MEETING GUIDE

Organized by:

The American Ceramic Society
www.ceramics.org

Materials Challenges In Alternative & Renewable Energy

February 26-March 1, 2012 | Hilton Clearwater Beach Resort | Clearwater, FL., USA

Co-organized by:

ASM International Everything Material. The Materials Information Society

SPS

TMS The Minerals, Metals & Materials Society

Endorsed by:

MRS Materials Research Society

SAMPE

www.ceramics.org/mcare2012

Welcome

Welcome to the Materials Challenges in Alternative & Renewable Energy Conference (MCARE 2012). This exciting, interdisciplinary forum is designed to bring together leaders in materials science and energy, to facilitate information sharing on the latest developments involving materials for alternative and renewable energy sources and systems.

We are happy that four of the premier materials organizations - The American Ceramic Society (ACerS), ASM International, The Minerals, Metals & Materials Society (TMS) and the Society of Plastics Engineers (SPE) - representing the disciplines of ceramics, metals and polymers, have joined forces to co-sponsor this conference of global importance. In addition, we are pleased to have the endorsement of the Materials Research Society (MRS) and the Society for the Advancement of Materials and Process Engineering (SAMPE).

MCARE 2012 includes nine "tutorial" presentations on leading energy technologies that will be given by global leaders in the field. In addition, the conference includes technical sessions addressing state-of-the art materials challenges involved with Solar, Wind, Hydropower, Geothermal, Biomass, Nuclear, Hydrogen, Batteries, Electric Grid/Smart Grid, Critical Materials Availability, and Nanocomposites/Nanomaterials, for Energy systems and applications.

This meeting was designed for scientists and engineers who are active in energy and materials science as well as those who are new to the field. The overall efficiency, effectiveness and practicality of potential future energy sources and systems are directly related to many materials related factors. Some of these key features include materials costs, availability and improvements in chemical, mechanical, electrical and/or thermal properties of materials now being considered, as well as the ability to produce and fabricate materials in forms and shapes that work effectively in areas of energy generation, storage and distribution.

Special thanks go to our sponsors, including Harper International, Lanzhou University of Technology, Savannah River National Laboratory, Toyota Research Institute North America, Sandia National Laboratories, and Dow Corning. Thank you to GM for providing a Chevy Volt and to Toyota for providing a FCHV for the Ride & Drive demo.

We are very excited that ACerS is committed to running this conference every two years. We believe the conference will continue to grow in importance, size, and effectiveness for the materials community.

Best regards,

George and Jack

George Wicks
Savannah River National Laboratory

Jack Simon
Technology Access

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Co-Organizing Societies

The American Ceramic Society
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TMS
The Minerals, Metals & Materials Society

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ASM INTERNATIONAL®
The Materials Information Society

Endorsing Societies

MRS Materials Research Society

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Organizing Committee

Conference Co-Chairs
Dr. George Wicks, Savannah River National Laboratory, Aiken, SC
Dr. Jack Simon, Technology Access, Aiken, SC

Technical Advisory Board and Topic Champions
Thad Adams, SRNL
Sivaram Arepalli, Sungkyunkwan University
Ming Au, SRNL
Geoffrey Brennecka, Sandia National Labs
Robin Brigmon, Savannah River National Lab
Subodh Das, Phinix
David Dorheim, DWD Advisors
Gary Fischman, Future Strategy Solutions
Bernadette Hernandez-Sanchez, Sandia National Lab
Natraj Iyer, Savannah River National Lab
Bruce King, Sandia National Lab
Dan Laird, Sandia National Lab
Edgar Lara-Curzio, Oak Ridge National Lab
Megan McCluer, U.S. Department of Energy
Mark Mecklenborg, ACerS
Rana Mohtadi, Toyota Research Inst. of N.A.
Gary Mushock, ASM International
Ralph Nichols, Savannah River National Lab
Ann Norris, Dow Corning
Gary Norton, U.S. Department of Energy
Ravi Ravindra, N.J. Institute of Technology
Steven Sherman, Savannah River National Lab
Bob Sindelar, Savannah River National Lab
Jay Singh, NASA
Rick Sisson, Worcester Polytechnic Institute
Ned Stetson, U.S. Department of Energy
Greg Stillman, U.S. Department of Energy
Hidda Thorsteinsson, U.S. Department of Energy
Mike Tupper, Composite Technology Development, Inc.
Eric Wachsman, Univ. of Maryland
Jy-An (John) Wang, Oak Ridge National Lab
Ragaiy Zidan, Savannah River National Lab
Mark Mecklenborg, The American Ceramic Society
Greg Geiger, The American Ceramic Society

Materials Challenges in Alternative & Renewable Energy Ride and Drive Program

Wednesday, February 29 – 4-7 p.m.

This is your chance to drive or ride as a passenger in a Chevy Volt and a Toyota Fuel Cell Hybrid Vehicle (FCHV) and speak with product experts from Toyota and GM. To participate as either a driver or a rider in one of these vehicles, please sign up in advance at the registration desk. Drivers and riders will be assigned specific times on a first-come, first-served basis. Space is limited.

Companion Coffee

Monday, February 27 – 9-10 a.m.

Companions, spouses and guests of conference attendees are invited to get to know one another at the companion coffee on the Water's Edge deck Monday morning.

Schedule At A Glance

Sunday – February 26, 2012

Registration	3 p.m. – 7 p.m.	Grand Ballroom Foyer
Welcome Reception Sponsored by Harper International	5 p.m. – 7 p.m.	Flamingo/Sandpiper Deck

Monday – February 27, 2012

Registration	7 a.m. – 5:30 p.m.	Grand Ballroom Foyer
Welcome & Plenary Sessions	8:45 a.m. – 12:15 p.m.	Salon EF
Companion Coffee	9 a.m. – 10 a.m.	Water's Edge Deck
Coffee Break	10:30 a.m. – 10:45 a.m.	Grand Ballroom Foyer
Networking Lunch	12:15 p.m. – 2 p.m.	Flamingo/Sandpiper Deck
Concurrent Technical Sessions	2 p.m. – 4:15 p.m.	Salons D, E, F, G
Networking Reception	4:30 p.m – 5:30 p.m.	Grand Ballroom Foyer

Tuesday – February 28, 2012

Registration	7 a.m. – 6 p.m.	Grand Ballroom Foyer
Concurrent Technical Sessions	8 a.m. – Noon	Salons D, E, F, G
Coffee Break	10 a.m. – 10:20 a.m.	Grand Ballroom Foyer
Networking Lunch	Noon – 1:30 p.m.	Flamingo/Sandpiper Deck
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Coffee Break	3:30 p.m. – 3:50 p.m.	Grand Ballroom Foyer
Poster Set up	4 p.m. – 6 p.m.	Water's Edge Ballroom
Poster Session 1 & Reception	7 p.m. – 9 p.m.	Water's Edge Ballroom

Wednesday – February 29, 2012

Registration	7:30 a.m. – 6 p.m.	Grand Ballroom Foyer
Concurrent Technical Sessions	8 a.m. – Noon	Salons D, E, F, G
Coffee Break	10 a.m. – 10:20 a.m.	Grand Ballroom Foyer
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Concurrent Technical Sessions	1:30 p.m. – 6 p.m.	Salons D, E, F, G
Coffee Break	3:30 p.m. – 3:50 p.m.	Grand Ballroom Foyer
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Poster Session 2 & Reception	7 p.m. – 9 p.m.	Water's Edge Ballroom

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Registration	7:30 a.m. – 4 p.m.	Grand Ballroom Foyer
Concurrent Technical Sessions	8 a.m. – Noon	Salons D, E, F, G
Coffee Break	9:40 a.m. – 10:30 a.m.	Grand Ballroom Foyer
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Coffee Break	3:30 p.m. – 3:50 p.m.	Grand Ballroom Foyer

2012 Plenary Speakers

Eric Peeters, Dow Corning Solar Solutions
Title: Innovation in Advanced Materials for Next Generation Technologies in Renewable Energy Sector

Biography: Peeters is the Global Solar Executive Director and Vice President. A rapidly growing sector that aims to develop and commercialize material solutions for the photovoltaic industry, Peeters is responsible for the overall strategic direction and operations of the solar business around the world. He joined Dow Corning in 1992, working as a chemical engineer at the company's manufacturing site in Barry, UK. Over the course of his 18-year career at Dow Corning, he has served in a number of science and business leadership roles in the U.S. and Europe, including Procurement, product line management, and Science & Technology. Peeters has a master's degree in Chemical Engineering from the Catholic University of Leuven in Belgium, and a Master in Technology Enterprise degree from the IMD in Lausanne, Switzerland.

Ned Stetson, U.S. DOE
Title: An Overview of U.S. DOE's Activities for Hydrogen Fuel Cell Technologies

Biography: Dr. Stetson is a Technology Development Manager for the U.S. Department of Energy's Hydrogen Program with over 18 years of experience in hydrogen storage materials and technology development. Stetson manages hydrogen storage projects, including the Metal Hydride Center of Excellence and the H-Prize. Prior to joining, he researched complex hydrides at the Univ. of Geneva. Stetson also spent over 10 years at ECD-Ovonics, where he was involved with the development of novel hydrogen storage materials and hydride-based hydrogen storage systems. He has also been active with the Compressed Gas Association, Society of Automotive Engineers, International Code Council and the International Standards Organization.

Megan McCluer, U.S. DOE Wind & Hydropower Technology Programs
Title: U.S. DOE Wind and Water Power Program

Biography: McCluer began her career at NASA Ames Research Center where she worked as an Aerospace Engineer in the Rotorcraft Aeromechanics Group for 12 years. She then served 4 years as the Project Manager for the U.S. Air Force's CV-22 Flight Test Program at Edwards Air Force Base. After volunteering to assist with disaster relief in the Gulf Coast, McCluer moved to private industry and became the Senior Engineering Program Manager for the Technology Department at Clipper Windpower. In Sept 2008 she was selected to become the Program Manager for the Wind and Hydropower Technologies Program at the DOE's Office of Energy Efficiency and Renewable Energy. She now serves as Senior Advisor for Wind Power Technologies at DOE. She has an Associate of Science in Civil Engineering from Franklin Institute of Boston, a Bachelor of Science in Aerospace Engineering from San Jose State University and a Master of Science in Aerospace Engineering from the University of Maryland, College Park.

Jim Ahlgrimm, U.S. DOE Wind & Hydropower Technology Programs
Title: U.S. DOE Wind and Water Power Program

Biography: Ahlgrimm is a team leader in the U.S. Department of Energy Wind and Water Power Technologies Program. He joined the program in 2002 and has served in various wind and hydropower technology development and deployment management roles. Currently he is responsible for program areas related to materials research and development. Jim has a B.S. in Aerospace Engineering from the U.S. Naval Academy, an MBA from the University of Maryland, and a Masters in National Resource Strategy from the National Defense University.

Bob Powell, General Motors Global R&D

Title: Materials Science for Automotive Electric Vehicle Transportation

Biography: Powell is the manager of the Electrochemistry and Battery Systems Group at the General Motors Global Research and Development Center. His group is responsible for identifying and developing advanced battery materials and supporting their integration into GM vehicle products. His thirty-three year career with General Motors has involved R&D in the fundamental materials and mechanisms of emission catalysis; electronic and structural ceramics, superconductivity, electro-rheological fluids. He was also responsible for magnesium and aluminum alloy and casting R&D for lightweight powertrains. He as published widely and holds twenty US patents. He received a B.S. from Alfred University and the M.S. and Ph.D. from the University of California at Berkeley. He is the recipient of the General Motors John Campbell Award for "fundamental contributions to creep deformation in magnesium alloys" and two TMS awards.

Bhakta Rath, Naval Research Laboratory

Title: Energy After Oil

Biography: Dr. Rath is the Associate Director of Research for Materials Science and Component Technology. He is recognized in the fields of solid-state transformations, grain boundary migrations, and structure-property relationships in metallic systems. He has published over 140 papers in these fields and edited several books and conference proceedings. He received a B.S. degree in physics and mathematics from Utkal University, an M.S. in metallurgical engineering from Michigan Technological University, and a Ph.D. from the Illinois Institute of Technology. Previously, he headed the Metal Physics Research Group of the McDonnell Douglas Research Laboratories in St. Louis until he came to NRL as Head of the Physical Metallurgy Branch. During this period, he was adjunct professor at Carnegie-Mellon University, the University of Maryland, and the Colorado School of Mines.

Tom Sanders, Savannah River National Laboratory

Title: State of Nuclear Energy in the World

Biography: Sanders the Associate Lab Director for Clean Energy Initiatives. He is responsible for developing new opportunities for the Lab in energy technology development. He was elected to a three year term as Vice President and President and Board Executive of the American Nuclear Society in 2008. Made rebuilding U.S. nuclear export industry through the development of Small Modular Reactors as his ANS executive initiative. Testified to Congress, Blue Ribbon Commission, and Secretarial Officers from DOE, DOS, DoD, NRC, and other agencies. Recently appointed to a second term on the Civil Nuclear Trade Advisory Committee, which serves the Secretary of Commerce on trade issues facing the U.S. civil nuclear industry. Recently elected to the International Nuclear Energy Academy. Chosen as a U.S. member of Russian President Medvedev's Global Energy Prize Committee. Co-founder and former Vice President of the American Council on Global Nuclear Competitiveness. Completed BS, MS and PhD in Mechanical/Nuclear Engineering at the University of Texas at Austin.

Steve Bossart, DOE, National Energy Technology Laboratory

Title: Materials Research for Smart Grid Applications

Biography: Bossart is a senior energy analyst at the National Energy Technology Laboratory (NETL). His primary area of study is the electric power sector with an emphasis on Smart Grid and its costs and benefits. He has 27 years of project management and analytical experience at the NETL and its predecessor organizations. He is author of over 70 publications covering a wide range of subjects including coal gasification, waste management, environmental controls for coal-based processes, nuclear decommissioning, and Smart Grid.

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Batteries and Energy Storage

Batteries are devices that convert chemical energy into electrical energy. There are many types of batteries available, representing a multi-billion dollar industry. Among the battery types of much interest are standard lead acid batteries and Li-ion batteries. Materials improvements are critical in making these energy systems more effective in the future.

Biomass

Biomass is energy derived from organic plant and animal matter including wood, crops, manure, and municipal solid wastes. When burned, the energy in biomass is released as heat but it can also be converted to other forms of energy like methane gas, ethanol and biodiesel. Biomass fuels currently account for about 3% of the energy used in the U.S.

Electric Grid

The Electric Grid is an interconnected network designed to deliver electricity from various energy sources, and involves controlling the generation, transmission and distribution of electricity. The grid cannot store significant amounts of power, so electricity must be generated as it is needed, by millions of consumers at any moment in time. Therefore, an efficient and effective control system is essential to match electric generation with use. It is critical to improve the reliability, efficiency and security of this system.

Geothermal

The U.S. produces more geothermal electricity that any other country, but this still amounts to less than ½ of one percent of all energy generated. Most geothermal reservoirs are deep underground but can find their way to the surface as volcanoes, hot springs and geysers. California has almost three dozen geothermal power plants that produce the largest fraction of U.S. energy from this source.

Hydrogen

Hydrogen can be produced from a variety of domestic sources, including fossil fuels as well as from renewable resources and can be stored in gas, liquid or solid forms. There is considerable work in progress on development of materials and systems for effective hydrogen storage. This alternative is considered a promising energy concept of the future, but like many alternatives, there currently is no infrastructure in place to produce, store, transport or distribute hydrogen effectively.

Hydropower

Conventional Hydropower is the most often used form of renewable energy in the U.S. Mechanical energy is produced and used by harnessing moving water. Over half of the U.S. hydroelectric capacity is located in Washington, California and Oregon, with the largest facility being the Grand Coulee Dam in Washington. Hydropower currently accounts for about 6% of the total electricity generated in the U.S.

Marine & Hydrokinetic Technologies are emerging advanced water power devices that capture energy from waves, tides, ocean currents, rivers, streams and ocean thermal gradients. There are several demonstration projects throughout the U.S. along with research to improve their manufacture, reliability, performance, increase market acceleration, and understand environmental effects.

Materials Availability for Alternative Energy

Tying all of the alternative energy technologies together is the availability of the materials needed to solve the issues for creating, storage and distribution of energy. The supply chain for the materials and parts that are necessary to create the new alternative energy scenario is crucial. Whether we find that materials are less available, or we find new uses for less expensive materials and materials systems, we will have to develop this supply chain to move forward. The theme of materials availability is, and will be, a major challenge as we develop our new and sustainable energy infrastructure.

Nanocomposites and Nanomaterials for Energy

There has been a tremendous increase in the use of nanocomposite materials to improve the existing energy systems based on conventional and renewable energy sources. It is important to know the possibilities and limitations of the use of nanomaterials in providing solutions for the current energy issues. We therefore need a better control and understanding of synthesis, processing, characterization, application as well as toxicity of nanomaterials and nanocomposites used for energy sources such as solar cells, fuel cells, and supercapacitors.

Nuclear

Nuclear power extracts usable energy from atomic nuclei by controlled nuclear reactions and most often, through nuclear fission. On a global scale, there are more than 400 operating nuclear power plants in more than 30 countries, which generate about 30% of the energy produced in the European Union and almost 20% of the energy produced in the U.S. Among the advantages of nuclear energy are no greenhouse emissions.

Solar Power

Solar power is energy derived from sunlight and can be converted into various forms of energy such as heat and electricity. The conversion to electricity can take place by photovoltaic (PV) or solar cells, as well as by use of solar power plants. There are currently more than a dozen major solar plants in the U.S., with most of these facilities located in California.

Wind

Wind power plants or wind farms often consist of many individual units. The largest wind farm located in Texas, consists of over 400 wind turbines that generate enough electricity to power about a quarter of a million homes each year. The U.S. is ranked second in the world in wind power capacity, only following Germany. In countries such as Denmark, about 20% of its electricity is generated from the wind.

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Presenting Author List

Oral Presenters

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Mahmoud, A.M.	1-Mar	9:20AM	Ballroom G	21
Malapaka, C.	29-Feb	3:10PM	Ballroom G	19
Marquis, F.D.	29-Feb	1:30PM	Ballroom D	19
Marra, J.	29-Feb	8:00AM	Ballroom F	17
McCluer, M.	27-Feb	2:00PM	Grand Ballroom	12
McGrail, P.	1-Mar	9:40AM	Ballroom G	21
Michopoulos, J.	29-Feb	4:30PM	Ballroom D	20
Mickiewicz, R.A.	28-Feb	11:00AM	Ballroom D	14
Mikhaylik, Y.V.	28-Feb	8:40AM	Ballroom F	13

Oral Presenters

Name	Date	Time	Room	Page Number
Milcius, D.	1-Mar	3:10PM	Ballroom E	22
Miller, A.K.	28-Feb	1:50PM	Ballroom D	15
Miller, D.A.	28-Feb	3:10PM	Ballroom D	15
Miller, D.A.	29-Feb	2:30PM	Ballroom D	19
Mishra, R.S.	28-Feb	2:30PM	Ballroom D	15
Mitlin, D.	28-Feb	2:50PM	Ballroom F	14
Mitlin, D.	28-Feb	8:00AM	Ballroom E	12
Mohtadi, R.	28-Feb	3:10PM	Ballroom E	14
Motyka, T.	1-Mar	9:00AM	Ballroom E	21
		N		
Najiba, S.	28-Feb	11:40AM	Ballroom E	12
Najoua, K.T.	1-Mar	9:40AM	Ballroom F	22
Najoua, K.T.	29-Feb	4:50PM	Ballroom G	19
Nguyen, B.N.	28-Feb	2:50PM	Ballroom D	15
Nishimura, C.	1-Mar	11:00AM	Ballroom E	21
		O		
Ortona, A.	29-Feb	8:00AM	Ballroom D	16
Ostapenko, S.	28-Feb	10:20AM	Ballroom D	14
		P		
Paolone, A.	1-Mar	2:50PM	Ballroom E	22
Paskevicius, M.	28-Feb	2:50PM	Ballroom E	14
Pay Gomez, C.	29-Feb	8:40AM	Ballroom E	17
Peeters, E.	27-Feb	9:00AM	Grand Ballroom	12
Pisano, A.P.	1-Mar	8:40AM	Ballroom G	21
Platt, H.A.	29-Feb	10:40AM	Ballroom D	16
Potter, B.	28-Feb	9:40AM	Ballroom D	14
Powell, B.R.	27-Feb	10:45AM	Grand Ballroom	12
Prochazka, J.	28-Feb	4:30PM	Ballroom F	15
Pundt, A.	28-Feb	10:20AM	Ballroom E	12
		R		
Ramaswamy, M.	28-Feb	9:40AM	Ballroom G	13
Rath, B.	27-Feb	2:45PM	Grand Ballroom	12
Reifsnider, K.	1-Mar	8:00AM	Ballroom F	22
Renugopalakrishnan, V.	29-Feb	8:00AM	Ballroom G	17
Robinson, D.B.	29-Feb	9:40AM	Ballroom G	17
Rolison, D.R.	28-Feb	11:00AM	Ballroom G	13
Rose, P.	1-Mar	10:20AM	Ballroom G	21
Rude, L.H.	1-Mar	10:40AM	Ballroom E	21
		S		
Sahlberg, M.	1-Mar	4:30PM	Ballroom E	22
Sanders, T.L.	27-Feb	11:30AM	Grand Ballroom	12
Sapori, B.	28-Feb	8:00AM	Ballroom D	13
Sartori, S.	29-Feb	3:50PM	Ballroom E	18
Sauder, C.	29-Feb	11:20AM	Ballroom F	18
Savage, P.B.	1-Mar	8:20AM	Ballroom D	21
Scheicher, R.H.	29-Feb	9:40AM	Ballroom E	17
Schneider, M.	1-Mar	8:40AM	Ballroom F	22
Schubert, H.	28-Feb	1:30PM	Ballroom F	14
Schubert, P.J.	29-Feb	10:40AM	Mangrove	18
Sedghi, A.	28-Feb	9:20AM	Ballroom G	13
Selvamanickam, V.	29-Feb	8:20AM	Ballroom D	16
Shahbazian-Yassar, R.	28-Feb	11:20AM	Ballroom F	13
Shahbazian-Yassar, R.	28-Feb	11:20AM	Ballroom G	13
Singh, G.	29-Feb	11:20AM	Ballroom D	16
Soboroff, M.	28-Feb	4:50PM	Ballroom D	15
Stafslien, S.J.	1-Mar	8:00AM	Ballroom D	21
Stetson, N.	27-Feb	9:45AM	Grand Ballroom	12
Sugama, T.	1-Mar	10:40AM	Ballroom G	21
Summers, W.A.	29-Feb	10:20AM	Ballroom F	18
Sun, D.	28-Feb	9:00AM	Ballroom E	12
Sunkara, M.V.	29-Feb	1:50PM	Ballroom G	19
		T		
Teprovich, J.A.	28-Feb	4:30PM	Ballroom E	14
Thanganathan, U.	1-Mar	10:20AM	Ballroom F	22
Tummala, R.	28-Feb	9:40AM	Ballroom F	13
Turick, C.	28-Feb	4:10PM	Ballroom G	15
		U		
Ugapathy, R.S.	29-Feb	9:00AM	Ballroom D	16
		V		
Vaidyanathan, R.K.	29-Feb	4:30PM	Ballroom G	19
Vegge, T.	29-Feb	9:00AM	Ballroom E	17
Vert, A.	1-Mar	8:20AM	Ballroom G	21
		W		
Walker, G.	29-Feb	4:30PM	Ballroom E	18
Wang, J.	28-Feb	5:10PM	Ballroom D	15
Wang, J.	29-Feb	4:50PM	Ballroom D	20
Wang, Q.	28-Feb	8:40AM	Ballroom E	12
Ward, P.A.	1-Mar	2:30PM	Ballroom E	22
Willauer, H.D.	29-Feb	11:00AM	Mangrove	18
Wood, A.	28-Feb	4:30PM	Ballroom D	15
Wu, J.	1-Mar	9:20AM	Ballroom F	22
		X		
Xia, G.	29-Feb	2:50PM	Ballroom F	19
Xu, J.	29-Feb	3:50PM	Ballroom G	19
		Y		
Yartys, V.	1-Mar	11:20AM	Ballroom E	21
		Z		
Zhang, J.	28-Feb	10:20AM	Ballroom F	13
Zhang, W.	28-Feb	2:10PM	Ballroom D	15
Zhang, X.	28-Feb	4:10PM	Ballroom F	15
Zlotea, C.	29-Feb	2:30PM	Ballroom E	18

Poster Presenters

Name	Date	Time	Room	Page Number
Ben Slama, R.	28-Feb	7:00PM	Waters Edge Ballroom	16
Blosser, M.	29-Feb	7:00PM	Waters Edge Ballroom	20
Chen, Y.	29-Feb	7:00PM	Waters Edge Ballroom	20
Cubeta, U.	29-Feb	7:00PM	Waters Edge Ballroom	20
Das, S.	29-Feb	7:00PM	Waters Edge Ballroom	20
Emily, J.N.	28-Feb	7:00PM	Waters Edge Ballroom	16
Greco, A.	28-Feb	7:00PM	Waters Edge Ballroom	16
Haglund, J.	29-Feb	7:00PM	Waters Edge Ballroom	20
Hubbard, L.R.	29-Feb	7:00PM	Waters Edge Ballroom	20
Kim, B.	28-Feb	7:00PM	Waters Edge Ballroom	16
Kumar, P.	29-Feb	7:00PM	Waters Edge Ballroom	20
Lee, E.	29-Feb	7:00PM	Waters Edge Ballroom	20
Lee, J.	29-Feb	7:00PM	Waters Edge Ballroom	20
Lee, J.A.	28-Feb	7:00PM	Waters Edge Ballroom	16
Lee, S.	28-Feb	7:00PM	Waters Edge Ballroom	16
Levchenko, A.A.	28-Feb	7:00PM	Waters Edge Ballroom	16
Meyer, K.	29-Feb	7:00PM	Waters Edge Ballroom	20
Najoua, K.T.	28-Feb	7:00PM	Waters Edge Ballroom	16
Ortona, A.	28-Feb	7:00PM	Waters Edge Ballroom	16
Park, K.	28-Feb	7:00PM	Waters Edge Ballroom	16
Ramireddy, B.	29-Feb	7:00PM	Waters Edge Ballroom	20
Robayo, M.D.	29-Feb	7:00PM	Waters Edge Ballroom	20
Rueschhoff, L.	29-Feb	7:00PM	Waters Edge Ballroom	20
Saadeddine, M.	28-Feb	7:00PM	Waters Edge Ballroom	16
Singh, P.	28-Feb	7:00PM	Waters Edge Ballroom	16
Sushant, K.	29-Feb	7:00PM	Waters Edge Ballroom	20
Takahashi, Y.	28-Feb	7:00PM	Waters Edge Ballroom	16
Vidu, R.	28-Feb	7:00PM	Waters Edge Ballroom	16
Wei, K.	29-Feb	7:00PM	Waters Edge Ballroom	20
Whitehead, J.	29-Feb	7:00PM	Waters Edge Ballroom	20
Xie, Z.	29-Feb	7:00PM	Waters Edge Ballroom	20
Yu, D.	29-Feb	7:00PM	Waters Edge Ballroom	20

Monday, February 27, 2012

Plenary: Materials Challenges in Alternative & Renewable Energy

Room: Grand Ballroom

Session Chairs: Jack Simon, Technology Access; George Wicks, Savannah River National Lab

8:45 AM

Opening Remarks
George Wicks, Jack Simon

9:00 AM

(MCARE-001-2012) Innovation in advanced materials for next generation technologies in renewable energy sector (Invited)
E. Peeters*, Dow Corning Europe S.A., Belgium

9:45 AM

(MCARE-002-2012) An Overview of U.S. DOE's Activities for Hydrogen Fuel Cell Technologies (Invited)
N. Stetson*, U.S. Department of Energy, USA

10:30 AM

Break

10:45 AM

(MCARE-003-2012) Materials Science for Automotive Electric Vehicle Transportation (Invited)
B. R. Powell*, General Motors Global R&D Center, USA

11:30 AM

(MCARE-004-2012) State of Nuclear Energy in the World (Invited)
T. L. Sanders*, Savannah River National Lab, USA

12:15 PM

Lunch

2:00 PM

(MCARE-005-2012) U.S. DOE Wind and Water Power Program (Invited)
M. McCluer*, J. Ahlgrimm, U.S. Department of Energy, USA

2:45 PM

(MCARE-006-2012) Energy After Oil (Invited)
B. Rath*, Naval Research Laboratory, USA

3:30 PM

(MCARE-007-2012) Materials Research for Smart Grid Applications (Invited)
S. Bossart*, R. Egidi, U.S. Department of Energy, USA

Tuesday, February 28, 2012

Hydrogen

H-Separations, H-Interactions and Effects on Materials

Room: Ballroom E

Session Chairs: Rana Mohtadi, Toyota Research Institute North America; Ragaiy Zidan, Savannah River National Laboratory

8:00 AM

(MCARE-008-2012) TEM Guided Microstructural Design of Magnesium Hydride Alloys with Capability for Room Temperature Volumetric Absorption Cycling (Invited)
D. Mitlin*, P. Kalisvaart, M. Danaie, University of Alberta and NINT NRC, Canada; S. Tao, Eindhoven University of Technology, Netherlands; B. Zahiri, University of Alberta and NINT NRC, Canada; H. Fritzsche, Canadian Neutron Beam Centre, Canada

8:20 AM

(MCARE-009-2012) Dense Membranes for Hydrogen Separation from Coal Gasification Stream
U. Balachandran*, T. H. Lee, C. Y. Park, J. E. Emerson, J. J. Picciolo, S. E. Dorris, Argonne National Laboratory, USA

8:40 AM

(MCARE-010-2012) Study on Influence of Hydrogen Processing on Microstructures and Mechanical Properties of Welded Joint of BT20 Titanium Alloy
Q. Wang*, D. Sun, R. Xu, Harbin Institute of Technology, China; J. Wang, Beihang University, China

9:00 AM

(MCARE-011-2012) Influence of Hydrogen on Hot Deformation Behavior and Microstructure of Pure Titanium
D. Sun*, Q. Wang, X. Han, J. Xiao, D. Jiang, Harbin Institute of Technology, China; J. Wang, Beihang University, China

9:20 AM

(MCARE-012-2012) Development of New Non Oxide Hybrid and Ceramic Membranes for Hydrogen Separation
L. Chareyre*, S. Cerneaux, V. Rouessac, A. Julbe, D. Cornu, Institut Europeen des Membranes (I.E.M.), France; E. Louradour, Ceramiques Techniques et Industrielles (C.T.I.), France

9:40 AM

(MCARE-013-2012) Hydrogen Separation & Purification Using Composite Inorganic Membranes
A. Alkali*, E. Gobina, Robert Gordon University, United Kingdom

10:00 AM

Break

10:20 AM

(MCARE-014-2012) Hydrogen interacting with nano-metals (Invited)
A. Pundt*, University of Goettingen, Germany

11:00 AM

(MCARE-015-2012) Microstructure and corrosion behavior of the Cu-Pd-X ternary alloys for hydrogen separation membranes
O. N. Dogan*, U.S. Department of Energy, USA; M. C. Gao, URS Corporation, USA; B. H. Howard, U.S. department of Energy, USA

11:20 AM

(MCARE-016-2012) Metallic membrane materials development for hydrogen production from coal derived syngas
O. N. Dogan, B. H. Howard, D. E. Alman*, U.S. Department of Energy, USA

11:40 AM

(MCARE-017-2012) Phase transition of lithium amidoborane at high pressure
S. Najiba*, J. Chen, Florida International University, USA

Nanocomposites/Nanomaterials

Nanocomposites and Nanomaterials I

Room: Ballroom G

Session Chairs: Woochul Kim, Yonsei University; Manorama Sunkara, CSIR-IICT, Hyderabad

8:00 AM

(MCARE-018-2012) Applications of Nanomaterials for Energy and Their Limitations (Tutorial)
S. Arepalli*, Sungkyunkwan University, Republic of Korea

8:40 AM

(MCARE-019-2012) Carbon Nanotube Papers: Microstructure and Biofuel Cell Electrodes (Invited)
V. A. Davis*, Auburn Unvierisity, USA

9:00 AM

(MCARE-020-2012) The role of nanomaterials for next generation energy storage devices – Supercapacitors (Invited)
D. Kalpana*, CSIR, India

9:20 AM

(MCARE-021-2012) Effect of Carbon nanotube counter electrodes on the behavior of Dye sensitized solar cells
A. Sedghi*, H. Nourmohammadi Miankushki, Imam Khomeini International University, Islamic Republic of Iran

9:40 AM

(MCARE-022-2012) Stuffed Lithium Garnets for All solid State Lithium Battery (Invited)
M. Ramaswamy*, Pondicherry University, India

10:00 AM

Break

10:20 AM

(MCARE-023-2012) Composite Aerogel Materials for Energy Storage (Tutorial)
S. Yang, Y. Cai, Y. Cheng, Duke University, USA; C. Varanasi, Army Research Office, USA; J. Liu*, Duke University, USA

11:00 AM

(MCARE-024-2012) Creating Next-Generation Electrochemical Power Sources via Architectural Design in 3D and on the Nanoscale (Invited)
D. R. Rolison*, J. W. Long, C. N. Chervin, M. B. Sassin, J. Wallace, J. F. Parker, N. W. Kucko, B. T. Willis, N. L. Brandell, U.S. Naval Research Laboratory, USA

11:20 AM

(MCARE-025-2012) Nanoscale Testing of Low Dimensional Materials for Energy Harvesting and Storage
R. Shahbazian-Yassar*, H. Ghassemi, A. Asthana, Y. Yap, Michigan Technological University, USA; M. Au, Savannah River National Laboratory, USA

Battery Technology

Novel Energy Storage Materials I

Room: Ballroom F

Session Chairs: Thad Adams, Savannah River National Lab; Ming Au, Savannah River National Lab

8:00 AM

(MCARE-026-2012) Lithium/air batteries: The next generation of rechargeable batteries beyond Li-ion chemistry? (Tutorial)
M. Au*, T. Adams, Savannah River National Laboratory, USA

8:40 AM

(MCARE-027-2012) Status of High Energy Rechargeable Li-S Battery Development at Sion Power (Invited)
Y. V. Mikhaylik*, I. Kovalev, C. Campbell, T. Kelley, J. Affinito, Sion Power Corporation, USA

9:00 AM

(MCARE-028-2012) Fabrication and Characterizations of Nanostructured Porous Si for Li-ion Batteries (Invited)
X. Sun, H. Huang*, Y. Zhuang, K. Chu, Wright State University, USA

9:20 AM

(MCARE-029-2012) Ionic conductivities in Li3xLa(2/3)-xTiO3 membranes of Li/Air batteries with controlled processing
C. Cooper*, APG, USA; M. Green, J. Wolfenstine, ALC, USA; A. C. Sutorik, G. Gilde, APG, USA

9:40 AM

(MCARE-030-2012) Solution Precursor Plasma Deposition of Nanostructured Co3O4 Anodes for Li – ion Batteries
R. Tummala*, R. K. Guduru, P. S. Mohanty, The University Of Michigan, USA

10:00 AM

Break

10:20 AM

(MCARE-031-2012) Nanostructured Materials for Energy Storage beyond Li-Ions (Tutorial)
J. Zhang*, J. Liu, J. Xiao, X. Li, W. Xu, G. Graff, Pacific Northwest National Laboratory, USA

11:00 AM

(MCARE-032-2012) Ultra High Energy Ball Milling Study of SiO-SnCoC Material as Anode for Lithium Batteries (Invited)
A. Abouimrane*, B. Liu, Argonne national Laboratory, USA; Y. Ren, University of Utah,, USA; Z. Fang, Argonne National Laboratory, USA; K. Amine, Argonne national Laboratory, USA

11:20 AM

(MCARE-033-2012) Lithium Intercalation in Low Dimensional Anodes Materials for Li-ion Batteries (Invited)
R. Shahbazian-Yassar*, H. Ghassemi, Y. Yap, Michigan Technological University, USA; M. Au, Savannah River National Laboratory, USA; Q. Gao, Michigan Technological University, USA

11:40 AM

(MCARE-034-2012) Synthesis and Characterization of Li2MSiO4 /C Cathode Materials for Lithium Ion Batteries
Y. Cen*, Worcester Polytechnic Institute, USA; C. Wang, Qingdao University of Science and Technology, China; R. D. Sisson, J. Liang, Worcester Polytechnic Institute, USA

Solar

PV Modules and Novel Approaches and/or Structures

Room: Ballroom D

Session Chairs: George Georgiou, NJIT; Bushan Sopori, National Renewable Energy Laboratory

8:00 AM

(MCARE-035-2012) Light Trapping and Optical Management in Solar Cells and Modules (Tutorial)
B. Sapori*, National renewal Energy Laboratory, USA

8:40 AM

(MCARE-036-2012) Investigation of Degradation Mechanism on Extended Damp Heat Aged PV Modules
A. W. Norris, B. Ketola*, Dow Corning Corporation, USA

9:00 AM

(MCARE-037-2012) Comparative Hazard Assessment of Photovoltaic Modules and Potential Modifications
D. Eisenberg*, M. Yu, C. Lam, University of California, Davis, USA; O. A. Ogunseitan, University of California, Irvine, USA; J. M. Schoenung, University of California, Davis, USA

9:20 AM

(MCARE-038-2012) Dielectric Core-shell Optical Nano-antenna for Extraordinary Solar Absorption Enhancement (Invited)
L. Cao*, North Carolina State University, USA

9:40 AM

(MCARE-039-2012) Nanostructure-mediated characteristics and device-level behavior of semiconductor-transparent conductive oxide (SC-TCO) nanocomposite thin films for photovoltaic energy conversion (Invited)
B. Potter*, G. Shih, R. J. Beal, S. DeValle, J. B. Kana-Kana, University of Arizona, USA

10:00 AM

Break

10:20 AM

(MCARE-040-2012) Crack Inspection in Si Solar Wafers and Cells Using Resonance Ultrasonic Vibrations (Tutorial)
S. Ostapenko*, Ultrasonic Technologies, Inc., USA

11:00 AM

(MCARE-041-2012) Characterization of the Mechanical Behavior and Material Properties of PV Module Encapsulants
R. A. Mickiewicz*, J. Lloyd, A. Stokes, T. Christian, D. Doble, R. Jaeger, P. Wu, J. Chapon, Fraunhofer Center for Sustainable Energy Systems (CSE), USA

11:20 AM

(MCARE-042-2012) Magnetic Field Assisted Assembly – Application to Solar Cell Integration
V. Kasi*, N. M. Ravindra, New Jersey Institute of Technology, USA

Hydrogen

New Methods and Novel Materials for H-Storage

Room: Ballroom E

Session Chair: Line Rude, Aarhus University; Rana Mohtadi, Toyota Research Institute North America

1:30 PM

(MCARE-043-2012) Recent Developments with Aluminum Hydride (Tutorial)
J. Graetz*, J. Wegrzyn, Y. J. Chabal, Brookhaven Natl Lab, USA; I. S. Chopra, The University of Texas at Dallas, USA; J. Reilly, Brookhaven Natl Lab, USA

2:10 PM

(MCARE-044-2012) Nitrogen-Based Composite Materials for Hydrogen Storage (Invited)
Y. Kojima*, T. Ichikawa, Hiroshima University, Japan

2:30 PM

(MCARE-045-2012) Stabilization of Aluminum Borohydride Through Adductation and Material Complexation
D. A. Knight*, R. Zidan, R. Lascola, T. Motyka, Savannah River National Laboratory, USA; R. Mohtadi, P. Sivasubramanian, Toyota Research Institute of North America, USA

2:50 PM

(MCARE-046-2012) Thermodynamic Destabilization of Complex Metal Hydrides (Invited)
M. Paskevicius*, D. A. Sheppard, Curtin University, Australia; U. Filsø, Aarhus University, Denmark; M. P. Pitt, Curtin University, Australia; T. R. Jensen, Aarhus University, Denmark; C. E. Buckley, Curtin University, Australia

3:10 PM

(MCARE-047-2012) Understanding and Altering the Properties of Low Stability Borohydrides for Onboard H2 Storage Applications (Invited)
R. Mohtadi*, P. Sivasubramanian, Toyota Research Institute North America, USA; T. Matsunaga, Toyota Motor Corporation, Japan; R. Zidan, D. Knight, Savannah River National Laboratory, USA

3:30 PM

Break

3:50 PM

(MCARE-048-2012) Development of Processes for the Reversible Dehydrogenation of High Capacity Hydrogen Carriers at Practical Conditions (Tutorial)
C. Jensen*, M. Chong, G. Severa, University of Hawaii, USA; E. Rönnebro, Pacific Northwest National Laboratory, USA; Z. Wang, Hawaii Hydrogen Carriers, LLC, USA; A. Karkamkar, T. Autrey, Pacific Northwest National Laboratory, USA

4:30 PM

(MCARE-049-2012) Elucidation of Hydride Interaction with Carbon Nanostructures and the Formation of Novel Nanocomposites for Reversible Hydrogen Storage
J. A. Teprovich*, R. Zidan, M. S. Wellons, D. A. Knight, R. Lascola, Savannah River National Laboratory, USA

4:50 PM

(MCARE-050-2012) Nanostructured metal hydrides for exploring candidate hydrogen storage systems (Invited)
D. Grant*, C. Fry, G. Walker, University of Nottingham, United Kingdom

5:10 PM

(MCARE-051-2012) Metal hydrides prepared by cold rolling: a new way to enhance hydrogen sorption (Invited)
J. Huot*, UQTR, Canada

Battery Technology

Novel Energy Storage Materials II

Room: Ballroom F

Session Chairs: Ali Abouimrane, Argonne national Laboratory; Jan Allen, U.S. Army Research Laboratory

1:30 PM

(MCARE-052-2012) Cathode Design an Stability of Li Batteries (Invited)
D. Kober, G. Gudday, M. Harth, O. Goerke, R. Bordia, H. Schubert*, Technische Universitaet Berlin.de, Germany

1:50 PM

(MCARE-053-2012) Nanostructured Materials as Potential Electrodes for Li-ion Batteries
F. Jiao*, B. Yonemoto, G. Hutchings, University of Delaware, USA

2:10 PM

(MCARE-054-2012) Nanostructured metals and metal oxides for HGH capacity anodes of Li-ion rechargeable batteries
M. Au*, T. Adams, Savannah River National Laboratory, USA

2:30 PM

(MCARE-055-2012) Improved Electrochemical Performances of Silicon Anodes Coated by P-doped C60 Films
A. Arie*, Parahyangan University, Indonesia

2:50 PM

(MCARE-056-2012) Supercapacitive Properties of Hydrothermally Synthesized Co3O4 Nanostructures (Invited)
D. Mitlin*, H. Wang, L. Zhang, C. Holt, B. Zahiri, B. C. Olsen, University of Alberta and NINT NRC, Canada

3:10 PM

(MCARE-057-2012) Investigation of Chemical Composition of Electrodes in Li-Ion Batteries
A. Fortier, S. K. Karna*, University of North Texas, USA

3:30 PM

Break

3:50 PM

(MCARE-058-2012) Engineering Electrochemically Active Nanoscale Silicon Based Hetero-structures (Invited)
P. Kumta*, University of Pittsburgh, USA

4:10 PM

(MCARE-059-2012) Nanofiber-Based Electrode Materials for Advanced Lithium-Ion Batteries (Invited)
X. Zhang*, North Carolina State University, USA

4:30 PM

(MCARE-060-2012) Three Dimensional Construction of Electrodes - Open Door to High Capacity Lithium Batteries (Invited)
J. Prochazka*, HE3DA, Inc., Czech Republic; L. Kavan, J. Heyrovsky Institute of Physical Chemistry, Czech Republic; M. Zukalova, J. Heyrovsky Institute of Physical Chemistry, Czech Republic

Biomass

Bioprocess Development

Room: Ballroom G

Session Chairs: Pratap Pullammanappallil, University of Florida; Robin Brigmon, Savannah River National Laboratory

1:30 PM

(MCARE-061-2012) Biomethane From Energy Crops and Organic Wastes (Tutorial)
D. P. Chynoweth*, University of Florida, USA

2:10 PM

(MCARE-062-2012) Evaluation of Fluorescence for Monitoring Plant Health for Bioenergy Applications (Invited)
R. Brigmon*, Savannah River National Laboratory, USA; K. McLeod, University of Georgia, USA; E. Doman, E. Wilde, Savannah River National Laboratory, USA

2:30 PM

(MCARE-063-2012) Comparison of Single and Two Stage Anaerobic Digestion of OFMSW
G. Ram Mohan, P. Pullammanappallil, P. J. Dube*, University of Florida, USA

2:50 PM

(MCARE-064-2012) Microbe-Derived Production of Fuel Components from Defined Renewable Waste
J. C. Biffinger*, R. E. Morris, L. Fitzgerald, E. Petersen, Naval Research Laboratory, USA; C. Ziemer, ARS-USDA, USA

3:10 PM

(MCARE-065-2012) Lactic acid metabolism of Escherichia coli and its use in recycling Poly-Lactide polymers
D. Chauliac*, K. Shanmugam, P. Pullammanappallil, University of Florida, USA

3:30 PM

Break

3:50 PM

(MCARE-066-2012) Degradation of automotive materials in palm biodiesel
M. Fazal, A. S.M.A. Haseeb*, H. H. Masjuki, University of Malaya, Malaysia

4:10 PM

(MCARE-067-2012) Electroactive Bio-Materials for Alternative Energy Processes (Invited)
C. Turick*, C. E. Milliken, Savannah River National Laboratory, USA

4:30 PM

(MCARE-068-2012) Biogasification of marine algae Nannochloropsis oculata
S. Buxy*, University of Florida, USA

4:50 PM

(MCARE-069-2012) Refractory Ceramic Lining Selection and Troubleshooting in Thermal Biomass Operations
D. Goski*, T. M. Green, D. J. Loiacona, Allied Mineral Products, USA

Hydropower

Material Challenges for Conventional and Marine Hydropower

Room: Ballroom D

Session Chairs: Alan Miller, Lockheed Martin Corp.; Bernadette Hernandez-Sanchez, Sandia National Laboratories

1:30 PM

(MCARE-070-2012) Materials Challenges and Developments in River Hydrokinetics (Invited)
E. C. Lovelace*, Free Flow Power, USA

1:50 PM

(MCARE-071-2012) Materials Challenges in the Huge Cold Water Pipes Required for Ocean Thermal Energy Conversion (Invited)
A. K. Miller*, Lockheed Martin Corp., USA; J. Halkyard, John Halkyard & Associates, USA; S. Shi, Houston Offshore Associates, USA; D. Dittenber, West Virginia Univ., USA

2:10 PM

(MCARE-072-2012) Material Challenges and Opportunities in Conventional Hydropower (Invited)
K. Zhang, W. Zhang*, B. T. Smith, Oak Ridge National Laboratory, USA; R. Dham, US Department of Energy, USA

2:30 PM

(MCARE-073-2012) Hydrokinetic Energy: Materials Challenges and Opportunities
K. Kandasamy, R. S. Mishra*, University of North Texas, USA

2:50 PM

(MCARE-074-2012) Tailoring Fiber Reinforced Composites Stiffness for Efficient Hydropower Systems (Invited)
B. N. Nguyen*, Pacific Northwest National Laboratory, USA

3:10 PM

(MCARE-075-2012) Degradation of Mechanical Properties in Composite Materials Subjected to Salt Water Environments
D. A. Miller*, J. Mandell, D. Samborsky, A. DiFronzo, Montana State University, USA

3:30 PM

Break

Electric Grid

Electric Grid

Room: Ballroom D

Session Chair: Jy-An Wang, Oak Ridge National Lab

3:50 PM

(MCARE-200-2012) Smart Grid Development by the U.S. Department of Energy (Invited)
D. Ton, S. Bossart*, U.S. Department of Energy, USA

4:30 PM

(MCARE-076-2012) Reversible Solid Oxide Fuel Cell Development at Versa Power Systems (Invited)
A. Wood*, H. He, T. Joia, Versa Power Systems Ltd., Canada

4:50 PM

(MCARE-077-2012) Gallium Nitride for Grid Applications
M. Soboroff*, U.S. Department of Energy, USA

5:10 PM

(MCARE-078-2012) Evaluation and improvement of conductor connectors for electrical power transmission system
J. Wang*, F. Ren, H. Jiang, E. Lara-Curzio, D. Lee, T. J. King, Oak Ridge National Laboratory, USA; J. Chan, G. Sibilant, Electrical Power Research Institute, USA; J. Graziano, E Inc., USA

General Poster Session

Room: Waters Edge Ballroom

7:00 PM

(MCARE-P001-2012) Characteristic of Li-La-Zr-O solid-state electrolyte thin film by RF magnetron sputtering for micro battery
S. Lee*, S. Jee, Y. Yoon, Yonsei University, Republic of Korea

(MCARE-P002-2012) The Effect of Carbon Loading and Fatty Acid Concentration on the Production of Biohydrogen by Anaerobic Fermentation of Agricultural Waste Feedstocks
J. N. Emily*, N. Mohammed, South Carolina State University, USA

(MCARE-P003-2012) Materials Selection Guide for Safe Design of Load Bearing Structures in Gaseous Hydrogen Environment
J. A. Lee*, NASA-Marshall Space Flight Center, USA

(MCARE-P004-2012) Hydrogen production by water electrolys: Effects of the electrodes materials nature on the solar water electrolysis performances
R. Ben Slama*, ISSAT, Tunisia

(MCARE-P005-2012) The Influence of cell morphology on the effective thermal properties of reticulated Si-SiC foams
S. Gianella, Erbicol SA, Switzerland; A. Ortona*, SUPSI, Switzerland

(MCARE-P006-2012) Combined Calorimetric and Volumetric Studies on MOFs for CO2 Separation Applications
A. A. Levchenko*, Setaram Inc, USA; R. Andre, E. Wirth, Setaram Instrumentation, France

(MCARE-P007-2012) In situ XAFS analysis of core shell CeZrO2 catalyst for the automotive application
Y. Takahashi*, Y. Yamada, Y. Ando, NORITAKE CO.,LIMITED, Japan; T. Hattori, KCM Corporation, Japan; M. Haneda, M. Ozawa, Nagoya Institute Technology, Japan

(MCARE-P008-2012) Microstructure and electrochemical properrties of La2NiO4+δ electrode prepared by screen-printing technique
K. Zhao, Q. Xu, D. Huang, Wuhan University of Technology, China; M. Chen, B. Kim*, Chonbuk National University, Republic of Korea

(MCARE-P009-2012) Thermal behavior studies of Ceria doped precursors produced by sol-gel method
C. Plapcianu, national Institute for Materials Physics, Romania; L. Stanciu, Purdue University, USA; R. Vidu*, University of California Davis, USA

(MCARE-P010-2012) P2O5-doped Fe2O3 for thermoelectric power generation
K. Park*, H. K. Hwang, J. Kim, K. Y. Kim, Sejong Uni., Republic of Korea

(MCARE-P011-2012) Electrochemically Doped CoSb3 Nanowires for High-Temperature Thermoelectric Materials
R. Vidu*, NanoRIS, USA; D. V. Quach, P. Stroeve, University of California Davis, USA

(MCARE-P012-2012) Simulation of performance insoles plans for the development of solar field in Algeria
M. Saadeddine*, M. Noureddine, université d'adrar, Algeria

(MCARE-P013-2012) Temperature dependent solar cell parameters – An Analysis
P. Singh*, N. M. Ravindra, New Jersey Institute of Technology, USA

(MCARE-P014-2012) Tribological Challenges in Alternative and Renewable Energy Applications
A. Greco*, V. Sista, K. Mistry, A. Erdemir, Argonne National Laboratory, USA

(MCARE-P015-2012) Physical properties of In2O3 nanomaterials grown by spray pyrolysis
K. T. Najoua*, N. Beji, M. Ajili, Z. Sboui, Laboratoire de Physique de la Matiere Condensee, Tunisia

(MCARE-P016-2012) Effect of the heat treatment on the structure, composition and optical properties of In2S3 prepared by chemical bath deposition
K. T. Najoua*, M. Kilani, J. Ouerfelli, Laboratoire de Physique de la Matière Condensée, Tunisia; M. Castagne, Université Montpellier II, France

Wednesday, February 29, 2012

Solar

Thin Films and Solar Thermal

Room: Ballroom D

Session Chairs: Ann Norris, Dow Corning; Sergei Ostapenko, Ultrasonic Technologies, Inc.

8:00 AM

(MCARE-156-2012) Si-SiC reticulated macroporous foams: processing, properties, and applications
A. Ortona*, S. Pusterla, C. D'Angelo, M. Barbato, SUPSI, Switzerland; S. Gianella, D. Gaia, Erbicol, Switzerland

8:20 AM

(MCARE-158-2012) Novel, Single-Crystalline-like Templates on Low-Cost, Flexible Substrates for High Efficiency Thin Film Photovoltaics
V. Selvamanickam*, University of Houston, USA; S. Sambandam, SuperPower, USA; R. Wang, C. Jian, G. Majkic, M. Yang, Y. Gao, E. Galtsyan, University of Houston, USA; X. Xiong, SuperPower, USA; A. Mehrotra, A. Freundlich, University of Houston, USA

8:40 AM

(MCARE-160-2012) Mysteries of CdTe Photovoltaic Technology
K. K. Chin*, NJIT, USA

9:00 AM

(MCARE-162-2012) Plasma/Laser Assisted Template Free Synthesis of Ultrafine/Nano Structured CdS films
R. S. Ugapathy*, R. Tummala, R. K. Guduru, P. S. Mohanty, The University Of Michigan, USA

9:20 AM

(MCARE-164-2012) Deep level defects in-CdS/p-CdTe Solar Cells
P. Kharangargh*, Z. Cheng, G. Liu, G. Georgiou, K. Chin, NJIT, USA

9:40 AM

(MCARE-167-2012) Growth Dynamics in Thin Films of Copper Indium Gallium Diselenide Sputtered from a Quaternary Target
J. A. Frantz*, R. Y. Bekele, J. D. Myers, United States Naval Research Laboratory, USA; V. Q. Nguyen, A. Bruce, S. V. Frolov, Sunlight Photonics, Inc., USA; M. Cyrus, J. S. Sanghera, United States Naval Research Laboratory, USA

10:00 AM

Break

10:20 AM

(MCARE-169-2012) Solar-Driven Fuel Production Using Metal Oxide Thermochemical Cycles (Invited)
M. D. Allendorf*, A. Ambrosini, E. N. Coker, A. H. McDaniel, E. B. Stechel, J. E. Miller, Sandia National Laboratories, USA

10:40 AM

(MCARE-171-2012) Solution Deposition of Thin Films and Patterns for Photovoltaics (Invited)
H. A. Platt*, S. E. Habas, C. J. Curtis, A. Miedaner, D. S. Ginley, National Renewable Energy Lab, USA; J. P. Novak, Y. Li, Applied Nanotech, Inc., USA; M. F. van Hest, National Renewable Energy Lab, USA

11:00 AM

(MCARE-173-2012) Solar Thermal Electrochemical Production of Energetic Molecules: Efficient STEP solar water splitting, carbon capture, and solar metals, fuel and bleach production
S. Licht, H. Wu, J. Asercion*, U. Cubeta, J. Lau, George Washington University, USA

11:20 AM

(MCARE-174-2012) Design and Development of ceramic composite and nano-structured materials for active solar air conditioning
G. Singh*, G. Singh, P. Singh, College of Engineering & Technology, Bikaner, India

Hydrogen

Theoretical Studies of H-Storage Materials and Additional Practical Use in Energy Storage System

Room: Ballroom E

Session Chairs: Martin Sahlberg, Uppsala University; Andrew Goudy, Delaware State University

8:00 AM

(MCARE-079-2012) Nano Materials for Hydrogen Storage (Tutorial)
P. Jena*, Virginia Commonwealth University, USA

8:40 AM

(MCARE-080-2012) Quasicrystals for Hydrogen Storage (Invited)
C. Pay Gomez*, M. Sahlberg, Uppsala University, Ångström Lab, Sweden

9:00 AM

(MCARE-081-2012) Descriptor based computational design of hydrogen membranes and battery electrolytes (Invited)
T. Vegge*, Technical University of Denmark, Denmark

9:20 AM

(MCARE-082-2012) Hydrogen Interaction with the Al Surface Promoted by Subsurface Alloying with Transition Metals (Invited)
F. Zhang, Y. Wang, M. Chou*, Georgia Institute of Technology, USA

9:40 AM

(MCARE-083-2012) What insights can be gained from ab initio studies of hydrogen storage systems? (Invited)
R. H. Scheicher*, Uppsala University, Sweden

10:00 AM

Break

10:20 AM

(MCARE-084-2012) Similarities in Energy Storage Methods for Vehicles (Tutorial)
S. W. Jorgensen*, General Motors R&D, USA

11:00 AM

(MCARE-085-2012) From nanostructured MgH2 to reversible hydrogen storage (Invited)
P. de Rango*, A. Chaise, B. Delhomme, D. Fruchart, S. Garrier, F. Longat, Institut Néel / CRETA, France; P. Marty, LEGI - INPG, France; S. Miraglia, B. Zawilsky, Institut Néel / CRETA, France

11:20 AM

(MCARE-086-2012) Metallic hydrides: a powerful class of materials for energy storage and conversion (Tutorial)
M. J. Latroche*, CNRS, France

11:40 AM

(MCARE-087-2012) Perspectives of H Storage and Battery Materials (Tutorial)
M. Fichtner*, Karlsruhe Institute of Technology, Germany

Nanocomposites/Nanomaterials

Nanocomposites and Nanomaterials II

Room: Ballroom G

Session Chairs: Jimmy Xu, Brown University; Sivaram Arepalli, Sungkyunkwan University

8:00 AM

(MCARE-088-2012) Engineering a Robust Artificial Photosynthetic System via Efficient Quantum Coherence (Tutorial)
V. Renugopalakrishnan*, Northeastern University, USA

8:40 AM

(MCARE-089-2012) Carbon Nanomaterials -The Route toward Applications in Energy (Invited)
W. Choi*, Florida International University, USA

9:00 AM

(MCARE-090-2012) Electrospin polyaniline nanofibers for Hydrogen storage applications
P. R. Ayalasomayajula*, S. Srinivasan, Nano RAM Technologies, India

9:20 AM

(MCARE-091-2012) Ultrasound Synthesis of Carbon Supported Pt-M1 (M1 = Fe, Co) Bimetallic Nanoparticles with Electrocatalytic Oxygen Reduction Reaction Activity
J. Jang*, E. Lee, Y. Kwon, Department of Chemistry and BK21 School of Chemical Materials Science, Sungkyunkwan University, Republic of Korea

9:40 AM

(MCARE-092-2012) Thermal stability of nanopores in palladium alloys used for hydrogen storage (Invited)
D. B. Robinson*, Sandia National Laboratories, USA; B. W. Jacobs, Protochips, Inc., USA; J. D. Sugar, M. D. Ong, M. E. Langham, Sandia National Laboratories, USA; L. R. Parent, I. Arslan, Pacific Northwest National Laboratory, USA

10:00 AM

Break

10:20 AM

(MCARE-093-2012) Three phase PZT-Cement-Al composites for structural health monitoring and energy harvesting applications
S. Banerjee*, Rutgers, The State University of New Jersey, USA; K. A. Cook-Chennault, Center for Advanced Energy Systems, USA

10:40 AM

(MCARE-094-2012) Thermochemical CO2 Splitting Using Thin Film Cobalt Ferrite/Alumina Active Materials
D. Arifin*, University of Colorado, USA; A. McDaniel, Sandia National Laboratories, USA; A. Weimer, University of Colorado, USA

Nuclear

Improved and Advanced Materials Systems for Fuel and NPP Components

Room: Ballroom F

Session Chair: Robert Sindelar, Savannah River National Lab; Gary Mushock, ASM International

8:00 AM

(MCARE-095-2012) Beyond Fukushima: Advanced Materials to Enable Enhanced Nuclear Power Systems (Tutorial)
J. Marra*, Savannah River National Lab, USA

8:40 AM

(MCARE-096-2012) Processing and Microstructural Characterization of Uranium Oxide
E. Luther*, C. Necker, R. Forsyth, P. Papin, D. Guidry, B. Mihaila, Los Alamos National Laboratory, USA

9:00 AM

(MCARE-097-2012) Development of a dynamic gas control technique to set a constant O/M ratio during sintering of UO_2
D. D. Byler*, Los Alamos Natl Lab, USA; J. B. Henderson, Netzsch Instruments NA, USA; K. J. McClellan, A. T. Nelson, Los Alamos Natl Lab, USA

9:20 AM

(MCARE-098-2012) Dynamic Sintering of UO_2 at constant Oxygen-to-metal Ratios
D. D. Byler, J. B. Henderson*, Netzsch Instruments North America, USA; K. J. McClellan, A. T. Nelson, Los Alamos National Laboratory, USA

9:40 AM

(MCARE-099-2012) Development of Diffusion Blocking Mechanisms during Processing of $GdO_{1.5}$ and UO_2-$GdO_{1.5}$
J. B. Henderson*, Netzsch Instruments North America, USA

10:00 AM

Break

10:20 AM

(MCARE-100-2012) Greenhouse Gas-Free Hydrogen Production Using Nuclear and Solar Energy (Tutorial)
W. A. Summers*, Savannah River National Lab, USA

11:00 AM

(MCARE-101-2012) Barrier behavior of Zr and V thin flms by electrodeposition method using ionic liquid for FCCI
S. Jee*, S. Lee, K. Lee, Y. Yoon, Yonsei Univ, Republic of Korea

11:20 AM

(MCARE-102-2012) Processing and characterization of SiC/SiC pin cladding reinforced with Hi-Nicalon S and SA3 fibers
C. Sauder*, S. Poissonnet, E. Buet, CEA, France

11:40 AM

(MCARE-103-2012) High Performance Homogenized Alloy 690 (Invited)
Y. Li*, K. Liu, X. Hao, R. Jiang, Y. Zhang, Institute of Metal Research,CAS, China

Biomass

Materials Challenges

Room: Mangrove

Session Chairs: David Dorheim, DWD Advisors, Inc.; Bhakta Rath, Naval Research Laboratory

8:00 AM

(MCARE-104-2012) Biodiesel Production through Ultrasound and Microwaves
S. C. Getty*, M. M. Kropf, Pennsylvania State University, USA

8:20 AM

(MCARE-105-2012) Biocoal: A Drop-In Fuel in Coal-fired Power Plants
E. Bar-Ziv*, Michigan Technological University, USA

8:40 AM

(MCARE-106-2012) An Innovative Biomass Waste Aerobic Degradation System for Hot Water
H. Li*, D. Yu, University of Nebraska-Lincoln, USA; Y. Yu, Nanjing University of Science & Technology, China

9:00 AM

(MCARE-107-2012) Effects of Fuel Grade Ethanol on Pump Station and Terminal Facilities
G. T. Quickel, DNV USA Inc., USA; J. A. Beavers*, DNV USA Inc., USA; F. Gui, N. Sridhar, DNV, USA

9:20 AM

(MCARE-108-2012) Material Challenges for Storing Alternative Fuels
J. S. Lee*, Naval Research Laboratory, USA; D. F. Aktas, University of Oklahoma, USA; R. R. Ray, Naval Research Laboratory, USA; J. M. Suflita, University of Oklahoma, USA; B. J. Little, Naval Research Laboratory, USA

9:40 AM

(MCARE-109-2012) Biocoal: A Novel Two-Stage Torrefaction-Pyrolysis for the Production of High-Grade Bio-Oil
E. Bar-Ziv*, J. Klinger, D. Shonnard, Michigan Technological University, USA

10:00 AM

Break

10:20 AM

(MCARE-110-2012) Rubber Reinforcement with Functionalized Lignin (Invited)
S. M. Dirk*, K. N. Cicotte, Sandia National Laboratories, USA; B. R. Hahn, D. A. Benko, The Goodyear Tire & Rubber Company, USA

10:40 AM

(MCARE-111-2012) Distributed Hydrogen Generation and Storage from Biomass
P. J. Schubert*, J. Paganessi, A. D. Wilks, M. Murray, Packer Engineering, Inc., USA

11:00 AM

(MCARE-112-2012) Advances in CO2 Hydrogenation to Value Added Hydrocarbons to Be Used as Liquid Fuel
H. D. Willauer*, Naval Research Laboratory, USA; M. T. Olsen, D. M. Drab, National Research Council, USA; R. Ananth, Naval Research Laboratory, USA; D. R. Hardy, Nova Research Inc, USA; R. Morris, F. W. Williams, Naval Research Laboratory, USA; F. DiMascio, Office of Naval Research, USA

Hydrogen

Adsorption, Catalysis and Means of Enhancing H-Interaction with Materials

Room: Ballroom E

Session Chairs: Theodore Motyka, SRNL; Astrid Pundt, University of Goettingen

1:30 PM

(MCARE-113-2012) Prospective of using structured nanoporous materials for hydrogen storage based on adsorption (Tutorial)
R. Chahine*, P. Bénard, E. Dundar, Hydrogen Research Institue, Canada; M. Richard, LTE-Hydro-Québec, Canada

2:10 PM

(MCARE-114-2012) Capacity, Kinetics and Evaluation of the Spillover Hydrogen Sorption Process (Invited)
T. Gennett*, NREL, USA

2:30 PM

(MCARE-115-2012) Nanoconfined materials for hydrogen storage (Invited)
C. Zlotea*, F. Cuevas, E. Léonel, T. Martens, M. Latroche, CNRS ICMPE, France; C. Matei Ghimbeu, R. Gadiou, C. Vix-Guterl, CNRS IS2M, France

2:50 PM

(MCARE-116-2012) Synthesis, crystal structure and properties of novel borohydrides (Invited)
B. C. Hauback*, C. Frommen, Institute for Energy Technology, Norway

3:10 PM

(MCARE-117-2012) Solid Carbon Ceramic Products to Enable Hydrogen from Decarbonized Fossil Fuels
J. W. Halloran*, University of Michigan, USA

3:30 PM

Break

3:50 PM

(MCARE-118-2012) Influence of carbon nanostructures on metal hydrides for hydrogen storage applications (Invited)
S. Sartori*, IFE, Norway

4:10 PM

(MCARE-119-2012) On the catalytic effect of TM additives on the Mg ↔ MgH2 kinetics of reaction (Invited)
D. Fruchart*, P. de Rango, O. Fruchart, G. Girard, S. Miraglia, L. Ortega, Institut Néel - CNRS, France; M. Shelyapina, St. Petersburg State University, Russian Federation; N. Skryabina, Perm State University, Russian Federation

4:30 PM

(MCARE-120-2012) Thermodynamic tuning of multicomponent hydride systems for hydrogen storage applications (Tutorial)
G. Walker*, University of Nottingham, United Kingdom

Nanocomposites/Nanomaterials

Nanocomposites and Nanomaterials III

Room: Ballroom G

Session Chair: Virginia Davis, Auburn Unviersity; Gary Mushock, ASM International

1:30 PM

(MCARE-121-2012) Nanomaterials in Photovoltaic R & D in India (Invited)
V. Kumar*, K. Kumari, Indian Institute of Technology, India; S. K. Srivastava, National Physical Laboratory, India

1:50 PM

(MCARE-122-2012) Nanostructured Multifunctional Metal Oxides and Nanocomposites for Solar Energy Harvesting and Niche Applications (Invited)
M. V. Sunkara*, CSIR-IICT, India

2:10 PM

(MCARE-123-2012) Strategies for the Efficiency Improvement of Photovoltaic Devices via Incorporation of Tailored Hybrid Nanostructures (Invited)
D. Kim*, Y. Jang, Y. Jang, S. Kochuveedu, U. Patil, Ewha Womans University, Republic of Korea

2:30 PM

(MCARE-124-2012) Strategies for improvement of efficiency of hydrothermally grown Zinc oxide (ZnO) nanorod dye-sensitized solar cells (Invited)
T. Bora, Asian Institute of Technology, Thailand; S. Sarkar, A. Makhal, S. N. Bose National Centre for Basic Sciences, India; S. Baruah, Uppsala University, Sweden; S. K. Pal, S. N. Bose National Centre for Basic Sciences, India; J. Dutta*, Sultan Qaboos University, Oman

2:50 PM

(MCARE-125-2012) Nano-structured Organic Photovoltaics: Design of the Ideal Structure (Invited)
W. Kim*, J. Kim, K. Kim, B. Jung, Yonsei University, Republic of Korea; S. Ko, KAIST, Republic of Korea

3:10 PM

(MCARE-126-2012) Efficient Sensitization of Nanocrystalline TiO2 Films by Metal-Free organic and Ru-Complexes for Application in Dye Sensitized Solar Cells (Invited)
C. Malapaka*, Indian Institute of Chemical Technology, India

3:30 PM

Break

3:50 PM

(MCARE-127-2012) Nano-heterogeneous structuring effects on thermal power factor and thermal conductivity (Invited)
G. Fernandes, Brown University, USA; S. Jung, Seoul National University, Republic of Korea; J. Kim, Brown University, USA; K. Kim, Seoul National University, Republic of Korea; Y. Park, F. Wahab, J. Xu*, Brown University, USA

4:10 PM

(MCARE-128-2012) Layered Ceramics for High-temperature Thermoelectric Generators
K. Scott, M. Saterlie, O. Graeve, S. Misture, D. Edwards*, Alfred University, USA

4:30 PM

(MCARE-129-2012) Nanocomposite-based Thermoelectric Devices for Energy Harvesting from Structural Components
R. K. Vaidyanathan*, O. Jacob, D. Vashaee, Oklahoma State University, USA

4:50 PM

(MCARE-130-2012) Effect of Sn-doped on physical properties of ZnO Thin films prepared by spray pyrolysis and grown on SnO2:F/glass
K. T. Najoua*, M. Ajili, Laboratoire de Physique de la Matière condensée, Tunisia; M. Castagne, Université de Montpellier II, France

Battery Technology

Novel Energy Storage Technologies

Room: Ballroom F

Session Chairs: Jason Zhang, Pacific Northwest National Laboratory; Reza Shahbazian-Yassar, Michigan Technological University

1:30 PM

(MCARE-131-2012) Magnesium Battery Research at Toyota: Current Challenges for the Next Generation of Electric Vehicles (Tutorial)
P. Fanson*, Toyota Motor Engineering & Manufacturing North America, Inc., USA

2:10 PM

(MCARE-132-2012) Electrical and Morphological Characterization of Monocultures and Co-cultures of Shewanella and Geobacter Bacteria in a Microbial Fuel Cell
K. E. Larson*, M. C. Shaw, California Lutheran University, USA

2:30 PM

(MCARE-133-2012) Materials Challenges in Developing High Voltage Li-ion Batteries (Invited)
T. R. Jow*, J. L. Allen, O. A. Borodin, U.S. Army Research Laboratory, USA

2:50 PM

(MCARE-134-2012) A Novel Iron-Polysulfide Redox Flow Battery
G. Xia*, X. Wei, L. Li, W. Wang, G. Yang, G. L. Graff, J. Liu, Pacific Northwest national Laboratory, USA

3:10 PM

(MCARE-135-2012) Correlation between Microstructure and Oxygen Removal in Solid-Oxide-Fuel-Cell-Modelelectrodes Pt(O2)/YSZ und Pd(O2)/YSZ
G. Beck*, Research Institute Precious Metals & Metals Chemistry, Germany

3:30 PM

Break

3:50 PM

(MCARE-136-2012) Energy Storage via Electrochemical Generation of CO as in Intermediate Product
I. Lubomirsky, V. Kaplan*, Weizmann Institute of Science, Israel

4:10 PM

(MCARE-137-2012) Characteristics of Pt/YSZ Nanocomposite Thin Films for Micro-SOFCs
H. Huang*, Wright State University, USA; M. Rottmayer, T. Reitz, Air Force Reearch Laboratory, USA

Wind

Wind Power

Room: Ballroom D

Session Chairs: Megan McCluer, U.S. Department of Energy; Jim Ahlgrimm, U.S. Dept. of Energy

1:30 PM

(MCARE-138-2012) The Role of Advanced Materials in Wind Energy (Tutorial)
F. D. Marquis*, Naval Postgraduate School, USA

2:10 PM

(MCARE-139-2012) Criticality of Defects in Wind Turbine Blade Materials and Manufacturing
D. Cairns*, J. Nelson, T. Riddle, M. Peterson, Montana State University, USA

2:30 PM

(MCARE-140-2012) Fatigue of Wind Blade Laminates: Effects of Resin and Fabric Structure Details
D. A. Miller*, D. D. Samborsky, J. F. Mandell, Montana State University, USA

2:50 PM

(MCARE-141-2012) Study of Effects of Surface Coatings on Envrionmental Degradation of Wind Turbine Blades through Environmental Wind Tunnel
J. Gou*, D. Ritson, S. Murray, M. Doherty, C. Harrison, S. Rice, J. Kapat, University of Central Florida, USA

3:10 PM

(MCARE-142-2012) Lightning Strike Protection of Composite Wind Turbine Blades
J. Gou*, F. Liang, J. Kapat, University of Central Florida, USA

3:30 PM

Break

3:50 PM

(MCARE-143-2012) Radar-wind farm interaction issues and mitigation via alternate wind turbine blade materials
J. J. McDonald, B. C. Brock, J. A. Paquette, S. E. Allen, K. W. Sorenson, E. D. Spoerke, J. Wheeler, D. A. Calkins, W. K. Miller, P. Clem*, Sandia National Laboratories, USA

4:10 PM

(MCARE-144-2012) Novel Flexible Membrane for Structural Health Monitoring of Wind Turbine Blades – Feasibility Study
S. Laflamme*, R. L. Geiger, Iowa State University, USA; G. Kofod, M. Kollosche, Potsdam University, Germany; C. Sumit, R. Khrisna, Iowa State University, USA

4:30 PM

(MCARE-145-2012) Robotic and Multiaxial Testing for the Constitutive Characterization of Composites (Invited)
J. Michopoulos*, Naval Research Laboratory, USA; J. Hermanson, Forest Products Laboratory, USA; A. Iliopoulos, Resident at Naval Research Laboratory, USA

4:50 PM

(MCARE-146-2012) Spiral notch torsion test for fracture behavior evaluation of polymeric composite materials for wind turbine applications
J. Wang*, F. Ren, T. Tan, E. Lara-Curzio, Oak Ridge National Laboratory, USA; P. Agastra, J. Mandell, Montana State University, USA; W. Bertelsen, Gougeon Brothers, Inc., USA; C. LaFrance, Molded Fiber Glass Companies, USA

Student Poster Contest & Design Contest

Room: Waters Edge Ballroom

7:00 PM

(MCARE-P017-2012) Multi-layered (Y2O3)0.08(ZrO2)0.92 / (Sc2O3)0.1(CeO2)0.01(ZrO2)0.89 Electrolytes
Y. Chen*, N. Orlovskaya, University of Central Florida, USA

(MCARE-P018-2012) Porous Media Burner Coupled with Thermoelectric Modules for Portable Power Generation
M. D. Robayo*, J. Hudson, E. Vinueza, J. Rodriguez, N. Orlovskaya, R. Chen, University of Central Florida, USA

(MCARE-P019-2012) Improving Electrostatic Energy Storage Density by Minimizing Voltage Tuning
K. Meyer*, Sandia National Laboratories, USA; Y. Jeon, Oregon State University, USA; H. Brown-Shaklee, Sandia National Laboratories, USA; D. Shahin, Missouri University of Science and Technology, USA; J. Ihlefeld, G. Brennecka, Sandia National Laboratories, USA

(MCARE-P020-2012) Nano facilitated charge transfer for an 11 electron redox couple for anodic charge storage: VB2
S. Licht, C. Hettige, J. Lau, J. Asercion, U. Cubeta*, George Washington University, USA

(MCARE-P021-2012) Assembly and Electrochemical Testing of Nano Silicon Lithium-Ion Batteries
L. Rueschhoff*, E. White, I. E. Anderson, S. W. Martin, Iowa State University, USA

(MCARE-P023-2012) The electrochemical enhancement of LiFePO4 by addition of surfactant via solid state method
J. Lee*, R. K. Singh, University of Florida, USA

(MCARE-P024-2012) A Fast, Low-cost Aerobic Biodegradation Energy System
D. Yu*, H. Li, University of Nebraska-Lincoln, USA

(MCARE-P025-2012) PEC Properties of Nanostructured Hematite: Effect of Silicon Ion
P. Kumar*, P. Sharma, Dayalbagh Educational Institute, India; R. Shrivastav, S. Dass, Dayalbagh Educational Institute,Dayalbagh, India; V. R. Satsangi, Dayalbagh Educational Institute, India

(MCARE-P026-2012) Portable Porous Media Burner for Thermoelectric Power Generation
E. Choi, A. DeWitt, T. Eman, J. Haglund*, N. Orlovskaya, R. H. Chen, University of Central Florida, USA

(MCARE-P027-2012) Nano-scale Thermoelectrics for Enhanced Power Conversion Application
K. Wei*, G. S. Nolas, University of South Florida, USA

(MCARE-P028-2012) Mineral Carbonation using Magnesium Oxide
K. Sushant*, Florida International University, USA

(MCARE-P029-2012) Synthesis of nanocystalline AlMgB14 powders by solid state synthesis technique
Z. Xie*, N. Orlovskaya, University of Central Florida, USA

(MCARE-P030-2012) Hierarchical TiO2 nanospheres fabricated by environmentally benign method for high efficiency photoanodes in DSSCs
M. V. Sunkara, B. Ramireddy*, P. Basak, CSIR-IICT, Hyderabad, India

(MCARE-P031-2012) Carbon-supported PtNi Nanoparticles Synthesized by Ultrasound for Oxygen Reduction Reaction in Fuel Cells
E. Lee*, SKKU Advanced Institute of Nanotechnology, Sungkyunkwan University, Republic of Korea; J. Jang, Center for Human Interface Nano Technology, Sungkyunkwan University, Republic of Korea; Y. Kwon, Department of Chemistry and BK21 School of Chemical Materials Science, Sungkyunkwan University, Republic of Korea

(MCARE-P032-2012) Charge Transfer Efficiency enhancement of Large Scale Graphene for Tri-iodide Reduction in Dye-Sensitized Solar Cells
S. Das*, Florida International University, USA; P. Sudhagar, Hanyang University, Republic of Korea; E. Ito, S. Lee, RIKEN-ASI, Japan; Y. Kang, Hanyang University, Republic of Korea; W. Choi, Florida International University, USA

(MCARE-P033-2012) Characterization of PECVD Thin Film Alumina for Electronic Passivation of Si Photovoltaics
L. R. Hubbard*, B. G. Potter, J. B. Kana-Kana, University of Arizona, USA

(MCARE-P034-2012) Silicon clathrates and their potential for photovoltaic applications
M. Blosser*, G. S. Nolas, University of South Florida, USA

(MCARE-P035-2012) The Use of Inexpensive All-Natural Organic Materials in Dye-Sensitized Solar Cells
J. Whitehead*, M. Shaw, J. Tannaci, California Lutheran University, USA

Thursday, March 1, 2012

Hydrogen

Engineering and Modification of H-Storage Materials for Applications

Room: Ballroom E

Session Chairs: Jacques Huot, UQTR; Sabrina Sartori, IFE

8:00 AM

(MCARE-147-2012) Condensed Phase Hydrogen Storage Materials Requirements for Automotive Applications (Tutorial)
D. L. Anton*, Savannah River National Laboratory, USA

8:40 AM

(MCARE-148-2012) Sorption and Heat Management Behavior of Complex Hydride-based Hydrogen Storage Tanks (Invited)
J. Bellosta von Colbe*, G. Lozano, J. Jepsen, T. Klassen, M. Dornheim, Helmholtz-Zentrum Geesthacht, Germany

9:00 AM

(MCARE-149-2012) Development of High Capacity Portable Power Systems (Invited)
T. Motyka*, Savannah River National Laboratory, USA

9:20 AM

(MCARE-150-2012) Metal Hydrides for Concentrated Solar Thermal Applications (Invited)
C. E. Buckley*, D. A. Sheppard, M. P. Paskevicius, Curtin University, Australia; D. N. Harries, University of Western Australia, Australia

10:00 AM

Break

10:20 AM

(MCARE-151-2012) Novel metal hydrides for hydrogen storage (Tutorial)
T. R. Jensen*, Aarhus University, Denmark

10:40 AM

(MCARE-152-2012) Solving the hydrogen storage challenge using metal borohydrides (Invited)
L. H. Rude*, T. R. Jensen, Aarhus University, Denmark

11:00 AM

(MCARE-153-2012) Materials development contributing to a distributed energy society (Invited)
C. Nishimura*, NIMS, Japan

11:20 AM

(MCARE-154-2012) Magnesium-based nanomaterials for hydrogen and energy storage (Invited)
V. Yartys*, Institute for Energy Technology, Norway

11:40 AM

(MCARE-155-2012) Mechanical Processing as Materials Preparation Tool: Alternative Energy and Related Applications (Tutorial)
V. Balema*, Aldrich Materials Science, Sigma-Aldrich Corporation, USA

Geothermal

Geothermal Systems and Applications

Room: Ballroom G

Session Chairs: Jy-An Wang, Oak Ridge National Lab; Greg Stillman, U.S. Dept. of Energy

8:00 AM

(MCARE-157-2012) Development of High Temperature Tools and Materials for Geothermal Applications (Invited)
F. Maldonado, S. Lindblom, J. Henfling*, Sandia National Laboratories, USA

8:20 AM

(MCARE-159-2012) Development of High Temperature Silicon Carbide Electronics
A. Vert*, C. Chen, A. Emad, A. Patil, A. Kashyap, T. Zhang, D. Shaddock, GE Global Research, USA; W. Johnson, Auburn University, USA

8:40 AM

(MCARE-161-2012) Harsh Environment MEMS for Energy and Power Applications
A. P. Pisano*, University of California, Berkeley, USA

9:00 AM

(MCARE-163-2012) High-Temperature Circuit Boards for Use in Geothermal Well Monitoring Applications
M. Hooker*, J. Walsh, M. Lizotte, Composite Technology Development, Inc., USA

9:20 AM

(MCARE-165-2012) Characterization of Low Temperature Geothermal ORC Systems Employing Non-azeotropic Working Fluid Mixtures (Invited)
A. M. Mahmoud*, A. I. ElSherbini, J. Lee, D. Luo, United Technologies Research Center, USA

9:40 AM

(MCARE-166-2012) Metal-Organic Heat Carrier Nanofluids for Geothermal Systems (Invited)
P. McGrail*, P. K. Thallapally, J. Blanchard, S. Nune, J. Jenks, PNNL, USA

10:00 AM

Break

10:20 AM

(MCARE-168-2012) Quantum Dots for Use as Tracers in Geothermal Reservoirs
P. Rose*, Energy and Geoscience Institute at the University of Utah, USA; D. Riasetto, J. Siy, M. Bartl, University of Utah, USA; M. Mella, K. Leecaster, Energy and Geoscience Institute at the University of Utah, USA

10:40 AM

(MCARE-170-2012) Self-degradable Cementitious Sealing Materials
T. Sugama*, T. Butcher, Brookhaven National Laboratory, USA

11:00 AM

(MCARE-172-2012) High Temperature, High Pressure Devices for Zonal Isolation in Geothermal Wells
J. Barker*, R. Taylor, P. Fabian, Composite Technology Development, Inc., USA

Hydropower

Hydropower Coatings

Room: Ballroom D

Session Chairs: Bernadette Hernandez-Sanchez, Sandia National Laboratories; Paul Savage, Brigham Young University

8:00 AM

(MCARE-175-2012) Rapid Biological Laboratory Assays for Evaluating the Performance of Antifouling Coatings and Materials Used to Construct Marine Hydrokinetic Devices (Invited)
S. J. Stafslien*, J. Daniels, J. Bahr, B. Chisholm, North Dakota State University, USA

8:20 AM

(MCARE-176-2012) Immobilization of Non-Peptide Mimics of Antimicrobial Peptides on Surfaces to Prevent Bacterial Biofilm Formation
P. B. Savage*, J. Snarr, Y. Li, X. Gu, L. Gao, Brigham Young University, USA

8:40 AM

(MCARE-177-2012) Biofouling Resistant Coatings Based on Zwitterions and Ceragenins for Marine Hydrokinetic Devices
M. Hibbs*, Sandia National Laboratories, USA; P. B. Savage, Brigham Young University, USA; L. Vanderwal, J. Daniels, S. Stafslien, North Dakota State University, USA; B. Hernandez-Sanchez, Sandia National Laboratories, USA

9:00 AM

(MCARE-178-2012) Sulfonium-Based Antibiofouling Coatings
S. M. Dirk*, M. B. Denton, M. F. Kirk, S. J. Altman, Sandia National Laboratories, USA; S. J. Stafslien, North Dakota State University, USA; B. A. Hernandez-Sanchez, Sandia National Laboratories, USA

9:20 AM

(MCARE-179-2012) Nanobased Coatings For The Prevention Of Corrosion And Biofouling For Marine Hydrokinetic Energy
B. A. Hernandez-Sanchez*, S. Altman, M. Kirk, S. Dirk, R. Rasberry, D. Enos, Sandia National Laboratories, USA; S. J. Stafslien, North Dakota State University, USA

9:40 AM

Break

10:00 AM

(MCARE-180-2012) Efficacy Testing Of Biofouling Resistant Materials For Marine Hydrokinetic Technology
S. J. Altman*, Sandia National Laboratories, USA; L. K. McGrath, LMATA Government Services LLC, USA; M. F. Kirk, Sandia National Laboratories, USA; S. J. Stafslien, North Dakota State University, USA; M. Hibbs, S. M. Dirk, K. N. Cicotte, Sandia National Laboratories, USA; M. Nagarajan, Owens Corning Science and Technology, LLC, USA; B. A. Hernandez-Sanchez, Sandia National Laboratories, USA

10:20 AM

(MCARE-181-2012) Evaluating the Environmental Risks of Biofouling Resistant Coatings for Marine and Hydrokinetic Technologies (Invited)
M. S. Greeley*, D. F. Glass-Mattie, M. S. Bevelhimer, Oak Ridge National Laboratory, USA

Materials Availability

Materials Availability for Alternative Energy

Room: Ballroom F

Session Chairs: Mike Tupper, Composites Technology Development; Gary Fischman, Future Strategy Solutions

8:00 AM

(MCARE-182-2012) Heterogeneous Functional Materials for Energy Storage and Conversion Systems
K. Reifsnider*, Q. Liu, F. Rabbi, U. South Carolina, USA

8:20 AM

(MCARE-183-2012) The role of raw materials in current and emerging energy technologies
B. Achzet*, University of Augsburg, Germany

8:40 AM

(MCARE-184-2012) Catalyzing Alternative & Renewable Energy Research
M. Schneider*, A. Schnyder, Chemspeed Technologies AG, Switzerland

9:00 AM

(MCARE-185-2012) Preparation of Organic-modified Ceria Nanocrystals with Hydrothermal Treatment
K. Kobayashi*, M. Haneda, M. Ozawa, Nagoya Institute of Technology, Japan

9:20 AM

(MCARE-186-2012) Synthesis of Pt doped Cr_2O_3/Bi_2O_3 Hybrid photocatalysts for Hydrogen Production from Water Splitting under Visible Light Irradiation
J. Wu*, Feng Chia University, Taiwan

9:40 AM

(MCARE-187-2012) Effect of spray solution flow rate on the physical properties of In_2S_3 grown by spray
Z. Seboui, N. Jebbari, K. T. Najoua*, Université de Tunis El Manar, Tunisia

10:00 AM

Break

10:20 AM

(MCARE-188-2012) Investigation on ammonium phosphate mixed heteropolyacid and SiO_2/polymer composite membranes
U. Thanganathan*, Okayama University, Japan

10:40 AM

(MCARE-189-2012) Mechanical and Physical Properties of Carbon S-Phase on Stainless Steel, Produced by Carbon Supersaturation
R. Hunger*, Bodycote Hardiff GmbH, Germany

Hydrogen

Analytical Methods and Characterization of Novel Hydrogen Storage Systems

Room: Ballroom E

Session Chairs: Thomas Gennett, NREL; Claudia Zlotea, CNRS ICMPE

1:30 PM

(MCARE-190-2012) The anelastic spectroscopy in the research on the hydrogen storage materials (Tutorial)
R. Cantelli*, Sapienza University of Rome, Italy; A. Paolone, O. Palumbo, CNR-ISC, Italy

2:10 PM

(MCARE-191-2012) Lifecycle analysis of a hydrogen storage material: formation, structure, and thermal decomposition mechanisms of $Al(BH_4)_3$ - TEDA adducts
R. Lascola*, D. A. Knight, R. Zidan, Savannah River National Laboratory, USA

2:30 PM

(MCARE-192-2012) Hydrogen Storage Characterization via Raman Spectroscopy
P. A. Ward*, R. N. Compton, University of Tennessee, USA

2:50 PM

(MCARE-193-2012) Relaxation processes and structural changes in LiH and NaH doped fullerene for hydrogen storage (Invited)
A. Paolone*, F. Vico, CNR & Sapienza university of Rome, Italy; F. Teocoli, Sapienza University of Rome, Italy; S. Sanna, CNR & Sapienza university of Rome, Italy; O. Palumbo, CNR-ISC, Italy; R. Cantelli, CNR & Sapienza university of Rome, Italy; D. Knight, J. A. Teprovich, R. Zidan, Savannah River National Laboratory, USA

3:10 PM

(MCARE-194-2012) Synthesis of SOFC electrolytes using e-beam deposition technique
D. Milcius*, Lithuanian Energy Institute, Lithuania; G. Laukaitis, K. Bockute, D. Virbukas, University of Technology, Lithuania

3:30 PM

Break

3:50 PM

(MCARE-195-2012) Best Practices in Characterizing Today's Most Advanced Hydrogen Storage Materials (Tutorial)
K. J. Gross*, H2 Technology Consulting LLC, USA

4:10 PM

(MCARE-196-2012) Thermodynamics and Kinetics of Complex Borohydride and Amide Hydrogen Storage Materials (Invited)
A. Goudy*, H. Yang, S. Sabitu, A. Ibikunle, T. Durojaiye, S. Orefuwa, Delaware State University, USA

4:30 PM

(MCARE-197-2012) Scandium-based Laves Phases for Hydrogen Storage (Invited)
M. Sahlberg*, Uppsala University, Sweden

4:50 PM

(MCARE-198-2012) Practical low-pressure hydrogen storage from nanoscale processing of complex and chemical hydrides
G. Round, Rutherford Appleton Laboratory, United Kingdom; S. Bennington*, Science and Technology Facilities Council, United Kingdom; S. Voller, Rutherford Appleton Laboratory, United Kingdom; A. Lovell, Science and Technology Facilities Council, United Kingdom; T. Headen, D. Royse, Rutherford Appleton Laboratory, United Kingdom; A. Nathanson, UCL, United Kingdom

5:10 PM

(MCARE-199-2012) NMR Tool for Characterization of Materials for Hydrogen Storage Application (Tutorial)
S. Hwang*, California Institute of Technology, USA

Monday, February 27, 2012

Plenary: Materials Challenges in Alternative & Renewable Energy

Room: Grand Ballroom
Session Chairs: Jack Simon, Technology Access; George Wicks, Savannah River National Lab

9:00 AM

(MCARE-001-2012) Innovation in advanced materials for next generation technologies in renewable energy sector (Invited)

E. Peeters*, Dow Corning Europe S.A., Belgium

The primary challenge of the PV industry is to reduce the cost of energy. Advanced materials and chemicals play a major role in helping the renewable energy sector succeed by bringing new innovative materials to market that enable next generation PV technologies. Eric Peeters will share information on latest developments in silicon-based materials that allow using less material, increase efficiency, improve durability and enable more efficient designs.

9:45 AM

(MCARE-002-2012) An Overview of U.S. DOE's Activities for Hydrogen Fuel Cell Technologies (Invited)

N. Stetson*, U.S. Department of Energy, USA

Hydrogen fuel cell technologies can provide clean, efficient electrical power for many near and long-term applications, ranging from portable power to automotive propulsion and large stationary power. As part of its mission to reduce dependency on imported petroleum and decrease greenhouse gas emissions, the U.S. Department of Energy supports research, development and demonstration activities to enable these technologies to be brought to market. This talk will provide an overview of the U.S. DOE's activities, including the current status of the technologies and materials challenges that still remain.

10:45 AM

(MCARE-003-2012) Materials Science for Automotive Electric Vehicle Transportation (Invited)

B. R. Powell*, General Motors Global R&D Center, USA

Materials and their processing are enabling for battery-based automotive electric vehicles. While Li ion batteries have effectively taken over the market for many consumer electronics devices; e.g., cell phones, computers, etc., the customer-driven criteria for success in automotive are remarkably more challenging; high power for speed and acceleration, high energy capacity for distance, rapid and convenient recharging, low cost, and of course safety, reliability, and durability (over years) in wide ranges of operating environments and driving conditions. The expectations place tremendous demands on scientists and engineers to discover/invent, develop, and manufacture advanced materials for electrodes, electrolytes, separators, current collectors and the dozens of other components in battery cells. Further, it is required that we have profound understanding of the mechanisms which determine cell performance and durability; to the extent that we can design and control battery systems such that reliable, robust models and operational algorithms can be created to meet the needs of this remarkable new era in transportation. An overview of General Motors' accomplishments and challenges in the materials science of battery systems will be presented.

11:30 AM

(MCARE-004-2012) State of Nuclear Energy in the World (Invited)

T. L. Sanders*, Savannah River National Lab, USA

U.S. President Dwight D. Eisenhower's 1953 "Atoms for Peace" speech at the UN laid the foundation for the present global nuclear enterprise. In his speech, he recommended the creation of the International Atomic Energy Agency. He offered nuclear technology developed in the U.S. to other nations as part of a broad nuclear arms control initiative. Since 1952, the world has produced over 400 nuclear power reactors and all but four nations have signed the nuclear non-proliferation treaty. Significant nuclear arms control treaties have been signed. Important international organizations related to nuclear matters have been established. The end of the Cold War, the events of September 11, 2001, and almost global support for the resurgence of nuclear energy have created a new opportunity to reinvigorate our commitment to peace and prosperity built around a new "Global Nuclear Future." For the U.S. to return to its former position as a visionary leader in the beneficial use of nuclear technology and materials on a global scale, it is imperative that steps be taken to reverse the conditions and decisions that led to the present situation-for the most part, the U.S. nuclear supply industry has moved offshore. This will require an integrated or holistic view of the global nuclear enterprise, from the cradle-to-the grave. Some of the realities of the global nuclear state will be outlined in this presentation.

2:00 PM

(MCARE-005-2012) U.S. DOE Wind and Water Power Program (Invited)

M. McCluer*, J. Ahlgrimm, U.S. Department of Energy, USA

The DOE Wind and Water Power Program works with industry, national laboratories, state, local and federal government agencies to advance wind and water power technology, reduce costs, and support the responsible wide-scale deployment of wind and water power as a national energy source. The goal is to deploy clean, affordable, reliable and domestic energy to reduce our dependence on foreign supplies and enhance national security, economic vitality and environmental stewardship. This presentation will describe what materials research the DOE Wind and Water Power Program is investing in and how that work contributes to the overall goals of the program. We will detail the areas of advancing technology; supporting grid interconnection; bolstering domestic manufacturing and creating jobs; overcoming barriers to deployment; and, investment in materials.

2:45 PM

(MCARE-006-2012) Energy After Oil (Invited)

B. Rath*, Naval Research Laboratory, USA

It is now evident that we are approaching a peak in global oil production to meet the ever increasing demand. Several projections indicate that total world consumption of oil will rise by nearly 60% between 1999 and 2020. In 1999 consumption was equivalent to 86 million barrels of oil per day, which has reached a peak of production extracted from most known oil reserves. These projections, if accurate, will present an unprecedented crisis to the global economy and industry. As an example, in the US, nearly 40 % of energy usage is provided by petroleum, of which nearly a third is used in transportation. The US Department of Defense (DOD) is the single largest buyer of fuel, amounting to, on the average, 13 million gallons per day. Additionally, these fuels have to meet different requirements that prevent use of ethanol or certain biodiesel additives. An aggressive search for alternate energy sources, both renewable and nonrenewable, is vital. The presentation will review national perspectives on the exploration of all potential alternatives and challenges on scale ups.

3:30 PM

(MCARE-007-2012) Materials Research for Smart Grid Applications (Invited)

S. Bossart*, R. Egidi, U.S. Department of Energy, USA

Our nation is transitioning to a Smart Grid which can sense and more optimally control the transmission, distribution, and delivery of electric power. The control of the electric power system is becoming more challenging with the addition of distributed renewable power sources, energy storage systems, electric vehicle charging, building and home energy management systems, smart appliances and devices capable of demand response, and other technologies.

These assets coupled with a smarter grid can provide many benefits including reducing peak demand and electricity consumption; better efficiency and reliability in distribution network, remote meter reading, improved outage management, automated feeder reconfiguration, improved maintenance by monitoring equipment health, and providing ancillary services to enhance grid stability and reliability. Materials research can enhance many applications made possible by smart grid. Materials research can result in reduced cost, increases in operating voltage and current, faster switching and sensing speed, better thermal management, greater efficiency, better protection, and longer life for many devices including solid-state circuit breakers, relays and switches, solid-state transformers, current limiters, static VAR compensators, high-voltage direct converters, and AC/DC inverters.

Tuesday, February 28, 2012

Hydrogen

H-Separations, H-Interactions and Effects on Materials

Room: Ballroom E
Session Chairs: Rana Mohtadi, Toyota Research Institute North America; Ragaiy Zidan, Savannah River National Laboratory

8:00 AM

(MCARE-008-2012) TEM Guided Microstructural Design of Magnesium Hydride Alloys with Capability for Room Temperature Volumetric Absorption Cycling

D. Mitlin*, P. Kalisvaart, M. Danaie, University of Alberta and NINT NRC, Canada; S. Tao, Eindhoven University of Technology, Netherlands; B. Zahiri, University of Alberta and NINT NRC, Canada; H. Fritzsche, Canadian Neutron Beam Centre, Canada

This presentation is separated into two sections: We will first discuss our recent cryogenic stage transmission electron microscopy (TEM) – based findings on the MgH2 to Mg (and vise versa) phase transformation. We show that both reactions proceed unevenly via sporadic nucleation, rather than by any “contracting volume” type of mechanism, and identify the dominant metal - hydride orientation relationships. By performing cryo-TEM on ball milled powders we discovered deformation twins in the microstructure. Density functional theory (DFT) analysis demonstrates that the twins significantly affect the kinetics of hydrogen diffusion. In the second portion of the presentation we highlight our recent alloy design efforts for both “bulk” thin films and thin film multilayers. The research culminates in the creation of several classes of catalysts that enable for relatively rapid room temperature volumetric absorption over multiple cycles at hydrogen pressures as low as 2 atmospheres. The same catalysts allow for ultra-rapid 250+ cycles elevated temperature absorption/desorption at hydrogen pressures between 1 and 3 atm. TEM analysis is again utilized to elucidate the key microstructural features that allow for such exquisite kinetics.

8:20 AM

(MCARE-009-2012) Dense Membranes for Hydrogen Separation from Coal Gasification Stream

U. Balachandran*, T. H. Lee, C. Y. Park, J. E. Emerson, J. J. Picciolo, S. E. Dorris, Argonne National Laboratory, USA

Our laboratory is developing hydrogen transport membranes (HTMs) for separating hydrogen from coal gasification streams. Extensive tests have been conducted with HTMs made by mixing Pd with Y2O3-stabilized ZrO2. With 90% H2/balance He at ambient pressure as feed gas, an ≈20-μm-thick membrane gave a flux of ≈32 cm^3[STP]/min-cm^2 at 500°C. A stable flux was measured over 600 h at 400°C. The present status of membrane development will be presented.

8:40 AM

(MCARE-010-2012) Study on Influence of Hydrogen Processing on Microstructures and Mechanical Properties of Welded Joint of BT20 Titanium Alloy

Q. Wang*, D. Sun, R. Xu, Harbin Institute of Technology, China; J. Wang, Beihang University, China

Hydrogen treatment is hopeful to refine the microstructure of weld seam of titanium alloy. This paper studies the impact of hydrogen treatment on the microstructure and the tensile property of weld seam of BT20 alloy by OM,XRD instrument, TEM and Instron machine. The results show that complete $\alpha+H\rightarrow\beta(H)$ transmission occurs during hydrogenizition at 800 centigrade degree for 30min. A lot of metastable β(H) and martensite α” form after water quenching and they decompose to α and δ during eutectoid treatment. The decomposition effect becomes heavier by rising the eutectoid temperature. Hydrogen is removed and recrystalization occurs in the process of dehydrogenisng at 750 centigrade degree for 8h in vacuum. After dehydrogenising the refinement of large grains in the fusion area is very obvious, but the original large grain boundaries are observed vaguely. After annealing, with the increasing of hydrogen content the tensile strength and plasticity of welded specimens decreased when they are hydrogenized at 650 centigrade degree. Through hydrogenising at 800 centigrade degree for 30min and quenching into water, then eutectoid at 300 centigrade degree for 8h, and dehydrogenising at 750 centigrade degree for 8h in vacuum, the ultimate strength decreases and the elongation increases a little in the joints by hydrogen treatment compared with those untreated.

9:00 AM

(MCARE-011-2012) Influence of Hydrogen on Hot Deformation Behavior and Microstructure of Pure Titanium

D. Sun*, Q. Wang, X. Han, J. Xiao, D. Jiang, Harbin Institute of Technology, China; J. Wang, Beihang University, China

It has been more reported on the hydrogenation process of titanium alloy, the influences of hydrogenation on the microstructure and properties of Ti alloy, and the hydrogen-induce thermal plasticity, but the hydrogen’s function and the microcosmic mechanism of the hydrogen-induce thermal plasticity in titanium alloy are still under study. In this work, the effects of hydrogenation on the hot deformation behavior and microstructure of pure titanium were studied, aiming at making clear the mechanism of hydrogen-induce thermal plasticity from the perspective of microstructure and dislocation motions. The results show that hydrogen in pure titanium crystal can reduce the flow stress of hot deformation; The flow stress peak is decreased best by 60% in a Ti-H crystal specimen deformed at 600~800 centigrade degrees and the peak flow stresses exhibit a trough behavior with the hydrogen concentration, that is, there is a minimum of peak flow stress at a certain hydrogen concentration. Through the analysis of microstructure, the great amounts of needle-like martensite and the small number of dislocations within the sub-grains in Ti-H crystal after hot deformation. These indicate that the hydrogen can increase the volume of β phase and can promote the dynamic recovery in the deformation process at high temperature, as a result, it decreases the flow stresses effectively.

9:20 AM

(MCARE-012-2012) Development of New Non Oxide Hybrid and Ceramic Membranes for Hydrogen Separation

L. Chareyre*, S. Cerneaux, V. Rouessac, A. Julbe, D. Cornu, Institut Europeen des Membranes (I.E.M.), France; E. Louradour, Ceramiques Techniques et Industrielles (C.T.I.), France

The improvement of innovative hydrogen production supplies represents a challenging objective. One solution to efficiently produce hydrogen would be the use of highly permselective membranes stable at high temperature (beyond 250°C). Silica-based membranes are serious candidates but their low resistance to water vapor is seriously prejudicial to their competitiveness. Based on previous results obtained at I.E.M., new non oxide membranes are designed in the system Si-M-C-N with M : a transition metal or metalloid. This work is divided into two major tasks, the first one is devoted to the synthesis of molecular precursors as single source and the second is focused on the deposition of these precursors by differents techniques to form active layers, such as Plasma Enhanced Chemical Vapor Deposition (P.E.C.V.D.), dip-coating, spin-coating and electrospray. With the objective to prepare quasi-dense active and selective membrane layers on porous ceramic supports (C.T.I.), we synthetized and characterized complex quaternary precursors "of Si-C-M-N". They should overcome the permeance and selectivity performances already obtained for the ternary phases "of Si-C-N".

9:40 AM

(MCARE-013-2012) Hydrogen Separation & Purification Using Composite Inorganic Membranes

A. Alkali*, E. Gobina, Robert Gordon University, United Kingdom

The main purpose of this work is to prepare a composite palladium membrane on ceramic alumina support by using the electroless plating method and to compare the hydrogen separation and purification performance of this membrane with that of an uncoated ceramic alumina support. In this study, a hydrazine based plating bath was used to prepare a palladium membrane on alumina support in a modified electroless plating method and tested for hydrogen permeation. The permeance of hydrogen was investigated across both the Pd membrane and the commercial alumina membranes. The permeation of a gas mixture (H2= 50%, CO= 28%, CO2= 10%, CH4= 8% and N2= 4%) was tested across the Pd membrane. In comparison, the results indicate a much higher performance by the Pd membrane than the uncoated coomercial alumina membrane in terms of hydrogen separation and purification. The results for commercial alumina membrane also show that the order of permeance of the gases do not follow the order of their kinetic diameter while the Pd membrane show a higher permeance for hydrogen compared to the gas mixture. This could be attributed to transport of the heavier components of the gas mixture. These results indicate a marked improvement in hydrogen separation and purification performance of Pd membranes prepared by electroless plating for high purity hydrogen especially for fuel cell applications.

10:20 AM

(MCARE-014-2012) Hydrogen interacting with nano-metals (Invited)

A. Pundt*, University of Goettingen, Germany

Hydrogen in metals (H-M) is a suitable and safe candidate for energy storage – however, high specific weight, hydride stability and time restrictions require materials improvements. Slow diffusion in light weight hydrides for example, hinders their practical use because of long loading times. One way to reduce the loading time is materials nano-sizing, since short paths result in short loading times. However, nano-sizing also changes the systems' physical properties. These changes are due to surface, interface and other defects contributions and, also, due to mechanical stress between the nano-system and its stabilizer. To give some examples: Surfaces and interfaces can act as local hydrogen sinks thereby increasing the local solubility tremendously. Mechanical stress of several GPa arises during hydrogen absorption between a film and its substrate. This high stress influences the hydride formation pressure. Furthermore, defect concentrations vary depending on the hydrogen content in the sample. Smooth sample surfaces become rough upon hydrogen uptake. Depending on sample thickness different pathways of stress release and defect generation are chosen. In this presentation, changes of physical properties are demonstrated and discussed on H-M model systems like thin films, multi-layers and clusters.

11:00 AM

(MCARE-015-2012) Microstructure and corrosion behavior of the Cu-Pd-X ternary alloys for hydrogen separation membranes

O. N. Dogan*, U.S. Department of Energy, USA; M. C. Gao, URS Corporation, USA; B. H. Howard, U.S. department of Energy, USA

Surface poisoning and corrosion have been shown to be the most significant degradation mechanisms acting on the membrane materials at elevated temperatures in syngas derived from coal containing impurities such as H2S. Cu-Pd alloys have demonstrated significant potential for being resistant against these degradation mechanisms. It has also been shown that Cu-Pd compositions containing ordered bcc (B2) crystal structure exhibit hydrogen permeability comparable to pure palladium. The B2 structure of the membrane alloys was successfully stabilized at higher temperatures by ternary element additions. Furthermore, the ternary alloy coupons were exposed to simulated syngas environments at 500C. Corrosion products were characterized using SEM and XRD. While additions of Al and Mg to the Cu-Pd alloys did not change the mass gain, additions of Y, La, Ti, and Hf increased the mass gain during the exposures.

11:20 AM

(MCARE-016-2012) Metallic membrane materials development for hydrogen production from coal derived syngas

O. N. Dogan, B. H. Howard, D. E. Alman*, U.S. Department of Energy, USA

To produce high purity hydrogen fuel from coal, hydrogen must be separated from synthesis gas (syngas), a product of coal gasification. Membrane technology can be used to achieve this goal. The U.S. Department of Energy has established a set of performance targets for hydrogen separation membranes for the syngas applications in its Hydrogen from Coal program. Although a variety of hydrogen separation membrane materials exist today, none of them is shown to be suitable for use in contaminant laden syngas at elevated temperatures. Surface poisoning and corrosion have been shown to be the most significant degradation mechanisms acting on the membrane materials at elevated temperatures in gases containing H2, CO2, CO, H2O, and impurities such as H2S, As, Se, and Hg. NETL is collaborating with several universities to understand the interaction between the constituents of syngas and the surface of metallic membrane materials. We will present the significant results from this collaboration.

11:40 AM

(MCARE-017-2012) Phase transition of lithium amidoborane at high pressure

S. Najiba*, J. Chen, Florida International University, USA

One of the major obstacles to the use of hydrogen as an energy carrier is the lack of proper hydrogen storage media. Lithium amidoborane has attracted significant attention as hydrogen storage medium due to its low dehydrogenation temperature. It releases ~10wt% hydrogen, which is beyond the DoE target, at around 90oC. It is essential to study the structural behavior of this potential material to improve its dehydrogenation behavior further and also to make rehydrogenation possible. In this study, the phase stability of this material with pressure was experimented in diamond anvil cell by using in-situ Raman spectroscopy. Two phase transitions were found at around 8.5 and 12 GPa which are characterized by sequential changes of Raman modes. These phases appear with the splitting of the N-H and B-H stretching modes, which indicates structural complexity increases with the applied pressure. Also, N-H stretching modes do not show redshift with pressure, which indicates there is no dihydrogen bonding in this material. The absence of dihydrogen bonding in this material is the interesting phenomenon, as dihydrogen bonding is the dominant bonding phenomenon in its parent compound ammonia borane. This observation will provide guidance to the improvement of the hydrogen storage properties of this material by giving insight into the structural details of this material.

Nanocomposites/Nanomaterials

Nanocomposites and Nanomaterials I

Room: Ballroom G
Session Chairs: Woochul Kim, Yonsei University; Manorama Sunkara, CSIR-IICT, Hyderabad

8:00 AM

(MCARE-018-2012) Applications of Nanomaterials for Energy and Their Limitations (Tutorial)

S. Arepalli*, Sungkyunkwan University, Republic of Korea

Nanomaterials are essential for development of high performance next generation alternative and renewable energy resources. Improved methods of energy conservation, production, storage and transmission using nanomaterials will provide quick solutions for the current energy issues as well. The present talk will focus on the application of carbon nanotubes and carbon nanostructures for energy production such as fuel cells, energy storage using supercapacitors and energy transmission using quantum wires. Incorporation of CNTs and other nanostructures will also be discussed for applications of hydrogen storage and rechargeable batteries. The limitations of CNT synthesis, safety and possible exposure issues will be presented.

8:40 AM

(MCARE-019-2012) Carbon Nanotube Papers: Microstructure and Biofuel Cell Electrodes (Invited)

V. A. Davis*, Auburn Unviersity, USA

Carbon nanotube papers, commonly called bucky-papers, have attracted immense interest in a range of applications for use in lightweight structural composites and fuel cell electrodes. In biofuel cells, carbon nanotubes are attractive because of their small size, large specific area and capacity for direct electron transfer with enzymes. There are two key issues that need to be addressed to optimize performance. First, a better understanding of the effects of processing on the interaction between the nanotubes and the enzymes and/or electrocatalysts is needed. Second, methods of controlling and quantifying the pore size distribution in the buckypapers is needed in order to optimize mass and electron transport. Progress in both areas will be described. For example, a cavity anode based on single-walled nanotube (SWNT) bucky-paper was developed for oxidation (and regeneration) of nicotinamide adenine dinucleotide (NADH) and oxidation of L-malate. Polymethylene green (PMG) was utilized as the electrocatalyst to produce NAD+ and anode performance was affected by whether the methylene green monomer was dispersed with the nanotubes prior to formation of the solid bucky-paper or deposited after bucky-paper production. In addition, we have developed a method using porometry to quantify the effects of composition and processing on pore size distribution. This will enable further optimization of electrode designs.

9:00 AM

(MCARE-020-2012) The role of nanomaterials for next generation energy storage devices – Supercapacitors (Invited)

D. Kalpana*, CSIR, India

Energy production relying on the combustion of fossil fuels and its environmental impact is forecast to have an adverse effect on world economic activity and ecology. This demand for more sustainable, efficient energy storage has provoked a renewed scientific and commercial interest in advanced capacitor designs in which the suite of experimental techniques and ideas that comprise nanotechnology are playing a critical role. Supercapacitors are the most promising electrochemical energy storage systems due to their pulse power supply, long cycle life, and high dynamic of charge propagation. The application of nanostructured materials with bespoke morphologies and properties to electrochemical supercapacitors is being intensively studied in order to provide enhanced energy density without comprising their inherent high power density and excellent cyclability. In particular, electrode materials that exploit physical adsorption or redox reactions of electrolyte ions are foreseen to bridge the performance disparity between batteries with high energy density and capacitors with high power density. In this lecture, some of the novel nanomaterial systems applied for electrochemical supercapacitors will be presented and show how material morphology, chemisty and physical properties are being tailored to provide enhanced electrochemical supercapacitor performance.

9:20 AM

(MCARE-021-2012) Effect of Carbon nanotube counter electrodes on the behavior of Dye sensitized solar cells

A. Sedghi*, H. Nourmohammadi Miankushki, Imam Khomeini International University, Islamic Republic of Iran

Dye-sensitized solar cells (DSSC) are based on a semiconductor formed between a photo-sensitized anode and an electrolyte. The counter electrode in these cells consists of fluorine-doped tin oxide (FTO) glass coated with platinum to afford more reversible electron transfer. In this research, Multi-Walled carbon nanotubes (MWCNTs) were used in DSSC counter electrode. Three types of counter electrode were studied: (i) pure platinum (Pt-CE), (ii) Pure carbon nanotube (MWCNT-CE) and (iii) Mixed platinum and carbon nanotube (Pt-MWCNT-CE). All of them were prepared by spraying on FTO glass and solar cell were fabricated by assembling them, TiO2 electrodes and Iodine electrolyte. A comparison of I-V curves of DSSC cells by light simulator showed almost similar efficiency of Pt-CE and MWCNT-CE. On the other hand, enhanced energy conversion efficiency was obtained by using Pt-MWCNT-CE and increased the efficiency up to about 20% in comparison with standard DSSC's. It could be related to chemical stability of the MWCNTs which were facilitated the electron-transfer kinetics, yielded the lowest transfer resistance and improved the photovoltaic activity for the reduction of electrolyte ions.

9:40 AM

(MCARE-022-2012) Stuffed Lithium Garnets for All solid State Lithium Battery (Invited)

M. Ramaswamy*, Pondicherry University, India

Integration of electrical energy generated by wind or solar technologies in to grid depends heavily on the availability of adequate high capacitive Batteries. Solid electrolytes promise the potential to replace organic liquid electrolytes and thereby improve the safety of next-generation high-energy lithium-ion batteries. In the last few years, a series of garnet-like structural compounds have been investigated as a novel family of fast lithium ion conductors. Among them $Li_7La_3Zr_2O_{12}$ (LLZ) has been paid much attention because of their stable nature against Li metal. The total (grain+grain boundary) conductivity around 10^{-4} Scm^{-1} at 25°C, good thermal stability and chemical stability against molten lithium and high densification of cubic LLZ suggested that this zirconium containing lithium garnet is a promising solid electrolyte for Li^+ rechargeable batteries. Disordered arrangement of Li^+ across tetrahedral and octahedral sites is prime factor for the observed high conductive in cubic LLZ. The electrochemical performance of all solid state thin film battery based on LLZ elctrolyte and also the advantage of all solid state batteries based on composites of 3 Dimensonally Ordered Macroporous (3DOM) garnet structured electrolyte and active material will be discussed.

10:20 AM

(MCARE-023-2012) Composite Aerogel Materials for Energy Storage (Tutorial)

S. Yang, Y. Cai, Y. Cheng, Duke University, USA; C. Varanasi, Army Research Office, USA; J. Liu*, Duke University, USA

A convenient, inexpensive and scalable method synthesizing hybrid carbon (C) and titanium dioxide (TiO2) composite aerogels were discovered. The hybrid aerogel can be directly used as active electrodes without the addition of binders or additives. As a result, the performance of Li ion battery (LIB)anodes using the hybrid aerogel is significantly improved over current LIBs based on carbon/titanium oxide composite. The reversible discharge capacity was stabilized at ~400 mA h g-1 at 168 mA g-1 scan rate and operating voltage between 0.05 and 3.00 V with excellent cyclic capacity retention. In addition, the loading density of the active monolithic material was 12.4 mg cm-2, which is much higher than the typical loading density of active materials in recent literature. This approach, however, is not limited to only C/TiO2 system. Other metal oxides mentioned above could also form composite aerogels with carbon to improve their potentials in electrochemical, photocatalytic, and photoelectronic devices.

11:00 AM

(MCARE-024-2012) Creating Next-Generation Electrochemical Power Sources via Architectural Design in 3D and on the Nanoscale (Invited)

D. R. Rolison*, J. W. Long, C. N. Chervin, M. B. Sassin, J. Wallace, J. F. Parker, N. W. Kucko, B. T. Willis, N. L. Brandell, U.S. Naval Research Laboratory, USA

Any future success in the global effort to shift energy usage away from fossil fuels will rely on electrical energy storage in batteries and electrochemical capacitors (ECs). A marked improvement in the performance of these power sources is critical for this effort, yet both are mature technologies that have always disregarded Moore's Law. Improved performance requires redesigning the reaction interphases in which the fundamental processes that store energy in batteries and ECs occur. Energy researchers are now rethinking the requisite multifunction—mass and charge transport, electronic and ionic conductivity, and electron-transfer kinetics—in light of nanoscience and architectural design in three dimensions. The design and fabrication of size- and energy-scalable three-dimensional multifunctional architectures from the appropriate nanoscale building blocks for chemical, physical, and physicochemical charge storage will be highlighted, including the use of "nothing" (void space) and deliberate disorder as design components as well as the importance of reexamining in a nanoscopic form those materials that yielded poor energy-storage performance when used in a macroscopic form.

11:20 AM

(MCARE-025-2012) Nanoscale Testing of Low Dimensional Materials for Energy Harvesting and Storage

R. Shahbazian-Yassar*, H. Ghassemi, A. Asthana, Y. Yap, Michigan Technological University, USA; M. Au, Savannah River National Laboratory, USA

Low dimensional materials have received considerable attention for their unique properties in energy storage (batteries) and energy harvesting (nanogenerators) devices. In this presentation, we cover the in-situ studies of zinc oxide nanowires (ZnO NWs) for piezoelectric energy harvesting and Silicon nanorods (NRs) for Li-ion batteries. Size scale effects were observed in ZnO nanowires and were explained by the modification of atomic structure at the nanowire surface. We also studied the mechanics of lithiated Si NRs to understand the effect of lithium intercalation into the structure of NRs.

Battery Technology

Novel Energy Storage Materials I

Room: Ballroom F

Session Chairs: Thad Adams, Savannah River National Lab; Ming Au, Savannah River National Laboratory

8:00 AM

(MCARE-026-2012) Lithium/air batteries: The next generation of rechargeable batteries beyond Li-ion chemistry? (Tutorial)

M. Au*, T. Adams, Savannah River National Laboratory, USA

Metal/air batteries use oxygen directly from the atmosphere to produce electricity. The cathode active material, oxygen, does not have to be stored in the batteries, which allows for higher total energy capacity in a smaller designed package. Very high energy density (2790 Wh/kg and 2800 Wh/L) can be achieved due to essentially unlimited cathode capacity. However, three major challenges still prevent Li/air batteries from practical application. The oxygen reduction and evolution both take place on the cathode and the effective and long-lasting bifunctional cathodes have not been developed yet. In order to reduce the products of the discharge, such as Li2O2 and Li2O, effective catalysts have to be discovered. Lastly, Li2O2 or Li2O are not soluble in the non-aqueous electrolyte and will clog the pores of the cathodes and eventually seize the cell. The recent investigation found that the lithium oxygen intermediate reacts with polycarbonate electrolyte and yield the stable LiCO3 that cast the shadow on reversibility of the LI/air cells. Focusing on these issues, we have conducted our initial investigation on cathode architecture, catalyst, electrolyte and the performance of the Li/air cells developed in out lab. We will discuss our results and share our vision for the future of this technology.

8:40 AM

(MCARE-027-2012) Status of High Energy Rechargeable Li-S Battery Development at Sion Power (Invited)

Y. V. Mikhaylik*, I. Kovalev, C. Campbell, T. Kelley, J. Affinito, Sion Power Corporation, USA

Sion Power Corporation in collaboration with BASF is working aggressively on realizing the impressive potential of the Li-S system for EV application. This presentation will discuss: 1. Fundamentals of Li-S electrochemical system including thermodynamics, reaction mechanisms and kinetics and their temperature dependence. 2. Li-S system active materials properties leading to several failure mechanisms limiting cycle life, charge efficiency, sulfur utilization and safety. 3. Current status of baseline 350 Wh/kg Sion Power cells and their high power and extreme low temperature variations. 4. Approaches pursued by Sion Power in collaboration with BASF towards increasing specific energy, cycle life, cells safety targeting to meet and exceed requirements for EV application. The core element of Sion Power's technology is a physically protected metallic lithium anode that allows substantial increase in cycle life and safety. With the Sion/BASF membrane system and dual phase-electrolyte, there was no thermal runaway for cells surpassing the melting point of metallic lithium (+181 oC). Physical membranes combined with improved cathodes have already more than tripled cycle life, in experimental 350 Wh/kg cell formats. As these new Li-S technologies are developed further, Sion is projecting to move from first generation of 350 Wh/kg Li-S cell to the Future 550 Wh/kg EV Li-S Cell.

9:00 AM

(MCARE-028-2012) Fabrication and Characterizations of Nanostructured Porous Si for Li-ion Batteries (Invited)

X. Sun, H. Huang*, Y. Zhuang, K. Chu, Wright State University, USA

High energy density Li-ion batteries can be achieved by developing and utilizing high capacity electrode materials. Si-based materials are promising anode candidate because of their high theoretical lithium storage capability (up to 4200 mAh/g). However, adaption of Si-based anode in Li-ion batteries for commercialization was hindered by the rapid capacity fading resulting from the dramatic volume variation during Li insertion and extraction. A well-designed microstructure or nanostructure can accommodate/resist the detrimental effect, which was recently demonstrated in Si nanowires and Si nanotubes etc. Recently we fabricated nanostructured porous Si by using anodization approach. Morphologies and thickness of the prepared porous Si were systematically studied by using SEM and the porosity was quantized with the help of OOF2 finite element analysis software. The pore size is in the range of 0.8-1.5um and thickness of the pore wall is 20-40nm in average. Lithium storage characteristics were investigated at both cyclic voltammetric and galvanostatic modes on the free-standing membranes as well as those mixed with carbon powders or supported on Si substrate. Si-wafer supported specimen showed high cycling stability. Specific capacities up to 1150mAh/g were achieved on free-standing membranes as well as those mixed with carbon powders.

9:20 AM

(MCARE-029-2012) Ionic conductivities in Li3xLa(2/3)-xTiO3 membranes of Li/Air batteries with controlled processing

C. Cooper*, APG, USA; M. Green, J. Wolfenstine, ALC, USA; A. C. Sutorik, G. Gilde, APG, USA

In Li/Air cells Li+ transport is limited by the membrane separating the electrolytes inciting need for high ionic transport properties. Controlled processing of membrane material Li3xLa(2/3)-xTiO3 perovskite was used to gain insight on its' ion transport properties. Literature typically demonstrates dry mixing of powders resulting in heterogeneity, thus an ethanol slurry was used to mix the initial powders to increase homogeneity in the pre-sintered powder. The temperatures were controlled to limit Li+ loss via volatility with reduction and control of calcination and sintering holds and temperatures yielding insight into possible over-sintering from literature. Sintering took place at 1200C with hold durations tested at 1, 6 and 12 hours and calcination temperatures of 900 and 1100C. High density maximizes grain-to-grain contact and minimizes pores improving ion transport. The pores are closed earlier during sintering of what will result in a high density sample, potentially decreasing the loss of Li+ at high temperatures which may increase lattice conductivity. Literature indicated density deviations up to 8% between pellets. This was resolved with cold isostatic pressing (CIP). Pellets were pressed via CIP to 30kpsi after uniaxial pressing and measured for density with the Archimedes method. Pressing via CIP improved sinterability and density consistency between samples.

9:40 AM

(MCARE-030-2012) Solution Precursor Plasma Deposition of Nanostructured Co3O4 Anodes for Li – ion Batteries

R. Tummala*, R. K. Guduru, P. S. Mohanty, The University Of Michigan, USA

Increasing demand for high energy density in Li – ion batteries has fueled intensive efforts for the search of high specific capacity anode materials to replace the carbon anodes. Cobalt oxide (Co3O4) with nanostructures has been found to be better alternative to carbon. However, most of the processing routes employ expensive or time intensive methods to obtain nanostructured Co3O4 powders, which then require further processing to obtain electrodes for battery assembly. Here we present a single step industrial scale solution precursor plasma deposition route to develop nanostructured, porous and flexible Co3O4 electrodes directly on a current collector. In this approach, a solution precursor comprising of water dissolved cobalt acetate is fed via an atomizer into a high temperature plasma plume for accelerated thermo-chemical reactions. The reaction products are then propelled toward the current collector by high pressure plasma jet to develop a film of Co3O4. Thus developed Co3O4 electrodes were binder and carbon free, and their microstructural analysis revealed nano particulate structure with desired amount of porosity. The films were then characterized by X-ray diffraction and microscopy studies. Electrochemical characterization indicated a theoretical capacity against Lithium. Absence of polymeric binders makes these electrodes suitable for high temperature battery applications.

10:20 AM

(MCARE-031-2012) Nanostructured Materials for Energy Storage beyond Li-Ions (Tutorial)

J. Zhang*, J. Liu, J. Xiao, X. Li, W. Xu, G. Graff, Pacific Northwest National Laboratory, USA

Li-air batteries and Li-S batteries are two of the most promising systems which have a theoretical energy density five to ten times of those of Li-ion batteries. The practical specific energy and cyclability of these batteries are strongly limited by the battery design, electrolytes, electrode materials and catalysts used in these batteries. To further develop these batteries for practical applications, a fundamental understanding on the reaction mechanisms during charge/discharge process of Li-air and Li-S batteries is required. In this presentation, our recent progresses on the effect of nano-structured materials on the performance of Li-air and Li-S batteries will be reported. We found that the performance of Li-air batteries strongly depends on nano-meso structure of carbon source used in air electrode. A newly developed air electrode consisting of a hierarchical arrangement of functionalized graphene sheets has demonstrated a record capacity of 15,000 mAh/g in a Li-air battery. Nanostructured sulfur/carbon electrodes also lead to a significant improvement on their capacity and cyclability. Fundamental mechanisms on the effect of nanostructured materials on the performance of these batteries will also be discussed.

11:00 AM

(MCARE-032-2012) Ultra High Energy Ball Milling Study of SiO-SnCoC Material as Anode for Lithium Batteries (Invited)

A. Abouimrane*, B. Liu, Argonne national Laboratory, USA; Y. Ren, University of Utah,, USA; Z. Fang, Argonne National Laboratory, USA; K. Amine, Argonne national Laboratory, USA

Amorphous state SiO has attracts much attention due to its high specific capacity (over 1400 mAh/g). However, this material suffers from its poor cycleability due to the volume expansion of the lithiated material. Tin-based alloys (Sn-Co-C) exhibit higher volumetric energy density than the conventional carbon anode and have been commercialized by Sony. In this work composite SiO-SnCoC system based on the SiO oxide and the SnCoC alloy is prepared and tested as anode material for Lithium batteries. Ultra high energy ball milling and SPEX ball milling methods were used to synthesize 50wt.% SiO-50wt.% Sn30Co30C40 electrode materials. Physical and chemical properties of this material were studied using various techniques like XRD, TEM and BET. The electrochemical performance shows that ultra-high energy ball milling sample yielded a specific capacity of reversible lithium insertion of 930 mAh/g under the current rate of 300 mA/g, which was much higher than the specific capacity obtained for the material prepared using the SPEX milling method (only 650 mAh/g@300mA/g). Samples prepared by both milling techniques exhibit good cycling performance. Indeed, no capacity fade was observed after 50 cycles. This result demonstrates that nanostructured SiO-SnCoC material is a promising anode for Lithium battery applications.

11:20 AM

(MCARE-033-2012) Lithium Intercalation in Low Dimensional Anodes Materials for Li-ion Batteries (Invited)

R. Shahbazian-Yassar*, H. Ghassemi, Y. Yap, Michigan Technological University, USA; M. Au, Savannah River National Laboratory, USA; Q. Gao, Michigan Technological University, USA

Silicon and titanate are promising materials for Lithium-ion batteries. This report focuses on the in-situ observation of lithiation and delithiation in Si nanorods and TiO2 nanotubes. The intercalation of

Li ions in Si nanorods was monitored during charging and the fracture of nanorods was quantified in terms of size. The electrochemical testing of these low dimensional structures were conducted inside a transmission electron microscope equipped with a novel in-situ electrical probing holder. In addition, the intercalation of crystalline anatase and amorphous TiO2 was studied and their fracture events were monitored in real time.

11:40 AM

(MCARE-034-2012) Synthesis and Characterization of Li2MSiO4 /C Cathode Materials for Lithium Ion Batteries

Y. Cen*, Worcester Polytechnic Institute, USA; C. Wang, Qingdao University of Science and Technology, China; R. D. Sisson, J. Liang, Worcester Polytechnic Institute, USA

The challenges of modern power sources demands electrode materials with high capacity and high power density. Due to the cost, safety and toxicity limitations of commercially used LiCoO2, Li[Ni, Mn, Co]O2 and LiMn2O4 cathode materials and low capacity of the vigorously studied LiFePO4, silicates with the general formula of Li2MSiO4 (M = Mn, Fe) have recently attracted much attention. Silicates provide a theoretical capacity of ~330 mAh/g. Even though they have relatively low electric conductivity, a reduction in particle size and coating with conductive carbon can significantly improve. Currently, most studies have focused on pure Li2MSiO4 compounds. It would be interesting to find out if Li2MSiO4 with mixed M of Fe, Mn and Co will provide superior performance to the pure phases as observed in the case of the layered LiMO2 cathodes (e.g. Li(Co1/3Mn1/3Ni1/3)O2). In our work, Li2MSiO4 with mixed M of Fe, Mn and/or Co was prepared by hydrothermal synthesis method. The product was coated with carbon nanomaterials to improve the electric conductivity and heat treated for complete crystallization. The structural, morphological and electrochemical characteristics of the mixed metal Li2MSiO4/C composites were investigated by X-ray diffraction, scanning electron microscopy, thermal gravimetric analysis and charge-discharge tests. The results are discussed in this presentation.

Solar

PV Modules and Novel Approaches and/or Structures

Room: Ballroom D
Session Chairs: George Georgiou, NJIT; Bushan Sopori, National Renewable Energy Laboratory

8:00 AM

(MCARE-035-2012) Light Trapping and Optical Management in Solar Cells and Modules (Tutorial)

B. Sapori*, National renewal Energy Laboratory, USA

The thickness of a solar cell is a very crucial parameter that must be carefully selected to achieve high performance of a solar cell. It is desirable to minimize the cell thickness to reduce the volume recombination and, concomitantly, lower the cell dark current, and boost the open circuit voltage and the fill factor. However, reducing the cell thickness can also lower its optical absorption and, hence, its photocurrent. To make up for the reduction in the cell thickness, it is often necessary to enhance the optical absorption by light trapping.Light trapping is a process of maximizing the absorption of light by controlling the optical design of the cell—through use of appropriately shaped interface geometries, and antireflection/reflection layers.Thus,light trapping simultaneously reduces the reflection and increases the absorption by increasing the optical length within the cell.The light trapping design can be quite complicated and, in general, requires a detailed optical management of light in the cell and the module.We have developed a software package,called PV Optics,for optimizing light trapping and for maximizing performance of a solar cell or a module.

8:40 AM

(MCARE-036-2012) Investigation of Degradation Mechanism on Extended Damp Heat Aged PV Modules

A. W. Norris, B. Ketola*, Dow Corning Corporation, USA

The power output over the lifetime of a photovoltaic (PV) module impacts the total number of kilowatt-hours (kWh) produced, which ultimately directly impacts the cost of generated electricity. For PV modules accelerated testing protocols, such as IEC 61215, have been used to assure that a 20 year lifetime is achievable. In particular, the accelerated aging Damp Heat (85°C/85% relative humidity) protocol has been used to indicate potential degradation mechanisms by increasing the temperature and humidity of the modules under test. This test was applied to compare the performance of PV modules encapsulated with silicone and ethylene vinyl acetate (EVA). These modules were aged in Damp Heat several times longer than the IEC standard of 1000 hours. The IV characteristics of these modules were periodically analyzed by the Sun Simulator to compare the influence of the encapsulant on module power output. At 3000 hours of exposure a significant reduction in power output was noted in the EVA set of modules, while minimal power degradation was observed in the silicone set. Analysis by electroluminescence (EL) imaging also indicated that factors other than corrosion at the electrical interconnects may have occurred. This presentation describes the analysis of the power output over time for silicone and EVA encapsulated modules after extended Damp Heat aging to help determine the degradation mechanisms.

9:00 AM

(MCARE-037-2012) Comparative Hazard Assessment of Photovoltaic Modules and Potential Modifications

D. Eisenberg*, M. Yu, C. Lam, University of California, Davis, USA; O. A. Ogunseitan, University of California, Irvine, USA; J. M. Schoenung, University of California, Davis, USA

Photovoltaics are currently viewed as a key source of sustainable energy when compared to traditional energy production methods, because of their potential for a smaller carbon footprint. Additional attributes, however, can influence the overall impact of photovoltaics on human and ecological health. In this work, the relative human health and environmental hazards associated with copper-indium-gallium-selenide/sulfide (CIGS) consumer modules and potential future product modifications have been studied. Hazard assessment has been performed through the customized application of established hazard scoring tools, specifically the Toxic Potential Indicator and Green Screen, developed by Fraunhofer IZM and Clean Production Action, respectively. The results provide a simple and effective way to distinguish the relative hazard amongst consumer modules and to identify ways in which CIGS modifications may or may not reduce their hazard scores. This assessment indicates that existing CdS buffer layer replacements can improve the current modules by rendering them less hazardous, with zinc based, indium-free, buffer layers offering the greatest improvement. It is also found that ethylene vinyl acetate encapsulant replacements such as thermoplastic polyurethane increase the hazard scores for the modules.

9:20 AM

(MCARE-038-2012) Dielectric Core-shell Optical Nano-antenna for Extraordinary Solar Absorption Enhancement (Invited)

L. Cao*, North Carolina State University, USA

The key challenge for massive utilization of solar energy is the high cost of existing solar conversion devices. Enhancing solar absorption by light trapping consists of a major strategy for the cost reduction and efficiency improvement of the device. Regardless that significant advances have been achieved so far, techniques to more efficiently trap solar light is needed to further lower the cost. We demonstrate a new approach to achieve extraordinary enhancement in the absorption of sunlight by exploring core-shell nanostructures. Unlike most existing techniques that typically employ one single mechanism for light trapping, our strategy capitalize on integrated contributions from multiple mechanisms We thoroughly examine the fundamental physics underlying the strong enhancement and propose new designs of high-performance light trapping for practical solar cells.

9:40 AM

(MCARE-039-2012) Nanostructure-mediated characteristics and device-level behavior of semiconductor-transparent conductive oxide (SC-TCO) nanocomposite thin films for photovoltaic energy conversion (Invited)

B. Potter*, G. Shih, R. J. Beal, S. DeValle, J. B. Kana-Kana, University of Arizona, USA

Interest in semiconductor nanophase composites for third-generation photovoltaic (PV) devices is widespread. Successful use of electronic and optical processes of import to PV energy conversion and unique to the nanoscale, however, is critically dependent on the control of multilength scale structure. Such issues as quantum-confinement-related spectral response, carrier generation and long-range charge transport are closely coupled through the structural attributes of the composite. The present work establishes the impact of semiconductor phase distribution (Ge, CdTe) within electrically active transparent-conductive-oxide matrices (ITO, ZnO) on the optical, electronic, and photoconductive response of the resulting nanocomposite. A sequential, RF sputtering technique and post-deposition thermal treatments are used to produce semiconductor structures ranging from isolated semiconductor quantum dots to interconnected, extended phase assemblies. Significant nanostructure-mediated modifications in optical absorption and carrier transport behavior will be discussed together with the performance characteristics of thin-film photovoltaic devices incorporating these nanocomposite materials.

10:20 AM

(MCARE-040-2012) Crack Inspection in Si Solar Wafers and Cells Using Resonance Ultrasonic Vibrations (Tutorial)

S. Ostapenko*, Ultrasonic Technologies, Inc., USA

Resonance Ultrasonic Vibrations (RUV) methodology was developed to accurately and automatically detect mechanically unstable wafers and cells with sub-millimeter length cracks and pinholes. RUV system provides a real-time in-line and off-line quality and process control tool to improve yield of automatic solar manufacturing lines. Experimental results of the RUV method are supported by FEA. Applicability of RUV technology in state-of-the art thin Si wafers and cells is demonstrated.

11:00 AM

(MCARE-041-2012) Characterization of the Mechanical Behavior and Material Properties of PV Module Encapsulants

R. A. Mickiewicz*, J. Lloyd, A. Stokes, T. Christian, D. Doble, R. Jaeger, P. Wu, J. Chapon, Fraunhofer Center for Sustainable Energy Systems (CSE), USA

Photovoltaic modules are composed of materials with widely varying mechanical and thermal properties. These properties can influence the performance and reliability of modules following exposure to external mechanical stress. Moreover, PV modules contain polymeric materials whose mechanical properties can vary over a wide range as a function of temperature. Since current mechanical loading tests for certification are performed at room temperature, they may not adequately reflect in-field mechanical stresses and failures. This work examines the impact of load testing at high and low temperature on module performance and cell integrity, with test modules characterized for performance and damage using a solar simulator and electroluminescence imaging. Additionally, the viscoelastic properties of the EVA encapsulant material were investigated in order to determine the level of cure of the laminated material. In particular, the stress relaxation properties of the EVA were probed and correlated with the gel content. Current methods to measure the gel content of the encapsulant material by solvent extraction are slow, destructive, and require use of hazardous chemicals. This new technique provides a means to quickly and non-destructively determine the gel content of the encapsulant in a laminated PV module and could be used for in-line quality control of the module manufacturing process.

11:20 AM

(MCARE-042-2012) Magnetic Field Assisted Assembly – Application to Solar Cell Integration

V. Kasi*, N. M. Ravindra, New Jersey Institute of Technology, USA

Magnetic Field Assisted Assembly is described in this study with an emphasis on application to large area devices such as solar cells. The proposed approach is shown to have significant advantages for reducing cost, increasing efficiency, reducing wastage and reducing the energy demands for repair, maintenance and integration of large area solar cell panels. Mathematical models for the assembly process are presented. A complete assembly system that includes a feedback mechanism for error correction and tolerance is described.

Hydrogen

New Methods and Novel Materials for H-Storage

Room: Ballroom E
Session Chair: Line Rude, Aarhus University; Rana Mohtadi, Toyota Research Institute North America

1:30 PM

(MCARE-043-2012) Recent Developments with Aluminum Hydride (Tutorial)

J. Graetz*, J. Wegrzyn, Y. J. Chabal, Brookhaven Natl Lab, USA; I. S. Chopra, The University of Texas at Dallas, USA; J. Reilly, Brookhaven Natl Lab, USA

Aluminum hydride (AlH_3) is a metastable, crystalline solid at room temperature that has a volumetric hydrogen density (148 g H_2/L) greater than twice that of liquid hydrogen and a gravimetric hydrogen density that exceeds 10 wt.%. It also exhibits a low heat of reaction (7 kJ/mol H_2) and rapid hydrogen evolution rates at low temperature (<100°C). Over the years, research groups from around the globe have led efforts to tackle the key challenges that limit the widespread use of aluminum hydride, yet considerable challenges remain. Recent efforts to characterize the structure, thermodynamics and kinetics of α-AlH_3 and the polymorphs (α', β and γ-AlH_3) have led to an improved understanding of the decomposition pathways and H_2 release rates. The application of surface coatings and catalysts have led to new methods to tailor the hydride stability and tune the hydrogen release rates as a function of temperature. In addition, a better understanding of aluminum-hydrogen interactions are paving the way for the development of new, low energy methods to regenerate aluminum hydride from aluminum metal and hydrogen gas at low pressure. This tutorial presentation will provide an overview of aluminum hydride research along with the most recent developments on efforts to tailor the decomposition kinetics and improve the regeneration efficiency.

2:10 PM

(MCARE-044-2012) Nitrogen-Based Composite Materials for Hydrogen Storage (Invited)

Y. Kojima*, T. Ichikawa, Hiroshima University, Japan

Ammonia borane (NH3BH3, AB) has emerged as attractive candidates for solid state hydrogen storage materials because of their high percentage of hydrogen (19.6 mass%) . The practical application of AB is greatly retarded by the higher dehydrogenation temperature at 393 K and the release of trace quantities of borazine. diborane and ammonia with the foaming. NH3BH3-based composite materials (MH/AB; M = Li, Na, K, Mg, Ca) were prepared by ball milling the mixture of AB and the corresponding alkali-metal hydrides and alkaline-earth metal hydrides. It was found that the NH3BH3-based composite materials suppressed the foaming and the impurity gasses with lower H2 desorption peak temperatures at 337-351 K (H2 desorption capacity: 6-9 mass%) . Ammonia (NH3) is also recognized as an attractive hydrogen (H2) carrier because it has a high hydrogen storage capacity of 17.8 mass% and it is easily liquefied under about 1 MPa at room temperature. However in order to release hydrogen from ammonia, high temperature of 623K is required even if active Ru-based catalysts are used. We found that alkali metal hydrides (LiH, NaH, KH) react with NH3 at room temperature, generating H2. After these H2 generations, alkali metal amides were able to store H2 at 373-573 K. The kinetic properties were shown to be better in the order of Li,Na,K.

2:30 PM

(MCARE-045-2012) Stabilization of Aluminum Borohydride Through Adductation and Material Complexation

D. A. Knight*, R. Zidan, R. Lascola, T. Motyka, Savannah River National Laboratory, USA; R. Mohtadi, P. Sivasubramanian, Toyota Research Institute of North America, USA

Aluminum borohydride, [Al(BH4)3,] possesses one of the highest hydrogen capacities of the metal hydrides, having almost 17 wt. % hydrogen available for desorption. The practicality of this material, however, is in question since this volatile and pyrophoric liquid not only tends to emit diborane during the hydrogen desorption process, but it also reacts rather energetically with only a trace amount of moisture in air. Our studies seek to stabilize aluminum borohydride through its complexation with other alkali metal borohydrides as well as by its adductation with Lewis base ligands of which lead to the formation of more stable and manageable solids. Presented here is the synthesis and hydrogen desorption/absorption analysis of alkali metal/aluminum borohydride complexes and Al(BH4)3/Lewis base adducts, along with an in-depth materials characterization in order to obtain a more accurate description of the materials' molecular structure and to determine a plausible desorption mechanism. The materials hydrogen sorption capabilities are measured using a standard Sieverts apparatus with additional thermal characteristics examined by TGA coupled with residual gas analysis. The materials and the associated sorption products are further characterized by X-ray powder diffraction, XRPD, Raman and FT-IR spectroscopy, and elemental analysis of select products by ICP atomic emission.

2:50 PM

(MCARE-046-2012) Thermodynamic Destabilization of Complex Metal Hydrides (Invited)

M. Paskevicius*, D. A. Sheppard, Curtin University, Australia; U. Filsø, Aarhus University, Denmark; M. P. Pitt, Curtin University, Australia; T. R. Jensen, Aarhus University, Denmark; C. E. Buckley, Curtin University, Australia

The need for a replacement fuel for vehicles is becoming ever more apparent as fossil fuel reserves begin to run out. Hydrogen is a lead contender to replace petroleum as a fuel for vehicles but one of the major hurdles is being able to safely store adequate quantities of hydrogen onboard vehicles. A hydrogen storage system must store high quantities of hydrogen (> 5 wt.% H_2) and it must absorb and desorb hydrogen within a suitable pressure and temperature window (1 – 100 bar and 0 – 100°C). A newly emerging area of research involves the alteration of the inherent properties of hydrogen storage materials to meet commercial targets by adjusting the reaction thermodynamics during hydrogen uptake and release. The thermodynamics can be changed by either reducing the metal hydride particle size below 10 nm or by altering the reaction pathway during hydrogen sorption. Research into both of these areas will be discussed. Focus will be directed towards encapsulation of complex hydride nanoparticles into ordered mesoporous carbon scaffolds and towards novel destabilization reactions involving complex hydrides.

3:10 PM

(MCARE-047-2012) Understanding and Altering the Properties of Low Stability Borohydrides for Onboard H2 Storage Applications (Invited)

R. Mohtadi*, P. Sivasubramanian, Toyota Research Institute North America, USA; T. Matsunaga, Toyota Motor Corporation, Japan; R. Zidan, D. Knight, Savannah River National Laboratory, USA

Global research efforts have been focused on complex metal hydrides for dense hydrogen storage onboard media. Most particularly, in depth investigations have been conducted on alkaline and alkaline earth metal borohydrides due to their high hydrogen content and ease of preparation; stemming from their high thermodynamic stability. This stability, while allowed for the preparation and manipulation of the original compounds; i.e. cationic and or anionic substitution with other elements, has been a hurdle towards their utilization due to the high temperatures required to release hydrogen in excess of 200 °C in most cases. Less stable borohydrides which are transition or aluminum metal based have not been of real focus due to their instability at ambient conditions, difficulty of preparation and isolation, and/or the generation of substantial amount of diborane observed upon their decomposition. We have been researching the synthesis and the stabilization of aluminum borohydride as hydrogen storage onboard media and the work presented will demonstrate the preparation procedure, unveil the hydrogen storage properties of the compounds prepared and show our strategies towards further improvements.

3:50 PM

(MCARE-048-2012) Development of Processes for the Reversible Dehydrogenation of High Capacity Hydrogen Carriers at Practical Conditions (Tutorial)

C. Jensen*, M. Chong, G. Severa, University of Hawaii, USA; E. Rönnebro, Pacific Northwest National Laboratory, USA; Z. Wang, Hawaii Hydrogen Carriers, LLC, USA; A. Karkamkar, T. Autrey, Pacific Northwest National Laboratory, USA

The majority of current research on the development hydrogen carriers is focused on the quest for new materials. Alternatively, an equally valid approach is to develop new chemical processes that enable practical hydrogen cycling pathways for well-known high-capacity materials. In our laboratories. we are using this approach to develop magnesium borohydride and liquid organic hydrogen carriers (LOHCs) as hydrogen storage materials . We have demonstrated the cycling of >11 wt% hydrogen from the direct, reversible dehydrogenation of Mg(BH4)2 to MgB2. However, this cycling required forcing conditions and we have more recently investigated the hydrogen storage potential of Mg(BH4)2 under more practical conditions. We have found that the dehydrogenation at 200 C results in the selective formation of Mg(B3H8)2. This process was found to be reversible at 250 C under 120 atm H2. The barrier to utilization of LOHCs for automotive applications is significantly lower than other storage media because they are cheap, abundant, and can be distributed using existing infrastructure. Additonally, the reversibly release 7-8 wt% H2 from LOHCs is free of the thermal management problems commonly associated with solid-state hydrogen absorbing materials. Our approach utilizes the PCP pincer complex, IrH2{C6H3-2,6-(OPBut2)2} as a catalyst for the dehydrogenation of the LOHCs.

4:30 PM

(MCARE-049-2012) Elucidation of Hydride Interaction with Carbon Nanostructures and the Formation of Novel Nanocomposites for Reversible Hydrogen Storage

J. A. Teprovich*, R. Zidan, M. S. Wellons, D. A. Knight, R. Lascola, Savannah River National Laboratory, USA

Numerous theoretical and experimental investigations have demonstrated that nanocomposites prepared from hydrides and carbonaceous nanostructures (graphene, CNT's, C_{60}, etc.) are unique materials for hydrogen storage. Initial work by our group has demonstrated that the intimate mixing of carbon nanostructures with complex metal hydrides (NaAlH4, LiBH4, and LiAlH4) improves the desorption/absorption of hydrogen in these materials. Fullerene (C_{60}) consistently outperformed the other carbonaceous nanomaterials examined. In order to identify the role of C_{60} in these nanocomposites, a systematic evaluation of spectroscopic and thermogravimetric data was performed. It was determined that the active hydrogen storage material is M_x-C_{60}-H_y and suggested that simple metal hydrides (i.e. LiH) can be used to prepare the nanocomposites. Utilizing an optimized Li:C_{60} ratio, our nanocomposite can reversibly store 5 wt % H_2

(T onset ~275 C) via a chemisorption mechanism with the material spectroscopically resembling a hydrogenated fullerene. However, our nanocomposite does not suffer from the same drawbacks as typical hydrofullerenes (T onset ~500 C and release of methane) because the fullerene cage remains mostly intact and is only slightly modified during multiple hydrogen desorption/absorption cycles.

4:50 PM

(MCARE-050-2012) Nanostructured metal hydrides for exploring candidate hydrogen storage systems (Invited)

D. Grant*, C. Fry, G. Walker, University of Nottingham, United Kingdom

The aim of this study is to explore the potential of layered nanostructures to improve kinetics, cycling behavior and integrity of cost effective metal hydrides for solid state hydrogen stores. To this end thin film multilayers have been produced by a Closed Field Unbalanced Magnetron Sputter Ion Plating system designed for multi axial scale up work allowing gram quantities to be analyzed for hydrogen uptake. The configuration used here was based on single axis rotation and multiple targets producing 150 alternating magnesium with nickel + transition element layers. X-TEM confirmed columnar growth and the Mg layers were 14±0.5 nm thick with the Ni transition layers ca. 1.5±0.5 nm. Pressure composition isotherms were recorded at 6 different temperatures from from 250°C to 350°C showing two plateaux consistent with modified MgH_2 and Mg_2NiH_4 (dehydrogenation $\Delta H=80.5\pm2.4$kJ/mol H_2 and $\Delta H=66.6\pm2.4$ kJ/mol H_2 respectively). Capacity of the multilayer was ca. 5 wt% ca. 90% of theoretical assuming a Mg/Mg_2Ni multilayer. Kinetics displayed a 90% uptake in only 44 s at 350°C and only 5 min at 250°C. Thin films offer a promising way of screening combinations of metal hydrides with tailored structures to improve the kinetics the system. The PVD configuration developed allowed gram quantities to be bulk analysed. The challenge is to translate such structures to cost effective bulk processing methods.

5:10 PM

(MCARE-051-2012) Metal hydrides prepared by cold rolling: a new way to enhance hydrogen sorption (Invited)

J. Huot*, UQTR, Canada

It has recently been shown that Severe Plastic Deformation (SPD) techniques could be used to obtain nanostructured metal hydrides with enhanced hydrogen sorption properties. Cold rolling is particularly interesting technique because it is easily scalable to industrial level. We will present our latest results on cold rolling different types of metal hydrides such as magnesium-based alloys, AB5 alloys, and Titanium-based alloys. In general, cold rolling is as effective as ball milling to enhance hydrogen storage properties of these compounds but with a tenfold reduction of processing time and energy. We also show that cold rolling could be performed on the hydride as well as on the alloy. The exact mechanism responsible for this enhancement may not be the same as in ball milling. In particular, particle size reduction and texture seems to play a leading role in the hydrogen sorption enhancement of cold rolled metal hydrides.

Battery Technology

Novel Energy Storage Materials II

Room: Ballroom F

Session Chairs: Ali Abouimrane, Argonne national Laboratory; Taiguang Jow, U.S. Army Research Laboratory

1:30 PM

(MCARE-052-2012) Cathode Design an Stability of Li Batteries (Invited)

D. Kober, G. Gudday, M. Harth, O. Goerke, R. Bordia, H. Schubert*, Technische Universitaet Berlin.de, Germany

This paper reports on experiment on variations in microstructural parameter and their correlation to stability of Li Batteries. Beside capacity and maximum power output the cycle stability is a key property for the usability of batteries. Until now the cycle stability is limited due to aging of the cathode array. Especially the high strain on Li penetration is a very critical issue. Analysis of commercial system showed, that the most design either put emphasis on lowering Youngs modulus or minimizing the contact area. Experimental variations on cathode microstructure have been carried out by changing particle size, hence, pore size and pore size distribution. Finally low strain materials are compared. Thus the three major contributions to the stress state of the materials such as strain, modulus and geometry have been addressed. The experiments indicate that a minimized stress situation correlates with good cycle stability. For the future a model must be developed which describe the microstructural parameters and their influence on stability.

1:50 PM

(MCARE-053-2012) Nanostructured Materials as Potential Electrodes for Li-ion Batteries

F. Jiao*, B. Yonemoto, G. Hutchings, University of Delaware, USA

A major goal of lithium battery research is to prepare electrodes that can sustain higher rates than present materials, for new high power applications such as HEV's. Here, we will show our recent progress in the synthesis of novel nanostructured materials as potential electrode materials for lithium-ion batteries. There is much current interest in mesoporous metal oxides, while it is still difficult to prepare metal oxides with a wall thickness below 3 nm. We will describe the synthesis of a wide range of mesoporous transition metal oxides by employing a novel nano-casting approach. The resulting nanostructured materials exhibit superior performance compared with their normal analogues. Also, we will discuss the electrochemical properties of nano-sized manganese oxides. Although manganese oxides have been intensively studied as potential cathode materials, understanding of their electrochemical behavior is still limited, particularly when the particle size is a few nanometers. In order to explore the size and morphology effects, we have prepared nanostructured manganese oxides with various morphologies. Our preliminary results show that these materials have unique electrochemical properties upon lithium ion intercalation compared to their micron sized counterparts. The detailed structural characterization and electrochemical studies will be presented.

2:10 PM

(MCARE-054-2012) Nanostructured metals and metal oxides for HGH capacity anodes of Li-ion rechargeable batteries

M. Au*, T. Adams, Savannah River National Laboratory, USA

The electric vehicles with 300 miles driving range require new batteries with capacity 4-5 times high than today's Li-ion batteries. The metals (such as Si, Sn and Al) and metal oxides (such as SnO2, Co3O4 and Mn2O3) have the higher theoretic capacity in the range of 500 ~ 4000 mAh/g. However, the large volume expansion and contraction of these metals and metal oxides during charge and discharge causes materials pulverization resulting in quick capacity decay. To accommodate the volume change and increase lithium ion mobility in the anodes, the aligned metal nanorods and the nanoporous hollow spheres of the metal oxides were developed. Our anodes made by aligned Al and Si nanorods demonstrated 1000-2000 mAh/g of capacity. By tuning the composition of Si nanorods, their electrochemical cycling life was improved significantly. The batteries made by the hollow nanoporous spheres of SnO2 demonstrated 400 mAh/g of capacity in multiply cycles. The good cyclability is contributed to the unique hollow spherical structured of these metal oxides. We will report the details in this presentation.

2:30 PM

(MCARE-055-2012) Improved Electrochemical Performances of Silicon Anodes Coated by P-doped C60 Films

A. Arie*, Parahyangan University, Indonesia

Silicon anodes of lithium secondary batteries were coated by Phosphorus doped fullerene C60 (P:C60) thin films using a plasma assisted thermal evaporation technique. The presence of phosphorus doping was confirmed by Raman and XPS analysis. In comparison with the undoped C60 coating layer, the electrochemical measurements showed that the P:C60 film contributes to the improvement of the capacity retention after the 50th cycle when discharged at a high C rate. It is attributed to the better Li-ion transfer and smaller charge transfer resistance at the interface between the anode and electrolyte.

2:50 PM

(MCARE-056-2012) Supercapacitive Properties of Hydrothermally Synthesized Co3O4 Nanostructures

D. Mitlin*, H. Wang, L. Zhang, C. Holt, B. Zahiri, B. C. Olsen, University of Alberta and NINT NRC, Canada

A hydrothermal process was employed to create a variety of Co3O4 nanostructures. We demonstrate that nominally minor differences in the synthesis temperature (50, 70° or 90°C) yielded profound variations in the oxide microstructure, with lathe-like, necklace-like and net-like morphologies of different scales resulting. This in turn resulted in significant variations in the supercapacitive performance that ranged from mediocre to superb. Specifically, the mesoporous net-like Co3O4 nanostructures that were synthesized at 50°C exhibited very favorable electrochemical properties: The net-like Co3O4 had a specific capacitance of 1090 F/g at a mass loading of 1.4 mg/cm2. At this high mass loading such performance has not been previously reported. SEM and TEM analysis of these samples revealed an interconnected array of sub-10 nm crystallites interspersed with a high volume fraction of pores that were on the same scale. The poorer performing microstructures were both coarser and much less porous.

3:10 PM

(MCARE-057-2012) Investigation of Chemical Composition of Electrodes in Li-Ion Batteries

A. Fortier, S. K. Karna*, University of North Texas, USA

Over the past few decades industry has almost exclusively adopted lithium (Li) ion batteries for use in portable electronics. However, the lag between practical and theoretical capacity for many types of Li-batteries indicates that there is still much improvement to be made in the field. Along with improving performance, battery research is also focused on extending the life cycle. One of the most common failures in Li-ion batteries is change in electrode's chemical composition. A known change in chemical composition that affects the functionality of the battery is formation of a layer called solid electrolyte interface (SEI) layer that forms at the interface of the anode and the electrolyte and results in material's opposition to the flow of electric current. In this study the main goal is to investigate the properties of the anode and the SEI layer, observe their crystallographic orientation and surface texture, and measure the stress state in battery before and after the battery failure. Comparison of the properties under study will be presented for new and failed batteries. Results are obtained using analytical tools involving SEM/FIB/EDS, XPS, XRD and MOSS. More insights on the electro-chemical behavior of batteries and its constituents will allow development of improved materials that will increase the performance of the electrodes and extend the life of many electronic devices.

3:50 PM

(MCARE-058-2012) Engineering Electrochemically Active Nanoscale Silicon Based Hetero-structures (Invited)

P. Kumta*, University of Pittsburgh, USA

Nanotechnology has revolutionized several areas of materials science and technology including the area of energy storage. Since Fuji discovered and demonstrated tin oxide nanocomposites as promising anode materials for lithium-ion batteries, there has been a resurgence of activities focused at identifying alternate materials to graphite, the currently used anode. Various strategies have been researched over the years comprising identifying new intermetallic anode systems, generation of a nanostructured disordered matrix containing the electrochemically active component upon electrochemical insertion of lithium as well as creation of nanowires, gels, and 'core-shell' structures. Our research over the years has been directed at synthesizing nanostructured composites comprising active and inactive phases generated directly ex-situ by exploiting novel low-cost synthetic approaches. Initial results have shown that the resulting intra-type nanocomposites exhibit stable capacities as high as 1000 mAh/g while novel vertically aligned CNTs containing nanoscale Si clusters based hybrid heterostructures exhibit impressive capacities as high as ~3000 mAh/g. Opportunities and challenges related to the synthesis and design of these nanostructured materials for next generation Li-ion batteries will be presented and discussed.

4:10 PM

(MCARE-059-2012) Nanofiber-Based Electrode Materials for Advanced Lithium-Ion Batteries (Invited)

X. Zhang*, North Carolina State University, USA

We use electrospinning technology to process different materials aimed at preparing novel composite nanofibers which can be used as anodes and cathodes for lithium-ion batteries. We present the fabrication of silicon/carbon (Si/C) anode and LiFePO4/carbon (LiFePO4/C) cathode composite nanofibers and the integration of these nanofibers in lithium-ion batteries to achieve high system performance. The anodes that are made from Si/C nanofibers have the advantages of both carbon (long cycle life) and Si (high lithium-storage capacity). The cathode material, LiFePO4/C nanofibers, also shows good electrochemical performance. The effect of the nanostructure on the electrochemical performance of these anodes and cathodes is presented. Their synthesis processes, electrochemical properties, and electrode reaction mechanisms are also discussed.

4:30 PM

(MCARE-060-2012) Three Dimensional Construction of Electrodes - Open Door to High Capacity Lithium Batteries (Invited)

J. Prochazka*, HE3DA, Inc., Czech Republic; L. Kavan, J. Heyrovsky Institute of Physical Chemistry, Czech Republic; M. Zukalova, J. Heyrovsky Institute of Physical Chemistry, Czech Republic

The thin-film lithium battery technology has made a significant progress in the past ten years and in many aspects it has reached the theoretical possibilities. While the thin-film battery is nearly optimized, the capacity limits of lithium accumulators can be further extended by an original construction of 3-D electrodes. The 3-D design, with electrodes several millimeters thick allows new features that have not been used in the battery industry yet. 3-D concept of the accumulator not only increases capacity of the individual cell but also significantly reduces size of the assembled modules. The new Li ion battery technology platform will be demonstrated on construction of prototypes and their electrochemical performance.

Biomass

Bioprocess Development

Room: Ballroom G
Session Chairs: Pratap Pullammanappallil, University of Florida;
Robin Brigmon, Savannah River National Laboratory

1:30 PM

(MCARE-061-2012) Biomethane From Energy Crops and Organic Wastes (Tutorial)

D. P. Chynoweth*, University of Florida, USA

The objective of this paper is to review the results and conclusions of research on biomass energy conducted under the sponsorship of the gas industry with periodic co-funding from other institutions. The scope of this program was to determine the technical and economic feasibility of production of substitute natural gas (SNG) from marine and terrestrial biomass and organic wastes using anaerobic digestion as a conversion process. This work began in 1968 and continued until about 1990, ending as a result of low energy prices in the U.S. and reduced emphasis in renewable energy. For each of these feedstock categories, growth or collection (in the case of wastes), harvesting, conversion by anaerobic digestion, and systems and economic analysis are addressed. Results from more recent studies will be presented on potential use of anaerobic digestion for stabilization of a recovery of nutrients from solid wastes during space missions and conversion of sugar beet wastes to methane and compost.

2:10 PM

(MCARE-062-2012) Evaluation of Fluorescence for Monitoring Plant Health for Bioenergy Applications (Invited)

R. Brigmon*, Savannah River National Laboratory, USA; K. McLeod, University of Georgia, USA; E. Doman, E. Wilde, Savannah River National Laboratory, USA

An assessment utilizing fluorescence for monitoring plant health was made at the Department of Energy's Savannah River Site (SRS) in Aiken, SC. Phytoremediation and monitored natural attenuation (MNA) processes at chlorinated solvent, heavy metal, and tritium contaminated sites could impact plants for use in biomass energy production. It is evident that environmental restoration efforts are most successful when the biotic community (primarily plant and rhizosphere communities) remains healthy. Plants were monitored in 6 different projects including greenhouse studies, lead phytoextraction from shooting range soil, and zinc phytoextraction. Two field-scale spray irrigations of contaminated groundwater were evaluated including chlorinated solvents and tritium uptake. A wetland system was tested where copper is the main contaminant of concern. Trees in a seepline area where chlorinated solvents are impacting groundwater were also tested. Due to the relatively low concentrations of contaminants at the field sites, little plant stress was observed. This project examined fluorometry as a tool to assess plant health through direct measurement of the plant photosynthetic capacity in stress situations. The photosynthetic capacity of the plants in the contaminated situations was not impacted, as measured with fluorometry, and could be a future biomass source for energy production.

2:30 PM

(MCARE-063-2012) Comparison of Single and Two Stage Anaerobic Digestion of OFMSW

G. Ram Mohan, P. Pullammanappallil, P. J. Dube*, University of Florida, USA

Concerns about rising energy costs have greatly increased the awareness of renewable fuels and alternative energy sources on a global scale.Anaerobic digestion of municipal solid wastes has the advantage of being able to produce a valuable end product, biogas, as well as reduce the volume of incoming waste streams.In a single stage system, biological and chemical reactions categorized into four stages namely, hydrolysis, acidogenesis, acetogenesis and methanogenesis, occur inside a single reactor.In a two-stage system biogas production is maximized by carrying out hydrolysis, acidogenesis and acetogenesis in the preliminary solids digester and then transferring the percolate from the solids digester to a second reactor, an anaerobic filter that is predominant in methanogens, for methanogenesis.In this paper, the performance of single-stage and two-stage system was compared at mesophilic(37C)and thermophilic(55C)temperatures.A synthetic source separated waste mix based on residential waste characteristics that included food waste, yard waste and paper waste was used for digestion.For single stage trials,experiments were performed in a 5L digesters in batch mode.In the two-stage system,5L solids digester was sequenced with a 12 L packed bed anaerobic filter reactor.During the course of each run soluble COD, pH, gas composition and production, and nutrient content was monitored on a daily basis.

2:50 PM

(MCARE-064-2012) Microbe-Derived Production of Fuel Components from Defined Renewable Waste

J. C. Biffinger*, R. E. Morris, L. Fitzgerald, E. Petersen, Naval Research Laboratory, USA; C. Ziemer, ARS-USDA, USA

A Shewanella containing bacterial consortia is being developed for wastewater pre-treatment that selectively increases the expression of long chain hydrocarbon components of aviation fuels and lubricants. This will result in a >70% overall reduction and re-use of waste/biomass through the conversion into usable power and heat. Native bacterial flora from a defined simulated human waste source are exposed to sequenced Shewanella spp. The chemical sensing and fuel technology section in the Chemistry Division of NRL performs basic and applied research to understand the underlying chemistry that impacts the use, handling and storage of current and future Navy mobility fuels. Research utilizing state of the art chemometric modeling is conducted to extract the critical chemical information from complex analytical data. These diagnostics will be utilized to correlate pyrolytic hydrocarbon content with bacteria population changes using GC-MS and GCxGC-MS and RT-PCR. The Shewanella spp. that increase alkane production are compared to strains that do not generate long chain hydrocarbons to identify potential genes necessary for optimal production/secretion of these components from waste. Alkane generating consortia (AGC) will be formulated and tested from the mixture of bacteria that result in the highest concentration of hydrocarbons (> C10) after pyrolysis.

3:10 PM

(MCARE-065-2012) Lactic acid metabolism of Escherichia coli and its use in recycling Poly-Lactide polymers

D. Chauliac*, K. Shanmugam, P. Pullammanappallil, University of Florida, USA

FDA approved, renewable PLA plastics are by far the most commercially viable alternative to petroleum-derived plastics. With 150 million tons of commodity plastics used every year, more and more brands turn their "non eco-friendly" packaging into PLA polymers. Although harmless when biodegraded in nature (under appropriate conditions), PLA polymers are not yet appropriately recycled and end up accumulating in landfills along with other plastics. The long-term goals of the proposed research are to elucidate ways of recycling the polymer after its intended initial use, i.e. develop a thermal / biological process that will enhance the rate of break down of polymers back to lactic acid and isolate the L- isomer of lactic acid for reuse. The specific objectives of the research are: (i)develop and optimize a process, which allows break down of the polymer into its simplest components: L and D-lactic acids (ii) Identify and characterize the enzymes that are responsible for the conversion of L-lactic acid into pyruvate in E. coli(iii) engineer and evolve a bacterial biocatalyst that can specifically and efficiently use D-lactic acid but not the L-lactic acid in the PLA syrup, leaving the remaining and abundant L-lactic acid in the medium to be further purified for reuse. The engineered biocatalyst will represent the first alternative to the expensive enantiomers separation performed chemically.

3:50 PM

(MCARE-066-2012) Degradation of automotive materials in palm biodiesel

M. Fazal, A. S.M.A. Haseeb*, H. H. Masjuki, University of Malaya, Malaysia

Recently, biodiesel is being considered as an attractive alternative fuel for automobiles because of its environmental benefits and the fact that it is made from renewable sources. However, corrosion of automotive materials in biodiesel is one of the concerns related to biodiesel compatibility issues. Biodiesel is more prone to absorb water which tends to condense on metal surface. Automotive fuel system and engine components are made from different ferrous and non-ferrous materials. Corrosion damage of different types of automotive materials was compared in both diesel and biodiesel. Due to exposure of different materials, changes in fuel properties were also examined. In order to reduce the corrosivity of biodiesel, different types of antioxidants and corrosion inhibitors were used. Degradation of metal surfaces were characterized by SEM/EDX, X-ray diffraction (XRD), x-ray photoelectron spectroscopy (XPS) etc. Changes in biodiesel were characterized by FTIR, GCMS, TAN analyzer etc. Among the metal investigated, copper is found to be least resistant in biodiesel. Use of TBA was found as an effective corrosion inhibitor for metals. Exposure of biodiesel to metals, particularly copper, led to catalytic enhancement of biodiesel properties. Possible degradation mechanisms for both metal and biodiesel were proposed.

4:10 PM

(MCARE-067-2012) Electroactive Bio-Materials for Alternative Energy Processes (Invited)

C. Turick*, C. E. Milliken, Savannah River National Laboratory, USA

Microorganisms often live and even thrive in extreme environments where survival and growth can only be accomplished through unique biochemistry. This includes molecules that possess utility in various aspects of alternative energy production. In particular, electroactive polymers produced by naturally occurring microorganisms enhance metal-oxide reduction and provide resistance to ionizing radiation for various organisms in the environment. These polymers are various forms of melanin pigments and contain quinone moieties that confer electron-shuttling capabilities. For instance, pyomelanin enhances electron transfer from metal-reducing bacteria to metal oxides and thus increases microbial growth rates. The redox-cycling capacity of pyomelanin can also be used to increase current production when bacteria are grown on electrodes, such as microbial fuel cells. Microbial fuel cells offer potential as alternative energy sources, especially in remote areas. Another example involves melanin producing fungal isolates from the Chernobyl nuclear facility that demonstrate enhanced growth in ionizing radiation fields. In this case eumelanin provides a means to quench harmful oxidizing effects of gamma radiation. When incorporated into a melanin-composite electrode, gamma irradiation produces an electric current. This has potential for incorporation into various aspects of alternative energy production.

4:30 PM

(MCARE-068-2012) Biogasification of marine algae Nannochloropsis oculata

S. Buxy*, University of Florida, USA

Current interest in the algal derived biofuels focuses on the production of lipids for conversion to diesel-fuel substitutes. However, this approach requires overcoming challenges like separation and extraction of the lipids. Another approach to biofuel production from algae will be via biogasification. The objectives of this study were to investigate the growth yields and productivity of marine algae, namely Nannochloropsis oculata and biogasification potential of it. Harvested algal cells were anaerobically digested in laboratory scale digesters to determine the extent and rate of degradation, methane production potential, and the effect of temperature, salinity and cell concentration on these biogasification parameters. Algae mainly consist of polysaccharides (included as cellulose, xylan and mannan), proteins, fatty acids, free amino acids and nucleic acids in varying proportion and lipids. Marine algae have low lignin and cellulose content and known to accumulate lipids which makes it easier to digest anaerobically and it should show high biochemical methane potential. Energy content of the biogas produced in this manner is comparable to that in the form of biodiesel per unit mass of algal cells. The algal cell slurry can be directly fed to the digester with no need for cell separation and lesser energy is spent to separate the biogas product, therefore the net energy produced from biogasification is much higher.

4:50 PM

(MCARE-069-2012) Refractory Ceramic Lining Selection and Troubleshooting in Thermal Biomass Operations

D. Goski*, T. M. Green, D. J. Loiacona, Allied Mineral Products, USA

There are innumerous creative alternative energy solutions incorporating high temperature processes and biomass emerging in the marketplace. These range from the small scale home heating level to the industrial large scale plants generating heat energy or alternative fuel gases. One of the limiting factors to the thermal efficiency and cost of these operations is the performance of the refractory ceramic containment materials. Different sources of biomass can contribute to different failure mechanisms in refractory linings. The authors will present a refractory selection and troubleshooting overview relating to differing biomass characteristics and operational conditions.

Hydropower

Material Challenges for Conventional and Marine Hydropower

Room: Ballroom D

Session Chairs: Alan Miller, Lockheed Martin Corp.; Bernadette Hernandez-Sanchez, Sandia National Laboratories

1:30 PM

(MCARE-070-2012) Materials Challenges and Developments in River Hydrokinetics (Invited)

E. C. Lovelace*, Free Flow Power, USA

For hydrokinetic renewable energy generation projects materials solutions are necessary to balance anti-biofouling, corrosion protection, strength, and cost attributes. Free Flow Power is developing hydrokinetic turbine arrays for commercial scale renewable energy generation on the Mississippi River. Tradeoffs between various composite and metal materials for the turbine blades and structure are discussed with respect to withstanding peak loads and high volume manufacturing costs. Anti-biofouling and corrosion resistant properties are discussed with respect to durability and both initial and maintenance costs. Current pilot in-river deployments of a prototype turbine to evaluate material behavior will be presented.

1:50 PM

(MCARE-071-2012) Materials Challenges in the Huge Cold Water Pipes Required for Ocean Thermal Energy Conversion (Invited)

A. K. Miller*, Lockheed Martin Corp., USA; J. Halkyard, John Halkyard & Associates, USA; S. Shi, Houston Offshore Associates, USA; D. Dittenber, West Virginia Univ., USA

The Cold Water Pipe (CWP) for a commercial-size (100MW) OTEC plant is 10m/33ft. in diameter by 1000m/3300 ft. in length. That is quite large. During the past four years, Lockheed Martin has worked out the minimum-cost configuration, materials, and fabrication method for an Advanced Composite CWP as part of its OTEC systems, and recently has validated key elements of the design, materials, and fabrication methodology at the 4m/13 ft. diameter required for a Pilot Plant. This paper reviews some elements of that overall work (including photos of the large-scale hardware), and as a specific materials challenge also focuses in some detail on seawater fatigue of the composite material, which is one of the two dominant design drivers. Recent hydrodynamic predictions of the bending fatigue loadings experienced by the CWP from wave-driven platform motions are shown, new data on the selected material's fatigue resistance to those loadings (after seawater conditioning) is also shown, and system-level implications of the preliminary fatigue design results are described.

2:10 PM

(MCARE-072-2012) Material Challenges and Opportunities in Conventional Hydropower (Invited)

K. Zhang, W. Zhang*, B. T. Smith, Oak Ridge National Laboratory, USA; R. Dham, US Department of Energy, USA

The conventional hydropower arena composes of both existing large and emerging small plants; each offering unique material challenges. For the former, there has been relatively limited opportunity for transforming the traditional materials (e.g. steel) to the new alternative materials (e.g. carbon fiber reinforced polymer) for the large hydro-turbine components. This is mainly due to the durability and deflection concerns under severe operating conditions (high rotational speed and vibrant flow velocity). Nevertheless, many material innovations have been driving up generation efficiency. Examples include 1) advanced materials and surface engineering for improving resistance to cavitation, erosion and abrasion of turbine, gate, spillway, and other water passage components; 2) self-lubricating materials for bearing faces to eliminate the risk of water oil pollution; and 3) onsite high-power laser technology for efficient equipment repair and rehabilitation. For the large number of undeveloped small hydro projects, there are more opportunities for using alternative materials for reducing cost of electricity. For instance, polyethylene, fiberglass reinforced polyester, and asbestos cement have resulted in great cost reductions for penstocks. Another example is plastics, carbon fibers or other new anti-corrosion materials offer possible low-cost, lightweight turbines for the low-head micro-scale applications.

2:30 PM

(MCARE-073-2012) Hydrokinetic Energy: Materials Challenges and Opportunities

K. Kandasamy, R. S. Mishra*, University of North Texas, USA

The energy in flowing river streams, tidal currents or other artificial water channels is being considered as viable source of renewable power. Hydrokinetic conversion systems, albeit mostly at its early stage of development, appear suitable for harnessing energy from such renewable resources. A number of resource quantization and demonstrations have been conducted throughout the world and it is believed that both in-land water resources and offshore ocean energy sector will benefit from this technology. This talk will give an overview of a major new effort on system level materials optimization for hydrokinetic energy. A comprehensive survey of various hydrokinetic systems reported to date has been done and a system level analysis on these emerging systems has been performed. This work integrates fundamental analysis and research with development of prototype systems. The results of this integrated approach will be presented along with guidelines and methodology for design and manufacturing of cost-effective hydrokinetic systems.

2:50 PM

(MCARE-074-2012) Tailoring Fiber Reinforced Composites Stiffness for Efficient Hydropower Systems (Invited)

B. N. Nguyen*, Pacific Northwest National Laboratory, USA

Fiber-reinforced polymer composites can offer important advantages over metals where lightweight, cost-effective manufacturing and high mechanical performance can be achieved. To date, these materials have not been used in hydropower systems. In view of the possibility to tailor their mechanical properties to specific applications, they now have become a subject of research for potential use in hydropower systems. The first step in any structural design that uses composite materials consists of evaluating the basic mechanical properties as a function of the composite microstructure. These properties are the elastic stiffness, stress-strain response, and strength. This article describes the evaluation of the elastic stiffness for some common injection-molded and compression-molded fiber polymer composites to preliminarily estimate whether they could be used in hydropower systems for load-carrying components such as turbine blades. To this end, the EMTA software developed at the Pacific Northwest National Laboratory has been applied to predict the elastic properties of these composites as a function of three key microstructural parameters: fiber volume fraction, fiber orientation distribution, and fiber length distribution. These parameters control the composite mechanical performance and can be tailored to achieve property enhancement.

3:10 PM

(MCARE-075-2012) Degradation of Mechanical Properties in Composite Materials Subjected to Salt Water Environments

D. A. Miller*, J. Mandell, D. Samborsky, A. DiFronzo, Montana State University, USA

This paper will present the recent trends in the mechanical characterization of composite systems under consideration for wind and Marine Hydro Kinetic (MHK) applications exposed to salt water environments. In initial testing, unidirectional ([0] and [90]) test samples were submerged for 1000 hours in synthetic sea water at 40°C, with the weight recorded at time intervals over the entire period. Static compressive and tensile strength properties at temperatures of 0°C, 20°C and 40°C were collected. Second round tests were completed utilizing a salt fog chamber to environmentally condition unidirectional, [0] and [90], samples. Additionally, [±45] laminates are currently submerged in sea water at 50°C for a third round of environmental test conditions. Both second and third round testing protocols will include both quasistatic and fatigue loadings. Initial results for the submerged samples show trends of reduced tensile and compressive strength with increasing moisture and temperature in the [0] samples. In the [90] samples, compression strength decreases but tensile strength is little affected as temperature and moisture increase. These trends were repeated in the quasi-static results of the salt fog treated samples. However, the reduction in properties was significantly less than the submerged samples, and tracks with the reduced moisture uptake into the salt fog samples.

Electric Grid

Electric Grid

Room: Ballroom D
Session Chair: Jy-An Wang, Oak Ridge National Lab

3:50 PM

(MCARE-200-2012) Smart Grid Development by the U.S. Department of Energy (Invited)

D. Ton, S. Bossart*, U.S. Department of Energy, USA

This presentation will provide an overview of smart grid development activities by the U.S. Department of Energy (DOE) Office of Electricity Delivery and Energy Reliability (OE). It encompasses smart grid goals, applications, values, barriers, and DOE program activities in the U.S. and internationally to address identified barriers. These activities aim to achieve both the DOE program metrics in improving electric system reliability, efficiency, and security and the program's long-term goals of a self-healing grid with full integration of demand response and customer participation. OE's Recovery Act Grid Modernization focus areas in deploying and demonstrating smart grid technologies will be highlighted, along with the computational tool being developed for analyzing smart grid technology benefits. R&D activities undertaken by the OE's Smart Grid R&D Program to implement its multi-year research agenda will be featured in the following five areas: integration of distributed energy resources, demand response, and plug-in electric vehicles; distribution automation; microgrids; standards and best practices; and communications and outreach. Lastly, recent progress on the International Smart Grid Action Network (ISGAN) projects and proposed activities will be presented.

4:30 PM

(MCARE-076-2012) Reversible Solid Oxide Fuel Cell Development at Versa Power Systems (Invited)

A. Wood*, H. He, T. Joia, Versa Power Systems Ltd., Canada

Versa Power Systems (VPS) is a developer of Solid Oxide Fuel Cell (SOFC) technology focused on SOFC stack and module development for commercial partners. In recent years VPS has been developing reversible SOFC (RSOFC) materials systems with a view to future commercial development of RSOFC stacks and modules. VPS has demonstrated significant technical improvements in RSOFC materials technology in a relatively short timeframe, and has begun to test these at the stack level. This paper will provide an update of RSOFC activities including cell and stack testing in both steady-state electrolysis operation and operating with RSOFC cycles (fuel cell and electrolysis cycling).

4:50 PM

(MCARE-077-2012) Gallium Nitride for Grid Applications

M. Soboroff*, U.S. Department of Energy, USA

As the United States transitions to a digital economy, the need to upgrade the nation's aging electric grid is becoming increasingly evident. Electricity demand is projected to increase by 30% between 2008 and 2035 and the U.S. electricity delivery system must be able to meet this demand and ensure the continued supply of reliable, secure electricity. Advanced power electronics will play a critical role in transforming the current electric grid into the next-generation grid. This work discusses devices based on the Gallium Nitride on Silicon materials system. In the short term the goal is to develop methods for fabricating electric utility-relevant GaN-Si devices through established wafer manufacturing. Longer term we hope to Integrate GaN-Si components into power electronic modules and systems that can be incorporated into electrical utility grids.

5:10 PM

(MCARE-078-2012) Evaluation and improvement of conductor connectors for electrical power transmission system

J. Wang*, F. Ren, H. Jiang, E. Lara-Curzio, D. Lee, T. J. King, Oak Ridge National Laboratory, USA; J. Chan, G. Sibilant, Electrical Power Research Institute, USA; J. Graziano, E Inc., USA

Conductor-connectors are critical components of the electrical power transmission system. Development of reliable and efficient connectors is important to both energy security and energy efficiency. In this project, an accurate protocol (Methodology for Estimating the Life of Power Line Conductor-Connector Systems Operating at High Temperatures, or MELCOT) has been developed to evaluate the reliability of splice connectors. By combining experimental testing and computer simulation via finite element analysis, an aging model is proposed. The successful results using this methodology to evaluate the performance of single-stage and two-stage splice connectors will be presented. In addition, preliminary efforts to develop new splice connectors and to improve connector surface conductivity will be discussed.

General Poster Session

Room: Waters Edge Ballroom

(MCARE-P001-2012) Characteristic of Li-La-Zr-O solid-state electrolyte thin film by RF magnetron sputtering for micro battery

S. Lee*, S. Jee, Y. Yoon, Yonsei University, Republic of Korea

Solid-state electrolyte thin films have been studied for application in solid-state ionic power devices such as thin film micro batteries and thin film micro supercapacitors due to their potential uses as main and alternative power sources in various applications. Besides many improvements of solid-state electrolyte, an advanced solid-state electrolyte is needed. Especially, ultra-thin electrolyte is being required for the microelectronic devices. In this study, lithium lanthanum zirconium (Li-La-Zr-O) thin films as solid-state electrolyte for thin film batteries have been investigated. The Li-La-Zr-O thin film electrolyte with garnet structure is prepared by radio frequency (RF) magnetron sputtering under atmosphere of argon (Ar) gas. We propose that the sandwich structure makes it possible to use a Li-La-Zr-O thin film as a thin film solid electrolyte without potential short circuiting of the Li-La-Zr-O thin film. Impedance measurements conducted at room temperature reveal ionic conductivities in the range of 10^-6 ~ 10^-7 S/cm for the various RF power conditions of the Li-La-Zr-O thin films. This result suggests that the Li-La-Zr-O solid-state electrolyte has potential as the ultra thin film electrolyte for application of micro thin film battery.

(MCARE-P002-2012) The Effect of Carbon Loading and Fatty Acid Concentration on the Production of Biohydrogen by Anaerobic Fermentation of Agricultural Waste Feedstocks

J. N. Emily*, N. Mohammed, South Carolina State University, USA

The purpose of this project is to conduct experiments which will use chemical kinetics as a control strategy for optimizing the design of an anaerobic bioreactor for the production of hydrogen by bacteria from cow manure acting on a variety of agricultural biomass substrates. A full factorial experimental design is employed to study the effect of carbon biomass concentration and the concentrations of major fermentation end products such as acetic, proprionic and butyric acid on the production of hydrogen from biomass using cow manure. Multi-variate regression analysis is used to model this relationship. We found that the optimization of the dark fermentation reaction of pretreated mixed microflora can be controlled by maintaining appropriate levels of simple volatile fatty acids by-products within the fermentation batch. This drives the metabolism of the mixed acid group toward the more efficient production of hydrogen via the acetic acid pathway. The incorporation of this type of kinetic control of bioreactor equilibrium can be used to maximize the production of hydrogen by the anaerobic dark fermentation of cellulosic feedstocks using mixed culture microflora.

(MCARE-P003-2012) Materials Selection Guide for Safe Design of Load Bearing Structures in Gaseous Hydrogen Environment

J. A. Lee*, NASA-Marshall Space Flight Center, USA

High pressure hydrogen gas environment has been known to have a deleterious effect on the mechanical properties of certain metals, particularly, the notched tensile strength, fracture toughness and ductility. The ratio of these properties in hydrogen as compared to Helium or Air is called the Hydrogen Environment Embrittlement (HEE) Index, which is a useful method to classify the severity of hydrogen embrittlement and to aid in the material screening for safe design for many hydrogen applications in aerospace, alternate and renewable energy sectors. In this paper, a material selection guide is proposed for selected groups of common metallic materials. The material selection guide is listed as a function of the material knock-down factor and the maximum operating hydrogen pressure at room temperature. In this scheme, the maximum allowable stress for a load bearing structure is equaled to the reduction of yield strength value resulting from a combination of the material knock-down factor plus the safety design factor. This material guide was developed base on NASA's historical experience in hydrogen embrittlement, fracture mechanics, damage tolerance assessment with space launch vehicles, and from a comprehensive NASA's hydrogen compatible material testing and world-wide database compilation.

(MCARE-P004-2012) Hydrogen production by water electrolys: Effects of the electrodes materials nature on the solar water electrolysis performances

R. Ben Slama*, ISSAT, Tunisia

Our contribution in the production of hydrogen, vector of energy, consists in testing the water electrolysis by photovoltaic solar energy. The realization of a certain electrolysers number whose electrodes are various materials, showed a clear difference from the point of view produced hydrogen flow, conversion efficiency, energy specific consumption and the electrodes lifespan. This made it possible to classify materials, by performances descending order, as follows: copper, lead, bronzes, aluminium, stainless, graphite and steel. However lead has a too low flow and aluminium corrodes quickly. Steel admits poor yield and lifespan. We then retain primarily copper like anode metal. To increase the hydrogen produced flow by electrolysis, the electrolysers parallel assembly choice is essential. According to the hour of the day, the parameters evolution: running soup, efficiency, and specific energy consumed differ from a material with another, which is explained by the fact why the power supply of solar origin, is variable in the day course. Keywords: Hydrogen - electrolysis - photovoltaic – electrodes - corrosion.

(MCARE-P005-2012) The Influence of cell morphology on the effective thermal properties of reticulated Si-SiC foams

S. Gianella, Erbicol SA, Switzerland; A. Ortona*, SUPSI, Switzerland

Ceramic foams are used in thermal application both as insulations and heat exchangers. Understanding the effect of foam morphology on their effective thermal conductivity is important for design engineers. In this work, the effects of parameters such as: porosity, cell inclination angle and ligament tapering are studied using Finite Elements (FE) method. For the purpose, an algorithm for the generation and meshing of tetrakaydecahedra was implemented and steady state thermal simulations performed. Results compared with experimental data from the literature showed good agreement. Influences were found by changing the above mentioned parametters

(MCARE-P006-2012) Combined Calorimetric and Volumetric Studies on MOFs for CO2 Separation Applications

A. A. Levchenko*, Setaram Inc, USA; R. Andre, E. Wirth, Setaram Instrumentation, France

The field of CO2 capture and sequestration (CCS) has gained a lot of attention in the recent years because of an increasing need to deal with green gas emissions and resulting from them global warming. Calorimetric techniques are the analytical tools especially suitable to assess energetics of processes involved in the CCS applications. When coupled with a high pressure gas dosing system a Calvet calorimeter is capable to measure such properties as adsorption capacity, heats of adsorption and kinetics for CCS materials under high pressure and supercritical conditions. The results on coupled experiments for some metal organic framework materials (MOFs) i.e. Cu-BTC (Basolite C300) are presented. The thermodynamic properties (both isosteric and directly measured enthalpies of adsorption) are presented and discussed. A combined gas sorption and calorimetric experiment has been shown to be particularly useful for materials characterization in CCS and MOFs particularly. A Calvet calorimeter provided an accurate measure of heats of adsorption of CO2 into the MOFs studied.

(MCARE-P007-2012) In situ XAFS analysis of core shell CeZrO2 catalyst for the automotive application

Y. Takahashi*, Y. Yamada, Y. Ando, NORITAKE CO.,LIMITED, Japan; T. Hattori, KCM Corporation, Japan; M. Haneda, M. Ozawa, Nagoya Institute Technology, Japan

Automotive exhaust catalyst with low amount of Ce (up to 30 wt%)has been developed. This was acheived by fabricating a core-shell nanostructure with CeO2 shell and ZrO2 as the core. In this invesigation, we analyzed the atomic nature of the components of the automotive exhaust catalysts by XAFS. Further, a comparison between the atomic behaviors of CeZrO2 catalyst and core-shell catalyst of CeO2 and ZrO2 has been carried out to understand the structure-property corelation.The results of the investigation will be presented and discussed.

(MCARE-P008-2012) Microstructure and electrochemical properrties of La2NiO4+δ electrode prepared by screen-printing technique

K. Zhao, Q. Xu, D. Huang, Wuhan University of Technology, China; M. Chen, B. Kim*, Chonbuk National University, Republic of Korea

La2NiO4+δ powders were derived from a ployaminocarboxylate complex precursor with diethylenetriaminepentaacetic acid (H5DTPA) as ligand. Particle morphology of the powders was tailored by adjusting the calcining temperature. Electrochemical cells with a three-electrode configuration of La2NiO4+δ/Ce0.8Sm0.2O1.9/Pt have been fabricated by the screen-printing technique. The electrochemical properties of La2NiO4+δ electrodes have been investigated with respect to the morphology of the starting powders and the resulting microstructures. Charge transfer at the electrode/electrolyte interface and oxygen exchange on the surface of the electrode were determined to be the main electrode processes, with the latter process dominating the overall electrode reaction. The electrocatalytic activity of the porous La2NiO4+δ electrodes was evaluated in relation to their microstructural features. The grain size and connectivity between the grains were found to be the key contributing factors to the electrocatalytic activity. Adopting superfine starting powder to fabricate the electrode is favorable to the electrocatalytic activity. At 800°C, the electrode prepared from superfine starting powder exhibited a polarization resistance of 0.38 Ωcm2, an overpotential of 103 mV at a current density of 200 mAcm-2 and an exchange current density of 102 mAcm-2.

(MCARE-P009-2012) Thermal behavior studies of Ceria doped precursors produced by sol-gel method

C. Plapcianu, national Institute for Materials Physics, Romania; L. Stanciu, Purdue University, USA; R. Vidu*, University of California Davis, USA

Ce1-x LnxO2-x 0<x<0.2) solid solution has been prepared by sol-gel method and then sintered in two ways: conventional sintering and Spark Plasma Sintering (SPS). The present study shows a comparison between the sintering methods, highlighting the influence of sintering conditions on the properties of material. Substituting a fraction of ceria with lanthanides creates oxygen vacancies in the crystals without adding electronic charge carriers. Some of the cerium(IV) oxide is reduced to cerium(III) oxide , which consequently increases the electronic conductivity of the material producing a better electrolyte for SOFC. Structural characterization of the compounds has shown a decrease in particle size for the SPS sintered compounds, reducing them from microns (conventional sintering) to a few hundred nanometers (SPS sintering). The SEM images of sintered samples at temperatures up to 1200 C have revealed homogenous micro and nanostructures respectively with some degree of grain growth during the sintering process. The kinetic parameters calculated using AKTS-Thermokinetics Software have been used to computing the reaction rate and progress under different heating rates and temperatures, and helped optimizing the sintering process.

(MCARE-P010-2012) P2O5-doped Fe2O3 for thermoelectric power generation

K. Park*, H. K. Hwang, J. Kim, K. Y. Kim, Sejong Uni., Republic of Korea

Thermoelectric power generation has been considered as a new technique to achieve energy savings and effective use of waste heat. In this respect, metallic oxides are suitable for new thermoelectric materials because they have good oxidation resistance, heat resistance, and low toxicity. In this study, we synthesized nano-sized Fe2-xPxO3 thermoelectric powders by solution combustion process. The synthesized powders showed spherical and nanocrystalline natures. The sintered Fe2-xPxO3 was crystallized the rhombohedral structure. No impurity phase was detected in the sintered samples. Higher P content promoted grain growth and microstructural densification, thus increasing electrical conductivity. The electrical conductivity σ was measured by using the direct-current (dc) four-probe method. The sign of the Seebeck coefficient was negative over the measured temperature range, indicating that the major conduction carriers were electrons. It was believed that the partial substitution of P for Fe was highly effective for improving the thermoelectric properties.

(MCARE-P011-2012) Electrochemically Doped CoSb3 Nanowires for High-Temperature Thermoelectric Materials

R. Vidu*, NanoRIS, USA; D. V. Quach, P. Stroeve, University of California Davis, USA

Because thermoelectric devices are still expensive and have low energy conversion efficiency, more efficient materials and technologies are needed to expand the commercial applications of thermoelectric devices. The binary skutterudite compound cobalt triantimonide CoSb3 is particularly interesting because it displays remarkable electrical properties. The overall performance of this material remains however low due to an excessive value of its lattice thermal conductivity. Thermoelectric properties of CoSb3 are largely affected by doping. This work will present our latest results on Ni and Te-doped CoSb3 nanowires for high temperature thermoelectric materials to increase conversion efficiency in thermoelectric devices and reduce thermal waste. Our approach to develop high-efficiency thermoelectric materials is to combine the chemistry and the size effects. In this paper, we present a method to produce doped CoSb3 nanowires in one step process by electrochemical deposition from aqueous solutions. Doped Ni and Te CoSb3 skutterudite were grown using template synthesis. We will present the electrochemical characterization of this system along with the chemical and morphological characterization (SEM, EDS). Combining chemistry and size effects to create new thermoelectric materials has the potential to result in a significant improvement in the power to weight ratio of the thermoelectric device.

(MCARE-P012-2012) Simulation of performance insoles plans for the development of solar field in Algeria

M. Saadeddine*, M. Noureddine, université d'adrar, Algeria

This study aims to simulate the thermal performance of solar air plans for various climatic and geographical contexts for the implementation of a solar system in a site should be done after estimating the productivity of the system depending on the local solar resource available really beautiful by day (clear sky) or by poor day (overcast). The results helped identify four operating modes and that through this characterization schemes that combine the various sites studied a very good correspondence between the performances and needs.

(MCARE-P013-2012) Temperature dependent solar cell parameters – An Analysis

P. Singh*, N. M. Ravindra, New Jersey Institute of Technology, USA

Earlier studies have shown that the performance of solar cells degrades with increase in temperature. The solar cell performance is determined by the device parameters such as short circuit current density (Jsc), open circuit voltage (Voc), fill factor (FF), and efficiency (η). Consequently, the temperature related study is critical for further improvement in performance and efficiency of the cells. This paper investigates, theoretically, the temperature dependence of performance parameters of solar cells in the temperature range of 273K to 523K. The analysis in this paper will be useful in predicting the performance of a single junction solar cell in the broader temperature range of 273K to 523K and can also be extended to study the temperature dependent performance of multi-junction, i.e., tandem solar cells. In this work, Voc, Jsc, FF and η of solar cells are calculated under ideal conditions and the results are compared with experimental and theoretical studies in the literature. Solar cells made from a variety of semiconductor materials are considered here.

(MCARE-P014-2012) Tribological Challenges in Alternative and Renewable Energy Applications

A. Greco*, V. Sista, K. Mistry, A. Erdemir, Argonne National Laboratory, USA

Friction and wear (i.e. tribological performance) are main drivers for energy loss and mechanical failures of many industrial systems; on a large scale estimates put the annual loss to US industries due to wear and friction at 2-6% of gross domestic product. Similarly, the current materials and lubricants used in energy conversion applications are met with certain limitations in their tribological performance which directly impact the associated cost of energy (COE). This presentation will outline the tribological demands of wind energy, hydropower, geothermal, and advanced vehicle applications, including common surface originated contact failures, specifically observed in wind turbines. Current areas of research and development will be presented on material and lubricant solutions to these early failures. Advanced surface treatments such as an Ultra-fast Boriding method has proven to be a cost effective process to enhance the wear resistance by an order of magnitude over conventional case carburizing. Also, new nano-particle based lubricant additives have demonstrated a near total mitigation of surface micro-pitting and friction reduction compared to conventional gear oils with organometallic extreme pressure additives. These current developments in R&D of surface treatments and lubricant additives further enable the cost efficient operation of alternative and renewable energy resources.

(MCARE-P015-2012) Physical properties of In2O3 nanomaterials grown by spray pyrolysis

K. T. Najoua*, N. Beji, M. Ajili, Z. Sboui, Laboratoire de Physique de la Matiere Condensee, Tunisia

In2O3 thin films have been successfully prepared on glass substrates using Spray pyrolysis technique. Characterization of the film was carried out by X-Ray diffraction (XRD), scanning electron microscopy (SEM) and by spectrophotometry . In this work, we study the physical properties of In2O3 thin films. X-ray diffraction pattern of indium oxide thin layers reveals a polycrystalline of cubic structure with (222) preferential orientation . Optical analysis by means of transmission $T(\lambda)$ and reflection $R(\lambda)$ measurements allow to determine the band gap energy value in the order of 2.9 eV . The In2O3 thin films grown by spray pyrolysis have a big potential use as a window material for photovoltaic devices such as Au/CuInS2/In2O3/SnO2:F in which CuInS2 is used as an absorber material and SnO2:F as an ohmic contact.

(MCARE-P016-2012) Effect of the heat treatment on the structure, composition and optical properties of In2S3 prepared by chemical bath deposition

K. T. Najoua*, M. Kilani, J. Ouerfelli, Laboratoire de Physique de la Matière Condensée, Tunisia; M. Castagne, Université Montpellier II, France

Indium sulfide thin films prepared by chemical bath deposition were annealed in vacuum for one hour at 200, 300 and 400 °C. The effect of this treatment on properties of the films was studied using X-ray diffraction, scanning electron microscopy, spectrophotometry. The cristallinity of the films showed a drastic improvement and the grain size increased. The investigation of optical properties shows that the band gap depends on the annealing temperature. After annealing, the surface morphology shows a substantial change in surface architecture. These results are discussed with respect to introduce the effect of annealing temperature in the physical properties.

Wednesday, February 29, 2012

Solar

Thin Films and Solar Thermal

Room: Ballroom D

Session Chairs: Ann Norris, Dow Corning; Sergei Ostapenko, Ultrasonic Technologies, Inc.

8:00 AM

(MCARE-156-2012) Si-SiC reticulated macroporous foams: processing, properties, and applications

A. Ortona*, S. Pusterla, C. D'Angelo, M. Barbato, SUPSI, Switzerland; S. Gianella, D. Gaia, Erbicol, Switzerland

Silicon carbide foams are, for their outstanding thermo-mechanical properties, good candidates for high temperature (1400°C) applications. Si-SiC reticulated foams with porosity >80% and pore size from 30 to 10 PPI have proven to withstand harsh conditions with low material degradation. These foams are currently employed in industrial porous burners for heat radiation applications. This work presents our research activities on effective foam properties measurements, simulation and optimization in view of several high temperature applications fields, among which stands concentrated solar power

8:20 AM

(MCARE-158-2012) Novel, Single-Crystalline-like Templates on Low-Cost, Flexible Substrates for High Efficiency Thin Film Photovoltaics

V. Selvamanickam*, University of Houston, USA; S. Sambandam, SuperPower, USA; R. Wang, C. Jian, G. Majkic, M. Yang, Y. Gao, E. Galtsyan, University of Houston, USA; X. Xiong, SuperPower, USA; A. Mehrotra, A. Freundlich, University of Houston, USA

We are developing a technology that combines the low-cost advantages of thin films with the high efficiencies achieved only with single crystalline PV. The innovation lies in the creation of an architecture using Ion Beam-Assisted Deposition (IBAD) that yields single-crystalline-like thin films even on polycrystalline substrates. MgO templates made by IBAD on flexible metal substrate have been used for epitaxial growth of germanium films using intermediate oxide layers. All layers were deposited by reel-to-reel magnetron sputtering and strongly (400) textured Ge films with an in-plane texture spread of just 1° FWHM were achieved. Optical properties of the germanium films are found to be comparable to that single crystal Ge and Hall mobility values of 518 cm2/Vs have been achieved. Epitaxial (100) GaAs has also been grown by molecular beam epitaxy (MBE) on the Ge films. While excellent epitaxial growth has been achieved in GaAs on flexible metal substrates, the defect density of the films showed a high value of 10^8 per cm^2. Cross sectional TEM of the multilayer architecture showed concentration of threading dislocations near the germanium-oxide interface. Defect reduction strategies are being employed and recent progress in use of single-crystalline-like templates on low-cost, flexible substrates for high-efficiency PV will be discussed in this presentation.

8:40 AM

(MCARE-160-2012) Mysteries of CdTe Photovoltaic Technology

K. K. Chin*, NJIT, USA

In spite of its spectacular commercial success, CdTe thin film solar cell technologiess is still often called: "MYSTERIOUS". In this talk we will discuss the fundamental difference of CdTe polycrystalline thin film from the traditional semiconductor materials, such as single crystalline Si and GaAs. CdTe thin film has multiple, multi-level, non-shallow, self-compensating native/impurity defect. By offering some basic understandings of these features of CdTe polycrystalline thin film, we try to resolve some of the mysteries of the CdTe PV technology.

9:00 AM

(MCARE-162-2012) Plasma/Laser Assisted Template Free Synthesis of Ultrafine/Nano Structured CdS films

R. S. Ugapathy*, R. Tummala, R. K. Guduru, P. S. Mohanty, The University Of Michigan, USA

Patterned structures are very useful for trapping the sun light in solar cells, and these are usually synthesized via elaborate template assisted/lithography/vapor deposition based techniques, which are not only time consuming but also expensive. Here we report a rapid and inexpensive synthesis of ultrafine/nano structures of CdS without use of templates/catalysts. Initially, thin films of CdS were developed from a solution precursor comprising Cadmium chloride, Thiourea and distilled water via plasma spray deposition technique on glass substrates. Then the ultrafine/nano structured surface patterns on CdS films with pillar morphology were achieved via pulsed lasing (wavelength = 248 nm). The growth of CdS pattern was believed to originate from hydrodynamic phenomena and its mechanism will be reported in detail. The phase and crystallinity was confirmed by X – ray diffraction. Optical transmission of the patterned CdS was observed to be uniform throughout the ultraviolet – visible range; however, the as-sprayed CdS films showed decreasing transmittance with increasing the energy of photon radiation. Microstructural characterization, optical reflectivity measurements and electrical properties will be presented.

9:20 AM

(MCARE-164-2012) Deep level defects in-CdS/p-CdTe Solar Cells

P. Kharangargh*, Z. Cheng, G. Liu, G. Georgiou, K. Chin, NJIT, USA

We characterize the thin film n-CdS/p-CdTe solar cells made with evaporated Cu as a primary back contact, using the temperature dependence of the reverse bias diode current (J-V-T) to determine the energy levels of deep defects. Since the solar cell quickly degrades (probably because of the well-established Cu diffusion from the back ohmic contact into CdTe) with measurement at temperatures greater than ~100°C, measurements are done below room temperature. . The results of our J-V-T measurements on solar cells made at NJIT, show that while modest amounts of Cu enhance cell performance, excessive high temperature process steps degrade device quality and reduces efficiency. Results identify the physical trap though the energy (activation) energy level. The location of and the amount of "trap" are derived from the voltage dependence of diode leakage using a Shockley-Read-Hall (SRH) recombination model.

9:40 AM

(MCARE-167-2012) Growth Dynamics in Thin Films of Copper Indium Gallium Diselenide Sputtered from a Quaternary Target

J. A. Frantz*, R. Y. Bekele, J. D. Myers, United States Naval Research Laboratory, USA; V. Q. Nguyen, A. Bruce, S. V. Frolov, Sunlight Photonics, Inc., USA; M. Cyrus, J. S. Sanghera, United States Naval Research Laboratory, USA

Thin film Copper Indium Gallium Diselenide (CIGS) has rapidly become an important photovoltaic material, competing for market share with silicon and other more established technologies. Typically, CIGS is deposited by co-evaporation or, alternately, by deposition of the metals with, or followed by, treatment in a selenium environment. These deposition techniques, while effective in the laboratory, have limitations from a large-scale manufacturing standpoint. In our laboratory, we have recently developed a deposition method that instead uses RF magnetron sputtering from a single quaternary target without additional selenization. The technique is more easily scalable than are many existing deposition methods. We have realized, for the first time, working devices using CIGS films that are sputtered in a single step and have demonstrated conversion efficiency as high as 10.2%. The sputtered films have a unique morphology – differing significantly from that of evaporated films – with small grains near the bottom contact, coalescing into larger grains with an inverted-pyramid structure. We study growth dynamics in these films by depositing films with varying deposition times and analyzing the films' morphological, chemical, and electronic properties.

10:20 AM

(MCARE-169-2012) Solar-Driven Fuel Production Using Metal Oxide Thermochemical Cycles (Invited)

M. D. Allendorf*, A. Ambrosini, E. N. Coker, A. H. McDaniel, E. B. Stechel, J. E. Miller, Sandia National Laboratories, USA

Worldwide demand for energy continues to increase as the economies of developing nations such as China and India expand. Although demand for all fuel types is predicted to increase, the rate of increase for liquid transportation fuels is particularly high. In this tutorial lecture, we will discuss a potential carbon-neutral approach to production of transportation fuels in which high-temperature thermochemical cycles are used to "re-energize" carbon dioxide and water by converting them to synthesis gas. In addition to an overview of this technology, the factors that must be considered in the design of materials optimized for such processes will be discussed. Our experience shows that design of the active material and the reactor must go hand in hand because decisions made in each area have implications for the other. We choose two important metal oxides with potential for use in such processes – ferrites and ceria – as case studies that illustrate the many tradeoffs that must be made between reactor design and the active material. From these examples it will become clear that there is no "ideal" material independent of the implementation. Instead, the reactor and material must be considered as a fully integrated system. Aspects that will be discussed include process thermodynamics, reaction kinetics and transport, and material stability and degradation issues.

10:40 AM

(MCARE-171-2012) Solution Deposition of Thin Films and Patterns for Photovoltaics (Invited)

H. A. Platt*, S. E. Habas, C. J. Curtis, A. Miedaner, D. S. Ginley, National Renewable Energy Lab, USA; J. P. Novak, Y. Li, Applied Nanotech, Inc., USA; M. F. van Hest, National Renewable Energy Lab, USA

The fabrication of solar cells requires covering large areas quickly, which makes solution-based approaches such as ink jet and aerosol jet printing, and ultrasonic spray coating excellent choices. These techniques use materials very efficiently, which will decrease the cost of silicon wafer and thin film solar cells. We have incorporated these tools into the Atmospheric Processing Platform (APP) at the National Renewable Energy Lab. Examples of solar cell components deposited in the inert environment of the APP include Ni and Cu lines, and thin films of earth-abundant FeS_2 pyrite. We have demonstrated near-bulk resistivities for Ni and Cu lines from printed precursors, along with respectable contact resistivities between the Ni lines and silicon wafers. The results from our more recent work on silicon wafer solar cells incorporating Ni/Cu bilayers as the top contact will be discussed. FeS_2 pyrite is of considerable interest because of its excellent absorption properties and low cost, so we have also developed inks to deposit it. The properties of these films will be discussed, along with the performance of heterojunction solar cells incorporating Bi_2S_3 as the n-type partner. These examples demonstrate the potential of solution processes to contribute to a wide range of solar cell technologies by increasing materials utilization and reducing cost.

11:00 AM

(MCARE-173-2012) Solar Thermal Electrochemical Production of Energetic Molecules: Efficient STEP solar water splitting, carbon capture, and solar metals, fuel and bleach production

S. Licht, H. Wu, J. Asercion*, U. Cubeta, J. Lau, George Washington University, USA

The Solar Thermal Electrochemical Production of energetic molecules converts solar energy at solar efficiency higher than that of the most efficient photovoltaics. Rather than electricity, a variety of useful chemicals are produced without CO2 emission by this new STEP process. STEP is a synergy of solar thermal and renewable energy electronic charge transfer, which captures sunlight and uses the global (visible + thermal) spectrum of sunlight. Solar thermal energy decreases the energy and enhances the kinetics of our molten electrosynthetic reactions. As one STEP example, carbon dioxide is converted to carbon at 34 to over 50% solar efficiency. Carbon capture, CO2-free iron production, bleach, magnesium and fuel generation by STEP will be presented. The new STEP approach for solar energy conversion is based on our theory and experimental observation, that even a semiconductor with bandgap smaller than the water splitting potential (E(H2O)=1.23V at 25°C) can split water at elevated temperature. Hence, silicon (band-gap 1.1 eV) was used to directly form hydrogen fuel from water at elevated temperature in a novel molten alkali hydroxide electrolyzer, and STEP generalizes this to the electrosynthesis of all endothermic products.

11:20 AM

(MCARE-174-2012) Design and Development of ceramic composite and nano-structured materials for active solar air conditioning

G. Singh*, G. Singh, P. Singh, College of Engineering & Technology, Bikaner, India

The research in the group is focused on the design and development of ceramic composite and nano-structured materials for active solar air conditioning. Reinforcement of BaTiO3 particles in ceramic composites body used to amplifying the process of thermoelectric cooling by using Thermoelectric cooling and ferroelectric effect in multilayer structure, the temperature significantly decreases This paper deals with the fundamental energy conversion principles. Using this process in zero energy building as a roofing tiles, the temperature of building can be maintained in solar cycles heating as well as cooling via active solar thermal energy conversion.

Hydrogen

Theoretical Studies of H-Storage Materials and Additional Practical Use in Energy Storage System

Room: Ballroom E

Session Chairs: Martin Sahlberg, Uppsala University; Andrew Goudy, Delaware State University

8:00 AM

(MCARE-079-2012) Nano Materials for Hydrogen Storage (Tutorial)

P. Jena*, Virginia Commonwealth University, USA

This talk will discuss how the novel properties of materials at the nanoscale can improve the thermodynamics and kinetics of hydrogen. In particular, I will discuss how carbon based nanostructures such as nanotubes and fullerenes can not only be used as catalysts to improve hydrogen uptake and release in complex light metal hydrides such as sodium alanate, but also how they can be functionalized with metal and B atoms to adsorb hydrogen in a novel quasi-molecular form. Such a bonding can improve the kinetics and thermodynamics of hydrogen sorption. I will also discuss the role of electric fields in hydrogen storage. These results, based upon density functional theory and quantum molecular dynamics, provide a fundamental understanding of the interaction of molecular hydrogen with hosts consisting of light elements. It is hoped that the understanding gained here can be useful in designing better materials for hydrogen storage. Results will be compared with available experimental data.

8:40 AM

(MCARE-080-2012) Quasicrystals for Hydrogen Storage (Invited)

C. Pay Gomez*, M. Sahlberg, Uppsala University, Ångström Lab, Sweden

Much attention is now being focused on Quasicrystals in the light of the recent Nobel Prize in chemistry. Although these exotic materials have been known to us since 1982, little has been known concerning the detailed atomic structures of icosahedral quasicrystals until recently. Based on the constituent atomic clusters in icosahedral quasicrystals, they can be classified into one of three families: Bergman-, Mackay- and Tsai-type quasicrystals. The Bergman-type family, also referred to as the Frank-Kasper type family (FK-type) is by definition structurally related to other well-known FK-type alloys such as LaNi5 and MgZn2 which are already being used commercially in high-capacity electrodes and hydrogen fuel cells. In spite of this fact, few investigations have been made in order to explore the hydrogen storage properties of quasicrystals and their related approximants. In this work we will give an introduction to the crystal chemistry of quasicrystals and approximants, highlighting their structural relation to simple FK-type alloys and their potential use as hydrogen storage materials.

9:00 AM

(MCARE-081-2012) Descriptor based computational design of hydrogen membranes and battery electrolytes (Invited)

T. Vegge*, Technical University of Denmark, Denmark

A calculational approach for the design of new energy materials with favorable thermodynamic stability and mass transport kinetics is presented. By combining density functional theory calculations on stable crystal structures and local coordination models with database methods, we perform large-scale screening studies of partial cat/anion substitution to predict new alloys/mixtures in the LiBH4 system, which stabilize crystalline phases with super-ionic lithium conduction. Experimental electrochemical impedance spectroscopy, X-ray diffraction and quasi-elastic neutron scattering data is also presented. Predictors for the kinetic properties of the materials are derived from combining DFT based materials screening with the nudged elastic band calculations and harmonic transition state theory to indentify simple materials parameters, e.g. the hydrogen binding energy, which correlate with the macroscopic diffusion rates Perovskite structured oxides with mixed electronic and protonic conduction for use as hydrogen permeable membranes. We demonstrate the possibility using such predictors to estimate diffusion rates based on O-H binding energy and temperature only, without determining transition states and vibrational frequencies, to design new mixed Perovskites with optimized hydrogen permeation. A novel hydrogen-pair transport mechanisms in Perovskites is also presented.

9:20 AM

(MCARE-082-2012) Hydrogen Interaction with the Al Surface Promoted by Subsurface Alloying with Transition Metals (Invited)

F. Zhang, Y. Wang, M. Chou*, Georgia Institute of Technology, USA

Dissociative chemisorption of H_2 on the Al surface is a crucial step for the regeneration of many promising hydrogen-storage materials such as alane and the alanates. This is believed to be closely connected to the catalytic reaction needed in order to drive the reversible hydrogen reactions in sodium alanate under favorable experimental conditions. We have performed first-principles calculations to study the physical processes associated with this system. We find that V and Nb are superior catalysts for the H_2 interaction with the Al(100) surface. The activation barrier for H_2 dissociation is significantly reduced to 0.4 eV and 0.2 eV, when V and Nb atoms are located at subsurface sites, respectively. In addition, the binding energy of an H atom on the surface can be enhanced by as large as 0.4 eV when V or Nb is introduced in the sub-layers of Al(100). The diffusion barrier for the adsorbed hydrogen is also reduced by about 0.1 eV, indicating increased hydrogen mobility. These results suggest that subsurface alloying with transition metals can significantly modify the surface properties such that the interaction with hydrogen is favorably promoted.

9:40 AM

(MCARE-083-2012) What insights can be gained from ab initio studies of hydrogen storage systems? (Invited)

R. H. Scheicher*, Uppsala University, Sweden

The exploration of materials suitable for hydrogen storage continues. Research efforts are driven by the prospect of a “hydrogen economy” that would allow us to gradually shift away from fossil fuel and replace it with hydrogen as energy carrier. Numerous challenging obstacles remain to be overcome before this goal could be reached; finding a system which can meet certain stringent requirements for hydrogen storage is one of these challenges. In this quest for the ideal hydrogen storage material, first-principles computational tools are heavily utilized to complement experimental studies, characterizing the electronic structure of promising systems or even predicting properties of new materials. The purpose of this talk is to provide an overview of the most recent theoretical studies undertaken by us in the field of hydrogen storage materials research. On selected examples, the application of our computational tool of choice, density functional theory, will be illustrated to show how ab initio calculations can be of use in the effort to reach a better understanding of hydrogen storage materials and to occasionally also guide the search for new promising approaches.

10:20 AM

(MCARE-084-2012) Similarities in Energy Storage Methods for Vehicles (Tutorial)

S. W. Jorgensen*, General Motors R&D, USA

The methods of energy storage available onboard vehicles are returning to a state of diversity that characterized the inception of the automotive age. In part this diversification is driven by overarching social issues such as environment stewardship, and the geopolitics and global economics of traditional energy sources. Interestingly, there is a synergy between many of the new and emerging energy storage systems at the research level. This similarity stems from two sources, a common set of requirements that a storage system must meet or exceed, and a certain amount of overlap in materials options and engineering techniques to build novel energy storage systems. There may be future opportunities to leverage the fundamental science gains in one area of energy storage research to improve the performance of other types of energy storage as well.

11:00 AM

(MCARE-085-2012) From nanostructured MgH2 to reversible hydrogen storage (Invited)

P. de Rango*, A. Chaise, B. Delhomme, D. Fruchart, S. Garrier, F. Longat, Institut Néel / CRETA, France; P. Marty, LEGI - INPG, France; S. Miraglia, B. Zawilsky, Institut Néel / CRETA, France

A systematic investigation of the co-milling process of MgH2 with transition metals was undertaken in order to develop large batches of suitable materials for hydrogen storage. The initiating role of additives was evidenced by in-situ neutron diffraction experiments. Because magnesium hydrogenation is very exothermic, the tank loading time is limited by heat exchange efficiency. To improve the thermal conductivity, ball-milled MgH2 was compacted with Expanded Natural Graphite. This compaction avoids macroscopic volumetric variations between metallic and hydriding states. However, a slow but continuous expansion of the compacts is observed on long term cycling. MgH2 tanks were developed and tested in different experimental configurations. A Phase Changing Material was used to store the heat of absorption and to reuse it during desorption. Thanks to the high reactivity of the nanostructured powders, the absorption can be initiated at room temperature. The specific-energy of these systems is of about 270 Wh/kg. The system volumetric-density is 42 gr/l. One of these tanks was connected to a Helion PEM-Fuel Cell. A numerical code taking into account heat exchanges and hydrogen mass flow was developed and validated by comparison with experimental results.

11:20 AM

(MCARE-086-2012) Metallic hydrides: a powerful class of materials for energy storage and conversion (Tutorial)

M. J. Latroche*, CNRS, France

Metal hydrides were discovered in the sixties and have been widely studied for both a fundamental and a practical point of view. Besides the interest in understanding the metal-hydrogen interactions, much research has been devoted to developing practical applications for this class of materials. Among them, storage and energy conversion are the most promising. Indeed, the metal hydrides are used in alkaline batteries Ni-MH, the biggest commercial success to date for these materials. The same materials are nowadays developed as negative electrode in Li-ion battery through a reversible reaction conversion. Important expectations are also expected in the hydrogen storage field to use this gas as an energy carrier in mobile or stationary tanks. Besides these well-known applications, other options are available for these compounds. Recently, new researches have been undertaken on the magneto-caloric effect observed for some of these magnetic metal hydrides and heat pumps or gas compressors are developed on the basis of their remarkable thermodynamic properties. The present paper will provide an overview of this class of materials with special emphasis on their interest for energy applications.

11:40 AM

(MCARE-087-2012) Perspectives of H Storage and Battery Materials (Tutorial)

M. Fichtner*, Karlsruhe Institute of Technology, Germany

The contribution will start with an introduction to the problem of energy storage. Chemical methods offer the highest energy density for storing energy; they are the most interesting option for high energy and high power applications such as automobiles and for seasonal storage of electric energy from renewables. Each storage method has its own perspectives, limits of its physical potential, technical limitations, associated with cost and safety issues. For storage of hydrogen or lithium, today s systems are based on intercalation materials which have the advantage of being well reversible and available on the market. However, as the energy density shall be improved by a factor of two (H storage materials) or five (battery materials), a paradigm change is necessary in the materials development in order to be able to reach these goals. From the current knowledge, only systems based on the conversion principle offer such high energy densities. Conversion materials are based on solid state chemical reactions where several reaction partners may be involved depending on whether the material is charged or discharged. The systems undergo a massive reconstruction of their structures, which is different in intercalation based systems. Several examples from H storage materials and battery research will be presented and discussed, and current directions of research in these fields will be outlined.

Nanocomposites/Nanomaterials

Nanocomposites and Nanomaterials II

Room: Ballroom G

Session Chairs: Jimmy Xu, Brown University; Sivaram Arepalli, Sungkyunkwan University

8:00 AM

(MCARE-088-2012) Engineering a Robust Artificial Photosynthetic System via Efficient Quantum Coherence (Tutorial)

V. Renugopalakrishnan*, Northeastern University, USA

At the heart of every photovoltaic device is a mechanism for photon-to-electrical transduction. Ideally, the device should capture light across a broad spectrum, and efficiently transfer this energy to the electrons. Photosynthesis is a collection of the most advanced and efficient systems nature has crafted to convert solar energy into an electrical potential and again into chemical compounds for energy storage. Bio-solar cells (BSSC) and bio-fuel cells represent the emerging frontier in green energy sources. In recent years Renugopalakrishnan et al., 2009 has reported several advances in the feasibility of bacteriorhodopsin (bR) as bio-photosensitizer in excitonic solar cells. His Lab has engineered mutants of bR to enhance thermo-stability and to favor charge separation. There are at least key components which implement the energy transfer step : (a) a hybrid mixture of engineered protein bR and quantum dots (QD) to absorb and trap the photon energy, (b) a thin layer of gold (Au) to produce the ballistic electrons and recycle the dye.

8:40 AM

(MCARE-089-2012) Carbon Nanomaterials -The Route toward Applications in Energy (Invited)

W. Choi*, Florida International University, USA

Advancements in the science and engineered carbon nanomaterials, graphene and carbon nanotubes, have created a great deal of promise for their application in a wide variety of fields including electronics, display, bio-sensors, battery and solar cells. This talk will focus on engineering of carbon nanomaterials, graphene and carbon nanotubes, and their applications in energy storage and flexible solar cells. Particularly, the interfaces of graphene-substrate, CNT-CNT and graphene-CNT will be used to highlight the challenges towards high efficiency energy applications. Various organized architectures of carbon nanomaterials can be fabricated using interfacial control and direct self assembly of these structures. Some of these structures offer excellent properties in Li-ion battery, dye sensitized solar cells and field emission applications. Our recent results of bonding energy characterization in nano scale will be introduced to offer the optimum structure of carbon nanomaterials. Our efforts on the strategies of manipulation of carbon nanomaterials towards high efficiency energy applications will be reviewed and critical issues will be highlighted.

9:00 AM

(MCARE-090-2012) Electrospin polyaniline nanofibers for Hydrogen storage applications

P. R. Ayalasomayajula*, S. Srinivasan, Nano RAM Technologies, India

Conducting polymer nanostructures combine the advantages of organic conductors and low dimensional systems and therefore should yield many interesting physicochemical properties and useful applications. The nanofibrillar morphology significantly improves the performance of polyaniline in many conventional applications involving polymer interactions with its environment. This leads to much faster and more responsive chemical sensors, new organic / polyaniline nanocomposites and ultra-fast non volatile memory devices. Nanofibers with diameters of tens of nanometers appear to be an intrinsic morphological unit that was found to “naturally” form in the early stage of chemical oxidative polymerization of aniline. In conventional polymerization, nanofibers are subject to secondary growth of irregularly shaped particles, which leads to the final granular agglomerates. The key to producing pure nanofibers is to suppress secondary growth. Based on this, two methods – interfacial polymerization and rapidly mixed reactions have been developed that can readily produce pure nanofibers by slightly modifying the conventional chemical synthesis of polyaniline without the need for any template or structural directing material. With this nanofiber morphology, dispersibility and processbility of polyaniline are now much improved.

9:20 AM

(MCARE-091-2012) Ultrasound Synthesis of Carbon Supported Pt-M1 (M1 = Fe, Co) Bimetallic Nanoparticles with Electrocatalytic Oxygen Reduction Reaction Activity

J. Jang*, E. Lee, Y. Kwon, Department of Chemistry and BK21 School of Chemical Materials Science, Sungkyunkwan University, Republic of Korea

We report on the preparation of carbon supported Pt containing bimetallic nanoparticles (NPs) with electrocatalytic activity for fuel cell applications. To form the bimetallic NPs, we chose 3d transition metals such as Co and Fe. In order to synthesize the NPs, sonochemical syntheses method was used. Ultrasound irradiation into carbon support, Pt(acac)2 and Fe(acac)3 or Co(acac)2 dispersed polyol solution could generate a reducing condition of the precursors which resulted in the formation of bimetallic NPs on carbon support. The structures of the nanoparticles were characterized by XRD, XPS, IR, SEM-EDS, HRTEM and STEM-HAADF. The NPs show narrow size distribution with averaging size of about 2 nm and no macroscopic phase segregation. Electrocatalytic oxygen reduction reaction (ORR) behavior of the materials was measured by rotating disk electrode (RDE) technique and compared with commercial Pt/C (TKK, 37.7 wt%). As a result, we obtained an enhanced electrocatalytic ORR activity than commercial Pt/C.

9:40 AM

(MCARE-092-2012) Thermal stability of nanopores in palladium alloys used for hydrogen storage (Invited)

D. B. Robinson*, Sandia National Laboratories, USA; B. W. Jacobs, Protochips, Inc., USA; J. D. Sugar, M. D. Ong, M. E. Langham, Sandia National Laboratories, USA; L. R. Parent, I. Arslan, Pacific Northwest National Laboratory, USA

Nanoporosity can offer improved charging and discharging kinetics in metal hydride electrodes and storage materials. We have synthesized nanoporous palladium and palladium alloy powders in a scalable fashion by reduction of palladium salts in a concentrated aqueous surfactant. Particle diameters are micrometer-scale, and each particle is perforated by pores tunable in the 3-10 nm range. In pure palladium, 3 nm pores are unstable at 150 C, but when alloyed with rhodium, they are stable up to 400 C on short timescales. These results are expected to be related to pore lifetime at more moderate temperatures. Electron tomography and elemental mapping after heating and/or hydrogen exposure help us understand the mechanism of the improvement, showing a dependence on pore geometry and rhodium distribution. Pore density and stability are also related to the presence of grain boundaries in the material. Improved stability can be obtained with minimal sacrifice of hydrogen storage properties. Sandia National Laboratories is a multi-program laboratory managed and operated by Sandia Corporation, a wholly owned subsidiary of Lockheed Martin Corporation, for the U.S. Department of Energy's National Nuclear Security Administration under contract DE-AC04-94AL85000.

10:20 AM

(MCARE-093-2012) Three phase PZT-Cement-Al composites for structural health monitoring and energy harvesting applications

S. Banerjee*, Rutgers, The State University of New Jersey, USA; K. A. Cook-Chennault, Center for Advanced Energy Systems, USA

Composite ferroelectric materials have been investigated for smart materials in applications such as structural health monitoring (SHM) of civil structures. Towards the development of structural health monitoring sensors and energy harvesting devices, researchers have developed diphasic cement based piezoelectric composites pertaining to their compatibility with materials commonly used for civil structural applications. The criteria that govern the applicability of these types of devices are their sensitivity and durability, which depend on electromechanical properties of the composite. The present work deals with the fabrication of PZT-Cement-Aluminum(Al) micro and nano, three phase composites. The composites show an enhancement in dielectric and piezoelectric properties with an increase in volume fraction of Al and PZT inclusions as compared to two phase PZT-Cement composites. Above a certain volume fraction of the Al inclusions the dielectric constant of the composites increase rapidly due to percolation of Al inclusions in the composite. This renders the composite inapplicable in the above mentioned applications. The percolation threshold and limit for the above composites are also determined. A comparative study of the change in material properties and percolation characteristics with variation of Aluminum volume fraction and size is also demonstrated here.

10:40 AM

(MCARE-094-2012) Thermochemical CO2 Splitting Using Thin Film Cobalt Ferrite/Alumina Active Materials

D. Arifin*, University of Colorado, USA; A. McDaniel, Sandia National Laboratories, USA; A. Weimer, University of Colorado, USA

This study explores the solar thermochemical CO2 splitting cycle of a CoFe2O4/Al2O3 material synthesized using atomic layer deposition to create a low bulk density reactive structure. The thermal reduction and oxidation, by both O2 and CO2, as well as the effects of pressure and reaction temperature on CO production during CO2 splitting are examined. The onset of oxygen evolution during thermal reduction of CoFe2O4/Al2O3 is 200-300oC lower than that observed for either CeO2 or a Fe2O3/ZrO2 composite. In addition, the CoFe2O4/Al2O3 material exhibits high thermal stability, with no sintering detectable up to 1460oC. The O2 oxidation kinetics is fast, with complete reoxidation accomplished within 60 seconds. On the other hand, the CO2 oxidation is much slower compared to O2 oxidation, and is greatly affected by the pressure and temperature of the reaction. This implies a surface mediated rate limiting process during the CO2 splitting step. Finally, the use of Raman spectroscopy confirms the mechanism in which the cycle progresses: during thermal reduction, cobalt ferrite spinel decomposes into its respective aluminate phase (iron aluminate and cobalt aluminate), and during oxidation, the spinel is reformed.

Nuclear

Improved and Advanced Materials Systems for Fuel and NPP Components

Room: Ballroom F

Session Chair: Robert Sindelar, Savannah River National Lab; Gary Mushack, ASM International

8:00 AM

(MCARE-095-2012) Beyond Fukushima: Advanced Materials to Enable Enhanced Nuclear Power Systems (Tutorial)

J. Marra*, Savannah River National Lab, USA

Increasing fuel oil and natural gas prices combined with worldwide energy demands increasing at an alarming rate and increased concerns about greenhouse gas (GHG) emissions have caused many to look negatively at long-term use of fossil fuels. This convergence of factors led to a growing interest in revitalization of the nuclear power industry within the United States and across the globe. However, on March 11, 2011 an earthquake centered near Japan and the resultant Tsunami caused significant damage to several reactors at the Fukushima Daiichi nuclear plant causing many to question the long-term future of nuclear power. As Japan and the international community begin to look at the lessons-learned from the Fukushima accident, advanced materials that eliminate or reduce the consequences of severe accidents will find increased application in advanced nuclear power systems. Ceramic and glass materials, which have long played a very important role in the commercial nuclear industry, offer some significant advantages under accident conditions. This presentation will review the sequence of events that led to the Fukushima Daiichi accident and discuss the critical role that ceramic and glass materials play throughout the nuclear fuel cycle and the critical material advancements required to enable the 'nuclear renaissance' in light of the recent events.

8:40 AM

(MCARE-096-2012) Processing and Microstructural Characterization of Uranium Oxide

E. Luther*, C. Necker, R. Forsyth, P. Papin, D. Guidry, B. Mihaila, Los Alamos National Laboratory, USA

Ceramic oxide nuclear fuel pellets are the most commonly employed fuel for the nuclear energy industry in the US and abroad. The nuclear industry uses standard fabrication methods; i.e. cold press and sinter, to generate hundreds of pellets per minute. Defects such as cracking and density variations are still inherent to this process. Various microstructural attributes can influence the properties of a fuel pellet. Porosity and grain structure are two aspects that have received considerable attention. These parameters influence factors such as fission gas release and the stability of the microstructure in pile. Efforts to model microstructural influences on properties are inhibited by a lack of data. By conducting research into controlling the microstructure of ceramic oxides, experiments that isolate phenomena that are microstructurally dependent are enabled and data collection to fill knowledge gaps is supported. In this study, pellets were fabricated using standard cold press and sinter techniques. The powders were conditioned and characterized prior to fabrication. Pellets were sintered under various conditions in order to observe the effects on grain growth. Scanning Electron Microscopy (SEM) and Electron Backscatter Diffraction (EBSD) were used to study grain size, size distribution, orientation and morphology. LAUR-11-04966

9:00 AM

(MCARE-097-2012) Development of a dynamic gas control technique to set a constant O/M ratio during sintering of UO_2

D. D. Byler*, Los Alamos Natl Lab, USA; J. B. Henderson, Netzsch Instruments NA, USA; K. J. McClellan, A. T. Nelson, Los Alamos Natl Lab, USA

The processing, properties, and performance of ceramic nuclear fuels have been researched for use in LWRs to determine the effects of variations in composition, density, structure and the oxygen-to-metal ratio (O/M) on fuel characteristics. Effects of these variations have a dramatic influence on the performance of fuels. A major contributor to the properties of nuclear fuels is O/M ratio due to the wide range of stoichiometries that the fuel can attain over the operating temperature range. Urania based nuclear fuels stoichiometries can range from ~$UO_{1.90}$-$UO_{2.54}$ depending on the partial pressure of oxygen (PO_2) and temperature that the fuel is exposed to. Variations in the stoichiometry can have deleterious effects on thermal and mechanical properties of the fuel. Research has been conducted to evaluate the effect of a controlled sintering atmosphere on the properties of urania and urania-pseudo binary compounds. A technique to dynamically change the PO_2 was developed to provide a means of controlling the O/M during the stages of sintering. During sintering, the oxygen activity varies as a function of temperature resulting in changes of the O/M of the sample. By setting a constant O/M, the thermal and physical properties of the fuel, as a function of O/M can be examined. The development of the technique and dynamic gas control system will be presented and discussed.

9:20 AM

(MCARE-098-2012) Dynamic Sintering of UO_2 at constant Oxygen-to-metal Ratios

D. D. Byler, J. B. Henderson*, Netzsch Instruments North America, USA; K. J. McClellan, A. T. Nelson, Los Alamos National Laboratory, USA

UO_2 and $(U,Pu)O_2$ are used in the vast majority of LWRs. They are therefore still the focus of intense research 50 years on. Much of this work has been aimed at gaining a better understanding of parameters which control the sinterability and quality of fuel pellets and hence the ultimate fuel performance. Most sintering studies are conducted using dynamic heating rates and a set partial pressure of oxygen (PO_2). This often results in oxygen-to-metal ratios (O/M) which vary throughout the measurement, depending on the starting O/M, PO_2, heating rate and temperature. This, of course, means that the defect structure and thus the diffusion mechanisms are dynamic. Furthermore, the fuel pellet may, depending on several factors, have both radial and longitudinal O/M gradients. These factors tend to mask the sintering physics and make data interpretation delicate. The purpose of this work was to study the sintering of UO_2 as a function of temperature and heating rate at constant set values of O/M. The O/M was controlled by varying the PO_2 throughout the measurements using a sophisticated control system which will be described in a separate presentation at this meeting. It is felt that these data will ultimately lead to a much better understanding of the diffusion mechanisms which control sintering. The results of this work will be presented and discussed in detail.

9:40 AM

(MCARE-099-2012) Development of Diffusion Blocking Mechanisms during Processing of $GdO_{1.5}$ and UO_2-$GdO_{1.5}$

J. B. Henderson*, Netzsch Instruments North America, USA

The importance and effectiveness of gadolinia as a burnable poison in the nuclear fuel cycle is well understood and documented. When mixed with an oxide fuel, for example UO_2, and sintered, it readily forms a solid solution. However, gadolinia also creates a sintering blocking mechanism which makes it difficult to reach the desired final density. Understandably, the addition of gadolinia to UO_2 affects the metal atom diffusion, and therefore densification, microstructure and thermophysical properties. In fact, even the sintering of single-phase $GdO_{1.5}$ and the evolution of its thermophysical properties is more complex than normally anticipated for most oxide ceramics. This is due, in part, to a phase transition which occurs in the range of 1250°C. The purpose of this work was to characterize the sintering behavior of $GdO_{1.5}$ to aid in understanding the more complex multi-component fuel systems. The mass change, densification, rate of densification, thermal conductivity, specific heat and transition energetics were measured during sintering. XRD measurements were also carried out on the starting powder and sintered material. The above-mentioned data were used to help explain the complex behavior of gadolinia during processing and will be presented in detail. Further, an effort will be made to explain the possible governing sintering blocking mechanisms in the more complex $(U,Gd)O_{2-x}$ system.

10:20 AM

(MCARE-100-2012) Greenhouse Gas-Free Hydrogen Production Using Nuclear and Solar Energy (Tutorial)

W. A. Summers*, Savannah River National Lab, USA

Hydrogen is a widely used industrial gas that is essential to petroleum processing, fertilizer production, petrochemicals, and synthetic fuels. Hydrogen has also been considered a candidate as a major energy carrier in a future carbon-free energy system (e.g. hydrogen economy). Almost all current hydrogen is produced by the steam reforming of natural gas or naphtha, resulting in significant quantities of carbon dioxide emissions. This paper will discuss carbon-free hydrogen production via water-splitting based on the use of high temperature heat from either nuclear reactors or solar central receivers. The leading thermochemical cycles and high temperature steam electrolysis systems will be discussed and compared. Major material challenges exist for each step in the process: (1) high temperature nuclear reactors; (2) solar receivers; (3) heat transport systems; (4) hydrogen production processes. The status of research in these areas will be reviewed and the prospects for development and demonstration of these technologies will be discussed.

11:00 AM

(MCARE-101-2012) Barrier behavior of Zr and V thin flms by electrodeposition method using ionic liquid for FCCI

S. Jee*, S. Lee, K. Lee, Y. Yoon, Yonsei Univ, Republic of Korea

The unique properties of U-Zr metal fuel in nuclear power plant, such as high thermal conductivity, proliferation resistance, ease of fabrication, and a good compatibility for sodium have stimulated research in Sodium-cooled Fast Reactor (SFR) for burning the long-lived fission products. It is very hard to use U-Zr metal fuel directly since actinide elements have a fuel-clad chemical reaction (FCCI) or eutectic reaction with stainless steel based cladding material even at just above 650 °C. The most common steady-state FCCI reaction is interchanged by diffusion of cladding components and rare earth fission products. The interaction layer in the cladding is very brittle and considered as having no strength. The barrier concept is needed to prevent the fission product interdiffusion as well as to prevent 'eutectic' melting during transient events. Zirconium (Zr) and vanadium (V) thin films onto a HT9 clad by electro-deposition using ionic liquid were carried out to prevent a FCCI and a eutectic reaction of rare earth fission products with clad material of nuclear power plant. Zr and V thin films were deposited with various pH values (2, 5, 8) at 140 °C for 5 hours. Diffusion couple tests at 660 °C for 25 hours showed that the Zr and V thin films showed a barrier behavior for FCCI between the metal fuel and the clad.

11:20 AM

(MCARE-102-2012) Processing and characterization of SiC/SiC pin cladding reinforced with Hi-Nicalon S and SA3 fibers

C. Sauder*, S. Poissonnet, E. Buet, CEA, France

Owing to the recent progress in the fabrication of stoichiometric fibers with a good stability under neutron irradiation, SiC/SiC composites are candidate of prime interest for nuclear applications in GenIV nuclear power plant (for example structural material for fuel containment in Gas Fast Reactor). In this work, it is proposed to study 2D braiding structure pins with two different PyC interphase texture. Mechanical tensile behaviour of composites are investigated and discussed with respect to microstructure analyses. The influences of very high temperature treatments under inert atmosphere have been studied to explore accidental situations. Residual mechanical tensile behaviours have been explored and a mechanism of degradation is proposed.

11:40 AM

(MCARE-103-2012) High Performance Homogenized Alloy 690 (Invited)

Y. Li*, K. Liu, X. Hao, R. Jiang, Y. Zhang, Institute of Metal Research,CAS, China

Alloy 690 is the most promising alloy applied to the SG tube for Pressurized Water Reactors. The trace elements such as S and N segregation become the most serious problems for manufacturing the homogenized high performance alloy 690. More attention should be paid to the solidification segregation behavior. The effect of S and N on the solidification segregation of alloy 690 was studied. The results indicate that S can strongly enlarge solidification zone of alloy 690 by decreasing the solidus. When S content increases from 20ppm to 1200ppm, the solidus drops about 40C. The gamma/CrS eutectic appears as S content reaches to 400ppm. The common solidified sample of 20ppm S has been analyzed by electron probe microanalysis. It is found that there exists sever segregation of S and Cr at the final solidified zone. The test results indicate that S segregation can induce the main alloying element Cr large positive segregation. The N has no influence on the liquidus, but decreases the solidus by 8K when N content increases from 10ppm to 1100ppm. With more N added to this alloy, the Cr, Ti C, S, N enriches at the residual liquid during the isothermal solidification process. And the segregation enrichment of these elements become much strong during isothermal solidification at 1628K. Accompanying by the sever segregation of Cr, Ti C, S, N, sulfides and chromium nitrides formed along the grain boundaries in the residual liquid.

Biomass

Materials Challenges

Room: Mangrove
Session Chairs: David Dorheim, DWD Advisors, Inc.; Bhakta Rath, Naval Research Laboratory

8:00 AM

(MCARE-104-2012) Biodiesel Production through Ultrasound and Microwaves

S. C. Getty*, M. M. Kropf, Pennsylvania State University, USA

With an ever increasing demand for fuels and new energy sources there becomes a growing need for new, innovative concepts of alternative and renewable energy sources. To meet this demand and become competitive with fossil fuels, industry must increase production of renewable energy while decreasing energy and costs of producing them. One such source of renewable energy, which has been changing rapidly in North America, is biodiesel. A novel processing approach developed at The Pennsylvania State University leverages high intensity, focused ultrasound and microwave heating to improve the material and energy efficiencies of the production of biodiesel. Technical approaches towards technology scale-up will be discussed along with the validation studies at industrial scales.

8:20 AM

(MCARE-105-2012) Biocoal: A Drop-In Fuel in Coal-fired Power Plants

E. Bar-Ziv*, Michigan Technological University, USA

Biomass torrefaction to produce biocoal gained interest as it solves hindrances encountered when using biomass for power generation. Biocoal is a premium drop-in fuel in pulverized-coal (PC) boilers aimed at the reduction of greenhouse gas and other emissions. Biomass torrefaction produces a material with properties similar to coal. Because these properties can be controlled and reproduced biocoal it can be utilized as a “drop-in” fuel replacement for traditional coal processes. Coal’s efficiencies and energy generation capabilities are well documented as well as its high level of greenhouse gas and other emissions. Biocoal offers many of the benefits of coal and also: (1) reduces emissions (NOx, SOx, mercury, CO2) significantly, (2) requires less raw-biomass energy, (3) uses low-cost equipment, and (4) decreases cost and is competitive with coal. The broad use of biocoal in small to large energy systems has received little attention, in spite of these advantages, because there are no commercial production torrefaction systems. Michigan Tech initiated a program that demonstrates the effectiveness of torrefaction and the applications of biocoal in coal-fired power plants. Our activity includes: (1) biomass development, (2) biomass torrefaction, using a torrefaction facility operating at a rate of 1 ton/hour, (3) co-firing of biocoal in PC boilers, (4) cost engineering and economic assessment for the power industry.

8:40 AM

(MCARE-106-2012) An Innovative Biomass Waste Aerobic Degradation System for Hot Water

H. Li*, D. Yu, University of Nebraska-Lincoln, USA; Y. Yu, Nanjing University of Science & Technology, China

As energy prices, population growth, and environment pollution continue to rise, the needs of sustainable renewable energy and waste treatment method are getting desperate. The U.S. alone generates over 250M tons of municipal solid waste per year two thirds of which is organic waste. However, most of this valuable energy resource is directly disposed through landfills and incineration by which enormous environmental damages have been inflicted. Only 7% is naturally decomposed to minimize environmental effects and produce fertilizers, since the traditional composting technology is too slow to be effective. Besides, massive green heat generated from the biodegradation is neglected and fully discharged. In this study, a biomass waste aerobic degradation system for hot water heating is developed to recover the free energy in a fast and effective manner. Lab testing using various biomass wastes demonstrates that, after the reaction occurs less than 12 hours, a sustainable heat output of 15~20W/kg wet biomass could be produced, and about 80% of energy could be recovered within 3 days. It is estimated that by just disposing 10kg of biomass waste every 3 days within this system, it can adequately support the daily domestic hot water needs (about 9 kWh/day) for a 4-member family. The study concludes this cost-effective system can be adopted widely for fast delivery of healthy fertilizer and domestic hot water.

9:00 AM

(MCARE-107-2012) Effects of Fuel Grade Ethanol on Pump Station and Terminal Facilities

G. T. Quickel, DNV USA Inc., USA; J. A. Beavers*, DNV USA Inc., USA; F. Gui, N. Sridhar, DNV, USA

There is significant interest within the North American pipeline industry in transporting fuel grade ethanol (FGE) as a result of the increased usage of ethanol as an oxygenating agent for gasoline and the potential use of ethanol as an alternative fuel. Several materials compatibility issues must be resolved before FGE can be safely transported in pipelines. Many of the issues related to corrosion of pipeline steels have been addressed in previous research projects. However, there is relatively little information on the effects of ethanol and ethanol - gasoline blends on other components in pipeline systems, such as pumps, valves, springs, and metering devices. The Pipeline Research Council International (PRCI) and the US Department of Transportation, Pipeline and Hazardous Materials Safety Administration (PHMSA) funded research to address these technical issues. The scope of the work includes a survey of knowledge and gaps, laboratory studies designed to close the gaps, and a guidelines document for the pipeline industry. This paper summarizes recent research results.

9:20 AM

(MCARE-108-2012) Material Challenges for Storing Alternative Fuels

J. S. Lee*, Naval Research Laboratory, USA; D. F. Aktas, University of Oklahoma, USA; R. R. Ray, Naval Research Laboratory, USA; J. M. Suflita, University of Oklahoma, USA; B. J. Little, Naval Research Laboratory, USA

Experiments were designed to answer the following questions: Are the material challenges for storing alternative fuels in contact with natural seawater different from those experienced with petroleum-based fuels? Is biodegradability of alternative fuels related to biodegradation of storage materials? Are chlorides and sulfur compounds from seawater found in alternative fuels after storage? Petroleum-based (JP5 and F76) and alternative (camelina-derived JP5, algal-derived F76) fuels were stored under typical storage conditions in the presence of natural seawater and uncoated carbon steel. Results indicate that seawater dissolved oxygen content decreased below 100 ppb within 2 days due to oxygen consumption by corrosion reactions at the carbon steel surfaces and respiration by aerobic microorganisms. Sulfides, produced by sulfate-reducing bacteria, and chlorides were co-located in corrosion products in both the seawater and fuel phases. Metabolic pathways for fuel degradation depended on the presence of transient oxygen. Catechols, indicative of aerobic degradation, and typically aerobic bacteria persisted after three-month exposures. The possibly that aerobic degradation is prolonged in corrosion-resistant materials and the concentrations of oxygen required to influence fuel degradation are under investigation.

9:40 AM

(MCARE-109-2012) Biocoal: A Novel Two-Stage Torrefaction-Pyrolysis for the Production of High-Grade Bio-Oil

E. Bar-Ziv*, J. Klinger, D. Shonnard, Michigan Technological University, USA

Barriers have been encountered when using raw biomass in pyrolysis for the production of bio-oils: formation of acids, large variability in the feedstock and bio-oil degradation. We have investigated biomass torrefaction, producing biocoal, and observed: (1) The component that mostly degrades is hemicelluloses. (2) Water, CO, CO2, organic acids are major products in the gas stream; and acids are not produced by cellulose and lignin. (3) Biocoal properties can be controlled, thus reducing feedstock variability. Consequently, we state that using biocoal in pyrolysis solves many of the hurdles and will provide a higher-grade bio-oil. In other words, doing a two consecutive stage torrefaction-pyrolysis process will produce up-graded bio-oils. We have shown the advantages of the two-stage pyrolysis process over the single-stage process. We propose to carry out a transformative comprehensive study on two-stage torrefaction-pyrolysis process and compare it with single stage pyrolysis. The study will be focused on establishing data bases in each of the stages for various types of biomass, from the forest and agriculture, that will enable to kinetically model these processes as well as to provide structural changes of each of the biomass components during their thermal degradation.

10:20 AM

(MCARE-110-2012) Rubber Reinforcement with Functionalized Lignin (Invited)

S. M. Dirk*, K. N. Cicotte, Sandia National Laboratories, USA; B. R. Hahn, D. A. Benko, The Goodyear Tire & Rubber Company, USA

Over five million metric tons of carbon black are used each year as reinforcing fillers in tires. A typical tire contains between 30-35% of carbon black, which generally improves the mechanical and electrical properties of the tire but adversely affects rolling resistance and fuel efficiency. Carbon black is made though energy intensive spray pyrolysis of petroleum at high temperatures. A green alternative to carbon black may be realized with the use of lignin. Over the past 60 years, literature reports have evaluated the use lignin as reinforcing filler in rubber compounds. It was observed that lignin displayed reinforcing properties far below those obtained with carbon black. Using lignin as a drop-in replacement for carbon black is not sufficient as negative effects are observed on properties such as tensile strength, tear resistance and abrasion resistance. Our research has focused on the modification of water soluble lignosulfonates via esterification and silylation reactions in order to improve the lignosulfonates organic solubility. The history of lignin as a rubber additive as well as initial results on lignin functionalization and rubber reinforcement with functionalized lignin will be discussed. Sandia is a multiprogram laboratory operated by Sandia Corporation, a Lockheed Martin Company, for the United States Department of Energy's National Nuclear Security Administration under contract DE-AC04-94AL85000

10:40 AM

(MCARE-111-2012) Distributed Hydrogen Generation and Storage from Biomass

P. J. Schubert*, J. Paganessi, A. D. Wilks, M. Murray, Packer Engineering, Inc., USA

A new paradigm is presented for local generation and storage of hydrogen, in which biomass is the only feedstock. A novel thermochemical conversion method produces hydrogen gas which can then be separated. The mineral ash produced contains carbon and silica. With proper stoichiometric ratios, post-processing of this ash produces pure silicon. This silicon can be converted into a storage media for hydrogen suitable for stationary or portable applications. In this way, local plant matter can be used to renewably produce and store hydrogen for fuel cells, prime movers, or for heat. This paper presents experimental results and overall system metrics.

11:00 AM

(MCARE-112-2012) Advances in CO2 Hydrogenation to Value Added Hydrocarbons to Be Used as Liquid Fuel

H. D. Willauer*, Naval Research Laboratory, USA; M. T. Olsen, D. M. Drab, National Research Council, USA; R. Ananth, Naval Research Laboratory, USA; D. R. Hardy, Nova Research Inc, USA; R. Morris, F. W. Williams, Naval Research Laboratory, USA; F. DiMascio, Office of Naval Research, USA

Novel catalysts and reactor technologies are being developed that can effectively transform carbon dioxide (CO2) into light olefins. These light olefins can subsequently be oligomerized to longer chain hydrocarbons to be used as liquid fuels. CO2 has been thought of as having too high of an energy barrier for polymerization, even in the presence of a catalyst. To overcome this challenge, novel approaches in catalyst development have led to thermodynamic improvements in the heterogeneous catalysis of the CO2 and H2 to hydrocarbons. Specifically, Fe/Mn supported on Al2O3 and promoted with K is an active catalyst for the hydrogenation of CO2 into light olefins. Furthermore, it has been demonstrated that Ni silica-alumina catalysts can oligomerize olefins into liquid hydrocarbons. The interest in moving these chemistries towards an integrated process has led to designing and testing suitable catalysts within fixed bed, tubular reactors. These small diameter tubular reactors are being modeled computationally to predict product formation so that they can be used as models for micro-channel processes. This presentation will discuss the progress in moving towards the integration of hydrogenation and oligomerization processes and the effects of catalyst composition and reactor design on CO2 conversion, olefin production, and selectivity toward C9-C16 product hydrocarbons.

Hydrogen

Adsorption, Catalysis and Means of Enhancing H-Interaction with Materials

Room: Ballroom E
Session Chairs: Theodore Motyka, SRNL; Astrid Pundt, University of Goettingen

1:30 PM

(MCARE-113-2012) Prospective of using structured nanoporous materials for hydrogen storage based on adsorption (Tutorial)

R. Chahine*, P. Bénard, E. Dundar, Hydrogen Research Institue, Canada; M. Richard, LTE-Hydro-Québec, Canada

In addition to sufficient usable volumetric and gravimetric capacities, viable materials based hydrogen storage systems need to satisfy a set of technical requirements including cost/efficiency, durability/operability, fast charging/discharging rates, cyclability, fuel purity, environmental health & safety, and loss of usable hydrogen. With traditional nanoporous adsorbents like activated carbon, it is cumbersome to predict the performance and the heat management requirements of such systems without prior experimentations. With the advent of structured nanoporous materials like metal organic frameworks, it is now possible to do so based solely on the unit structure and composition of the adsorbent. A case study will be presented.

2:10 PM

(MCARE-114-2012) Capacity, Kinetics and Evaluation of the Spillover Hydrogen Sorption Process (Invited)

T. Gennett*, NREL, USA

With the tremendous interest in spillover-type materials for hydrogen storage, NREL and DOE have dedicated considerable resources to demonstrate the reproducible synthesis of specific materials and to develop, validate and perform the requisite capacity measurements. Despite the fact that processes involving spiltover-hydrogen have been known for over 40 years in the catalysis community, the nature of this phenomenon has not been fully investigated or clarified. Without direct spectroscopic evidence, the debate regarding the chemical nature of the activated hydrogen moieties, their diffusion mechanism and ultimate hydrogen sorption capacities is still ongoing. Our approach to resolve some of these critical issues with spillover for hydrogen storage applications include the validation of syntheses and the rigorous characterization of a specifically selected set of materials that have an apparent enhanced hydrogen sorption capacity beyond what is expected for physisorption of dihydrogen, i.e., possibly metal catalyzed hydrogen spillover. After volumetric instruments, we evaluate the materials spectroscopically with diffuse reflectance infrared fourier transform spectroscopy (DRIFTS), neutron scattering and nuclear magnetic resonance (NMR) to identify specific reversible interactions between the receptor material and the hydrogen atoms. A summary of our collaborative results will be presented.

2:30 PM

(MCARE-115-2012) Nanoconfined materials for hydrogen storage (Invited)

C. Zlotea*, F. Cuevas, E. Léonel, T. Martens, M. Latroche, CNRS ICMPE, France; C. Matei Ghimbeu, R. Gadiou, C. Vix-Guterl, CNRS IS2M, France

In the clean energy field, nanosizing and nanoconfinement of materials is a key issue for the design of new hydrogen storage media. Among a wide variety of materials, hybrids containing metals embedded in porous structures are currently explored for their promising hydrogen storage and energy conversion properties. The present work reports on the synthesis and properties of hybrid materials obtained by in situ formation of Mg-based nanoparticles and nano-alloys/compounds within porous ordered carbon templates. Metal nanoparticles are synthesized by decomposition of organometallic precursors or reduction of metallic salts directly within the ordered porous carbon. The pores of the host material serve as a nanoreactor for confining the synthetic reaction of nanoparticles and hamper their coalescence into larger aggregates. Nanoscale effects on fundamental and hydrogen sorption properties are addressed. Experimental results reveal that the contribution of free energy from surfaces cannot be longer ignored. The hydrogen sorption kinetics of metal nanoparticles are significantly enhanced by downsizing the particle size. The hydrogen sorption thermodynamic properties of metallic nanoparticles and nano-alloys/compounds are determined and compared to the bulk counterparts.

2:50 PM

(MCARE-116-2012) Synthesis, crystal structure and properties of novel borohydrides (Invited)

B. C. Hauback*, C. Frommen, Institute for Energy Technology, Norway

Borohydrides are attractive materials for hydrogen storage because of their high gravimetric H-density. They suffer, however, from sluggish kinetics, high desorption temperatures and poor reversibility. This talk will present several novel borohydrides that have been obtained by mechano-chemical reactions (ball milling) between an alkali/alkaline earth borohydride and a different metal chloride. This method allows the synthesis of unsolvated compounds that have not been obtained by alternative chemical methods. The following topics and materials will be presented in detail: 1.) $Ca_3(BH_4)_3(BO_3)$: a product obtained from borohydride oxidation, containing both B-H and B-O bonds. 2.) $LiCe(BH_4)_3Cl$: The first mixed-metal and anion substituted rare-earth borohydride. 3.) $NaBH_4$-NaCl: chloride substitution in sodium borohydride. 4.) $Tb(BH_4)_3$ and $Er(BH_4)_3$: two new solvent-free rare-earth borohydrides. In addition the effect of different transition metal based dopants on the decomposition temperature of representative borohydrides like $NaBH_4$ and $Mg(BH_4)_2$ will be covered.

3:10 PM

(MCARE-117-2012) Solid Carbon Ceramic Products to Enable Hydrogen from Decarbonized Fossil Fuels

J. W. Halloran*, University of Michigan, USA

Hydrogen fuel can be obtained by decarbonizing fossil hydrocarbons with pyrolysis to separate the fossil hydrogen gas from the solid fossil carbon. The hydrogen gas product is accompanied by about 90 wt% solid carbon co-product, which can be utilized as carbon ceramics to in applications such as bricks, masonry, concrete and other building products. Developing very large markets for this solid carbon is critical to the economics of the pyrolytic decarbonization. This paper analyzes the prospects for fossil carbons used in a range of applications in the built infrastructure in terms of the required materials development, projected market size, and realistic market value. Solid carbon production methods are discussed including methane decomposition for nanoparticulate carbons and coal pyrolysis for macroscopic coke-like carbons.

3:50 PM

(MCARE-118-2012) Influence of carbon nanostructures on metal hydrides for hydrogen storage applications (Invited)

S. Sartori*, IFE, Norway

The synthesis of nano-sized particles infiltrated in carbon structures has being investigated as an alternative way to improve the properties of metal hydrides for hydrogen storage applications. The kinetics of this type of materials has been found to be significantly improved but the possible change in thermodynamics is still not clear. The successful wet or melt infiltration of nanoparticles of $Mg(BH_4)_2$, $NaAlH_4$ and MgH_2 into carbon fibers and activated carbons have been demonstrated by small-angle neutron scattering (SANS) performed at the JEEP II reactor at IFE. With the complementary *in situ* small-angle X-ray scattering (SAXS), it has been possible to underline important differences in the morphology and surface area of the hydride particles when they are nano-confined in the porous scaffolds, compared to their values in the bulk state. In this talk the latest work concerning SANS, SAXS and wide-angle X-ray scattering investigations of several hydrides will be presented. TEM, NMR and desorption data will contribute in some cases to clarify the properties of the nanocomposites. The interaction of the hydrides with the carbon structures will also be taken into account.

4:10 PM

(MCARE-119-2012) On the catalytic effect of TM additives on the Mg ↔ MgH2 kinetics of reaction (Invited)

D. Fruchart*, P. de Rango, O. Fruchart, G. Girard, S. Miraglia, L. Ortega, Institut Néel - CNRS, France; M. Shelyapina, St. Petersburg State University, Russian Federation; N. Skryabina, Perm State University, Russian Federation

For years, TM, TM-alloys and TM-compounds (oxides, halides) were demonstrated very active agents to improve markedly the kinetics of H-absorption/desorption forming metal (and complex) hydrides. This was achieved by applying nanostructuration on both Mg and TM components, namely using the ball-milling technique. Undertaken as well as on many different types of hydrides the process was proven due to TM metal or reduced TM-metal particles. The present report focuses on the nature and the role of the TM//Mg-MgH2 interface on the nucleation/growth opposite transformations Mg ↔ MgH2.

4:30 PM

(MCARE-120-2012) Thermodynamic tuning of multicomponent hydride systems for hydrogen storage applications (Tutorial)

G. Walker*, University of Nottingham, United Kingdom

Many metal hydrides and complex hydrides with a high hydrogen capacity (e.g. magnesium hydride and lithium borohydride) have a large enthalpy of dehydrogenation, ΔH_{dehyd}, which results in the temperature needed for a 1 bar equilibrium pressure, the T(1 bar), being too high for hydrogen fuel cell vehicle applications (i.e. >> 100 °C). However, there has been a lot of progress made in reducing the enthalpy of dehydrogenation by combining the hydride phase with either another element or compound in order to reduce the overall enthalpy of reaction. For example, the ΔH_{dehyd} for magnesium hydride can be reduced by over 50 kJ mol^{-1} via a concerted reaction with germanium forming magnesium germanide: $2\ MgH_2 + Ge \rightarrow Mg_2Ge + 2\ H_2$ Examples will be given for binary hydrides and complex hydrides. An issue with these multicomponent reactions is that they tend to be kinetically slow at temperatures below 200 °C. In situ diffraction studies have been undertaken to explore these reaction pathways and identify kinetic barriers. Solutions to these kinetic barriers being investigated in the field will be discussed such as nanostructuring and nanoconfinement.

Nanocomposites/Nanomaterials

Nanocomposites and Nanomaterials III

Room: Ballroom G
Session Chair: Virginia Davis, Auburn Unviersity; Gary Mushock, ASM International

1:30 PM

(MCARE-121-2012) Nanomaterials in Photovoltaic R & D in India (Invited)

V. Kumar*, K. Kumari, Indian Institute of Technology, India; S. K. Srivastava, National Physical Laboratory, India

During the last decade, excitement aroused by nanomaterial R & D and resurgence of interest in photovoltaics have been rather spectacular. The two distinguishing attributes of a nanomaterial, namely large surface area and enlargement of band gap due to quantum confinement effects, make nanomaterial particularly attractive for PV device development. Some aspects of this confluence of interest in Indian R & D efforts will be reviewed. Several groups in India are looking into inorganic – organic composite materials for PV applications with CNT, ZnO, CdS, and TiO2 nano-particles. We will also present activity on nano- phosphors for up-conversion and down-conversion approaches for PV as also the attempts to use plasmonics to improve solar cells. CdSe QDs of different sizes (5-8 nm) were synthesized by chemical route using TOPO as well as greener oleic acid (OA) as surface passivating ligands, and subsequently dispersed in MEH-PPV and P3HT to investigate the effect of QDs on the structural, opto-electronic and change transport and PV properties. Arrays of large area aligned silicon nano-wires have been fabricated at room temperature by electrochemical etching of silicon wafers. An average reflectivity < 4 % in the relevant spectral range is achieved. “Black silicon” solar cells have been demonstrated by conventional diffusion process with an absolute ~1% efficiency improvement.

1:50 PM

(MCARE-122-2012) Nanostructured Multifunctional Metal Oxides and Nanocomposites for Solar Energy Harvesting and Niche Applications (Invited)

M. V. Sunkara*, CSIR-IICT, India

Mounting global energy demands with increasing environmental concerns has translated into an urgency to tap the ‘SUN’, a sustainable and green energy source. Design and development of novel nanostructured materials with exotic architectures is an area of research being pursued. Our group is actively participating in creating a library of materials suitable for applications as alternate photo-anodes for DSSCs as well as visible light active photocatalysts for decontamination of environmental pollutants. In this endeavor, we focus on easily up-scalable, low temperature and eco-friendly synthetic routes for designing nanostructured metal oxides, control morphology, desired phases, high surface area, band-gap control, porosity and self-assembly for applications as alternate photo-anodes. Some of the semiconducting metal-oxides identified for the purpose are SnO2, ZnO, Fe2O3 and TiO2 and over the years several strategies have been optimized. These nanoparticles were independently stabilized in-situ using polyelectrolytes (chitosan), and oleyl amine to form polymer inorganic nanocomposites and these are being tried for their suitability in photovoltaic applications.

2:10 PM

(MCARE-123-2012) Strategies for the Efficiency Improvement of Photovoltaic Devices via Incorporation of Tailored Hybrid Nanostructures (Invited)

D. Kim*, Y. Jang, Y. Jang, S. Kochuveedu, U. Patil, Ewha Womans University, Republic of Korea

Unconventional approaches for enhancing solar cell performance have gained tremendous interest. An increase in the charge carrier generation can be achieved by introducing novel materials such as metal nanoparticles, periodic nanostructures, and carbon structures into conventional solar cells. In particular, various types of carbon materials including nanotubes, nanofibers, and graphene have been used to ensure high electrical conductivity, which is essential for increasing the electron collections in solar cells. In this study, we introduce a distinctly different and facile strategy to integrate carbonized TiO2 thin layers into conventional TiO2-based DSSCs. Ordered arrays of TiO2 dots in carbon matrix were fabricated via calcining UV-stabilized block copolymers containing inorganic precursors and integrated thus-prepared hybrid elements into both sides of pristine TiO2 layer. The mechanism of the enhancement of power conversion efficiency was investigated in terms of electrical impedance analysis and charge carrier mobility.

2:30 PM

(MCARE-124-2012) Strategies for improvement of efficiency of hydrothermally grown Zinc oxide (ZnO) nanorod dye-sensitized solar cells (Invited)

T. Bora, Asian Institute of Technology, Thailand; S. Sarkar, A. Makhal, S. N. Bose National Centre for Basic Sciences, India; S. Baruah, Uppsala University, Sweden; S. K. Pal, S. N. Bose National Centre for Basic Sciences, India; J. Dutta*, Sultan Qaboos University, Oman

Highly efficient solar cells with power-conversion efficiency (PCE) ~ 5-5.5% can be routinely fabricated by using hydrothermally grown Zinc oxide (ZnO) nanorod (NR) photoelectrodes and N719 dye in the dye-sensitized solar cells (DSSCs) configuration. An additional "indirect excitation" of dye can be introduced by using the sensitivity of Förster resonance energy transfer (FRET). The efficiency of light harvesting dynamics of the ZnO NRs was slightly lower (40 % with an acceptor dye oxazine) than for ZnO NPs (74 %) as studied by picosecond-resolved, time-correlated single-photon-count (TCSPC) spectroscopy. Upon decorating the nanorods with gold (Au) nanoparticles, due to the formation of the Schottky barrier at the ZnO/Au interface and the higher optical absorptions of the ZnO/Au photoelectrodes arising from the surface plasmon absorption of the Au nanoparticles, enhanced PCE of ~6.5% for small-area (0.1 sq. cm) solar cells were observed. For a better understanding of the charge-transfer processes at the semiconductor/metal interface photo-selective picosecond-resolved luminescence studies has been done and the study reveal the mediating role Au layer in promoting photo-induced charge transfer. For large area DSSC (1 sq. cm), ~130% enhancement in PCE (from 0.50% to 1.16%) was achieved after incorporation of the Au nanoparticles into the ZnO NRs.

2:50 PM

(MCARE-125-2012) Nano-structured Organic Photovoltaics: Design of the Ideal Structure (Invited)

W. Kim*, J. Kim, K. Kim, B. Jung, Yonsei University, Republic of Korea; S. Ko, KAIST, Republic of Korea

Organic photovoltaics (OPVs) have recently received increasing attention as alternatives to inorganic solar cells because of their light weight, compatibility with flexible electronics, and low production cost. The PCE of OPVs has been dramatically increased by the BHJ structure, charge trapping remains problematic for further increases of the PCE because of the complicated device structure. Therefore, the ordered bulk heterojunction (OBHJ) OPV was suggested as a solution to reduce carrier loss by providing direct carrier transport paths. We propose an ideal device structure of an ordered bulk heterojunction organic photovoltaics. We also suggest a parameter related to the power conversion efficiency of the device, which could be served as a rule of thumb for experimentalists. To produce maximum power conversion efficiency, (1) the size of a pillar and spacing between them has to be on the order of the exciton diffusion length and (2) thickness of the active layer has to be at least greater than half of the photon mean free path, i.e., inverse of the absorption coefficient.

3:10 PM

(MCARE-126-2012) Efficient Sensitization of Nanocrystalline TiO2 Films by Metal-Free organic and Ru-Complexes for Application in Dye Sensitized Solar Cells (Invited)

C. Malapaka*, Indian Institute of Chemical Technology, India

Nanotechnology has tremendous applications in health, energy and agriculture. As the fossil fuels are fast depleting, there is a search for alternative energy resources such as solar energy all over the world. Dye-sensitized solar cells (DSSCs) have attracted significant attention as low-cost alternatives to conventional solid-state photovoltaic devices and their performance is remarkably insensitive to angle of incidence and temperature change. The best photovoltaic performance among DSSCs, both in terms of conversion yield and long term stability, has so far been achieved with polypyridyl complexes of ruthenium. The high efficiencies of the ruthenium(II)-polypyridyl DSSCs can be attributed to their wide absorption range from the visible to the near infra-red (NIR) regime. In this regard the ruthenium sensitizers H112, H102 and H105, PTZ1, HRD1 and HRD2, BDF, mLBD1 and mLBD2,BPFC, H101 synthesized in our laboratory obtained encouraging photovoltaic performance results. H102 and H105 sensitizers showed maximum solar to electricity conversion efficiencies(η) of upto 8.39%, 8.76% respectively in DSSC. Detailed synthesis and photovoltaic performance of these metal-free organic, and ruthenium sensitizers in test cell DSSCs will be presented.

3:50 PM

(MCARE-127-2012) Nano-heterogeneous structuring effects on thermal power factor and thermal conductivity (Invited)

G. Fernandes, Brown University, USA; S. Jung, Seoul National University, Republic of Korea; J. Kim, Brown University, USA; K. Kim, Seoul National University, Republic of Korea; Y. Park, F. Wahab, J. Xu*, Brown University, USA

Underlying the numerous interesting thermoelectric devices and structures is the same governing principle – Boltzman transport. As a result, the Seebeck coefficient and electrical conductivity are interlocked in such a way that one goes up with the Fermi energy while the other goes down. It can be shown that instead of maximizing the Seekbeck coefficient, one should ascertain an "optimal" value that is common to all materials and dimensionalities, at which the thermal power factor is maximal. The electrical and thermal conductivities are also coupled, but not as tightly such that their ratio can be increased as demonstrated with nanostructuring of materials to reduce phonon mean free length more than the electron's. By deploying a new strategy, nano heterogeneous structuring, one could introduce an extra degree of freedom into the system, and with which, to spatially transfer electrons from the secondary subsystem to the primary one while retaining Seebeck coefficient's optimal value and adding more scatterings to phonons. Here below we present our explorations of this new approach, starting from a simplest – a highly-ordered silicon nanopore membrane coupled to nanoparticles to more complex ones – random networks of nanotubes subjected to periodic nanoscale hole etching.

4:10 PM

(MCARE-128-2012) Layered Ceramics for High-temperature Thermoelectric Generators

K. Scott, M. Saterlie, O. Graeve, S. Misture, D. Edwards*, Alfred University, USA

Thermoelectric generators (TEGs) have been used in niche low-power, low-temperature applications for decades, but many conventional thermoelectric a materials are intermetallic compounds which limits their use under oxidizing conditions at high temperature. Oxide thermoelectric materials may offer significant advantages over conventional thermoelectric materials for industrial and automotive waste heat recovery, but the performance of oxide materials lags behind conventional TE materials. Significant advances have been made in the development of p-type thermoelectric oxides over the past decade, the but he performance of n-type oxides limits device performance. We are investigating beta-gallia rutile intergrowths, and other natural superlattice structures, as potential thermoelectric materials. This presentation will discuss the fabrication and thermoelectric characterization of these materials.

4:30 PM

(MCARE-129-2012) Nanocomposite-based Thermoelectric Devices for Energy Harvesting from Structural Components

R. K. Vaidyanathan*, O. Jacob, D. Vashaee, Oklahoma State University, USA

For reducing energy usage, improved energy harvesting techniques are crucial. Energy harvesting by utilizing the temperature difference between two surfaces is known as thermoelectric (TE) energy generation. We propose to incorporate nanocomposite TE devices onto structural components so that waste energy can be harvested during the service of these components e.g., furnace linings and structural panels. By using nanocomposite TE materials, it will be possible to increase the electrical conductivity while simultaneously reducing the thermal conductivity so that the ZT may be enhanced even at low efficiencies. We have developed a thick film TE device fabrication method that can be used with such structural components. These devices are inexpensive to manufacture and appropriate for energy harvesting needs ensuring ease of fabrication compared to a thin film approach. The process uses a three-layered structure consisting of metal contacts and TE material that are sintered and diced into thick films for device fabrication. This method can be extended to other TE materials irrespective of the temperature range.

4:50 PM

(MCARE-130-2012) Effect of Sn-doped on physical properties of ZnO Thin films prepared by spray pyrolysis and grown on SnO2:F/glass

K. T. Najoua*, M. Ajili, Laboratoire de Physique de la Matière condensée, Tunisia; M. Castagne, Université de Montpellier II, France

Transparent conducting thin films of tin-doped zinc oxide (TZO) have been deposited on SnO2:F/glass by the chemical spray technique, starting from zinc acetate (CH3CO2)2Zn2H2O and tin chloride SnCl2. The effect of changing the tin-to-zinc ratio from 0 to 1 at.% on the structural, optical and electrical properties of ZnO:Sn thin layers, has been thoroughly investigated. It was found that X-Ray diffraction results reveal that TZO films have an hexagonale Wurtzite structure with (002) preferred orientation. The maximum transmittance is around 80% for the 0.6 at.% Sn doped thin films. The band gap energy, calculated for samples is around 3.28 eV. A minimum resistivity ρ of 5.4 x 10-4 Ω.cm is obtained for the undoped thin layer. Doping with Sn4+ in the ZnO influences the volume composition of ZnO:Sn thin films, makes the film surface roughness decrease until 0.6 at.% Sn and leads to the decreasing of average grain size. Keywords. Tin doped zinc oxide (TZO), chemical spray pyrolysis, structural properties, optical properties, electrical properties.

Battery Technology

Novel Energy Storage Technologies

Room: Ballroom F
Session Chairs: Jason Zhang, Pacific National Laboratory; Reza Shahbazian-Yassar, Michigan Technological University

1:30 PM

(MCARE-131-2012) Magnesium Battery Research at Toyota: Current Challenges for the Next Generation of Electric Vehicles (Tutorial)

P. Fanson*, Toyota Motor Engineering & Manufacturing North America, Inc., USA

In order to realize the vision sustainable mobility in the automotive sector, new green technologies such as plug-in hybrid and all electric powertrains are under development. In order to enable this technology, advanced battery systems with superior capacity and low cost will be necessary. Current lithium ion technology is limited to a theoretical energy density of approximately 2000 Wh/l. Current research at the Toyota Research Institute of North America (TRINA) is focused on the investigation of post-lithium ion technologies, such as magnesium-based batteries, which offer the potential of higher volumetric energy densities and therefore vehicles with a much larger range. In order to develop advanced Mg batteries, new electrolyte, cathode, and anode materials are all needed. For the electrolyte, TRINA has developed a novel organomagnesium material which is compatible with both a Mg metal anode and a high capacity, reversible sulfur-based cathode. Current research efforts are focused on the development of higher voltage, oxide-based cathodes as well as electrolytes with improved voltage stability and corrosive properties. As an alternative strategy, TRINA is also developing novel intermetallic anodes that are compatible more conventional high voltage, ionic electrolytes.

2:10 PM

(MCARE-132-2012) Electrical and Morphological Characterization of Monocultures and Co-cultures of Shewanella and Geobacter Bacteria in a Microbial Fuel Cell

K. E. Larson*, M. C. Shaw, California Lutheran University, USA

The diminishing supply of fossil fuels has led to a global effort to develop renewable energy sources such as microbial fuel cells (MFCs), which produce electricity via the breakdown of organic matter by bacteria. The purpose of this study was to design and build an MFC and electrical characterization apparatus in order to measure and analyze the electrical output of single cultures of the Shewanella and Geobacter bacterial species, as well as the potential synergistic interactions of co-cultures of these species. Results that will be presented include (i) measurements from a zinc-copper galvanic cell in the MFC structure, with a 0.98% error from the standard reduction potential; (ii) a negative control producing a 1-5 mV MFC output; and (iii) an MFC using bacteria samples taken from the benthic zone of a nearby water source, which produced a 30-59 mV MFC output. We will also describe data from MFCs comprising monocultures and co-cultures of Shewanella and Geobacter species to explore potential synergistic interactions between them. Finally, scanning electron micrographs of the bacteria/electrode morphologies for each case will be presented as a foundation for subsequent studies with nanostructured electrodes. We conclude that these results show the feasibility of both mono and co-cultured MFCs comprising Shewanella and Geobacter bacteria.

2:30 PM

(MCARE-133-2012) Materials Challenges in Developing High Voltage Li-ion Batteries (Invited)

T. R. Jow*, J. L. Allen, O. A. Borodin, U.S. Army Research Laboratory, USA

Li-ion batteries with an energy density of 200 Wh/kg are widely used in today's portable electronic devices such as smartphones, laptop and tablet computers. To further increase the energy density for broader applications, lithium alloy based anodes such as LixSi with a capacity of many times of lithiated graphite are used. However, the Li-ion batteries incorporating such anodes could achieve higher energy density but deliver limited cycle life with low rate capability. Alternatively, the use of high voltage cathodes such as 4.7 V LiNi0.5Mn1.5O4 and 4.8 V LiCoPO4, which are of the same intercalation type as the state-of-the-art LiCoO2 cathodes, coupled with lithiated graphite anode appears to be a viable approach for increased energy density without sacrificing the cycle life. However, such approach faces two materials challenges. The first is that the state-of-the-art electrolytes would not support the 5 V operations. The second is that the structure stability of the high voltage cathodes that is needed to sustain repeated intercalation and de-intercalation cycles has not been well established. Recent efforts in developing high voltage electrolytes that are compatible with high voltage cathodes and stabilizing structures of high voltage cathodes including modeling in both cases will be reviewed and discussed.

2:50 PM

(MCARE-134-2012) A Novel Iron-Polysulfide Redox Flow Battery

G. Xia*, X. Wei, L. Li, W. Wang, G. Yang, G. L. Graff, J. Liu, Pacific Northwest national Laboratory, USA

A novel iron-polysulfide based redox flow battery system is developed for renewable energy storage applications. This system employs alkali metal ferricyanide/ferrocyanide and alkali metal polysulfide as the redox electrolytes. This new flow battery has an open circuit voltage of 1.1 volts (fully charged). When proper electrodes, such as pre-treated graphite felts, are used, over 75% energy efficiency and at least

98% columbic efficiency can be retained with good stability over 100 charge-discharge cycles. The remarkable advantages of this system over the current state-of-the-art redox flow batteries include:1) less corrosive and relatively environmentally benign redox solutions used; 2) excellent energy and utilization efficiencies; 3) low costs for electrolytes and cell components. The major drawbacks of the present cell designs are sulfur species crossover and relatively low power density, which need to be further improved.

3:10 PM

(MCARE-135-2012) Correlation between Microstructure and Oxygen Removal in Solid-Oxide-Fuel-Cell-Modelelectrodes Pt(O2)/YSZ und Pd(O2)/YSZ

G. Beck*, Research Institute Precious Metals & Metals Chemistry, Germany

Pt and Pd films have been prepared on (111) and (100) orientated as well as on polycrystalline yttrium-stabilized zirconia (YSZ) by pulsed laser deposition (PLD) and subsequent annealing. The metal films on all substrates are (111) orientated. On single crystalline (111) orientated YSZ the films are single crystalline as well. On YSZ(111) with defects these defects can also be found within the films (mostly twins). The films on (100) orientated and polycrystalline YSZ are polycrystalline. The grain boundary angle and the grain size in these polycrystalline films depend on the substrate. The closer the texture of the substrate is to the (111) orientation, the larger is the ordering within the films. Besides, µm-sized droplets and holes as well as voids of up to ca. 100 nm size (located at the interface between the substrate and the film) can be found. During polarisation, oxygen is formed at the anode Pt(O2)/YSZ and Pd(O2)/YSZ, respectively. This oxygen formation occurs mainly at the triple phase boundary, but also at holes and grain boundaries (also at twin grains). Within dense metal films or dense parts of the metal film bubbles are built. These bubbles are formed close to grain boundaries, at twin grains or at the position of voids. Accordingly, dense metal films are aging during polarisation and the electrochemical behaviour is changing drastically.

3:50 PM

(MCARE-136-2012) Energy Storage via Electrochemical Generation of CO as in Intermediate Product

I. Lubomirsky, V. Kaplan*, Weizmann Institute of Science, Israel

The capacity of the largest resources of renewable energy, wind and solar, are weather- and time-dependent. The variability of the supply leads to the large cost of the infrastructure relative to the total cost of the renewable-energy-based systems. This problem can be alleviated if a reliable method for storing and transporting the harvested energy is found. Electrochemical conversion of CO2 into CO is one of the most promising solutions. We have found such a combination of electrode materials (Ti-Al alloys and graphite) and electrolyte (mixture of molten Li2CO3 and Li2O) that do not undergo detectable at 900°C. The process can be carried out at a current density of up to 0.5 A/cm^2. At a current density of 0.1 A/cm^2, the process has 100% Faradaic efficiency and 90% thermodynamic efficiency. The gases produced at the cathode and anode compartments are at least 99% pure CO and O2 respectively. In the absence of oxygen, the melt does not absorb SO2 and NOx decomposes upon on contact with the melt. The proposed technique of CO2 to CO conversion has a number of advantages: a) it does not require precious metals or other expensive materials; b) it does not use or produce environmentally hazardous or polluting materials; c) it has a potential for continuous operation with flue gases of power stations; e) the method is sulfur tolerant; e) the conversion efficiency of CO2 to CO is close to 100%.

4:10 PM

(MCARE-137-2012) Characteristics of Pt/YSZ Nanocomposite Thin Films for Micro-SOFCs

H. Huang*, Wright State University, USA; M. Rottmayer, T. Reitz, Air Force Reearch Laboratory, USA

Thin micro- solid oxide fuel cell (µSOFCs) were demonstrated recently and power densities at the intermediate temperatures were improved significantly. The architecture of the µSOFCs was made up of dense YSZ electrolyte and porous Pt electrode membranes supported on Si wafer. The technical challenge of using Pt electrode is to control and stabilize the porosity of the Pt, which is critical to achieve fast electrode kinetics and stability of the long-term operation. Pt/YSZ nanocomposites combine the high catalytic properties of Pt and acceptable ionic conductivities of YSZ, which can be a promising alternative electrode for micro SOFCs. Recently we have conducted research on 1) PVD processing of Pt/YSZ nanocomposite thin films and 2) structural, morphological, and electrical characterizations of the electrode thin films. SEM imaging results exhibited that the Pt/YSZ thin films are dense crack-free, and homogeneous. The particle size is less than 40nm in average. The Pt atoms/particles are homogeneously distributed in the YSZ matrix or vice versa. The composite thin films with less Pt content exhibited poor crystallinity, but both YSZ and Pt crystallinity increased with increasing the Pt contents. The percolation threshold was determined in the range of 30 to 50% of Pt.

Wind

Wind Power

Room: Ballroom D
Session Chairs: Megan McCluer, U.S. Department of Energy; Jim Ahlgrimm, U.S. Dept. of Energy

1:30 PM

(MCARE-138-2012) The Role of Advanced Materials in Wind Energy (Tutorial)

F. D. Marquis*, Naval Postgraduate School, USA

The global energy demand is growing at an alarming rate, drawing primarily on the use of fossil fuels. In short term there is an urgent need to achieve higher energy efficiency, significant energy savings and increase supplies from all forms of renewable energy. The wind energy available on the earth atmosphere is much larger then the current world power consumption. Its potential on land and near shore is believe to exceed 72 TW. This is equivalent to 54 millions of tons of oil per year, or over five times the total combined world power from all sources. In addition wind power is clean and renewable without any form of emissions or residues and it does not involve the depletion of any form of fuel. The growth in new capacity has exceeded 30 percent over the last five years and is expected to continue and/or exceed this trend for many years to come. Advanced materials are playing an important role in addressing several important challenges that need to be overcome in order to drive the industry to the full mature stage. This paper discusses the current and potential roles of advanced materials in typical direct sub-systems such as blades and rotors, drive train and generators, tower and foundations. In addition it brings into attention the potential role of advanced materials in energy storage and power grid as secondary enablers to the full development of wind energy.

2:10 PM

(MCARE-139-2012) Criticality of Defects in Wind Turbine Blade Materials and Manufacturing

D. Cairns*, J. Nelson, T. Riddle, M. Peterson, Montana State University, USA

Modern wind turbines have attained a level of maturity with respect to power generation and acceptance. The wind turbine blades are manufactured with composite materials on large scales at commodity prices compared to aerospace structures. Wind turbine blades can be over 50m in length. In this paper, we explore the criticality of material and manufacturing defects for the reliability of wind turbine blades. Defects in the composite material laminate, the assembly process (including adhesive bonds) are examined with respect to inspection techniques, durability, and damage tolerance. Discussions on a damage tolerance philosophy are provided for composite wind turbine blades. This includes inspection, damage growth, and residual strength. While preliminary, these discussions are intended to provide a framework for material suppliers, wind turbine manufacturers, and wind turbine operators for an improved understanding of the criticality (size, type, and location) of defects in composite wind turbine blades.

2:30 PM

(MCARE-140-2012) Fatigue of Wind Blade Laminates: Effects of Resin and Fabric Structure Details

D. A. Miller*, D. D. Samborsky, J. F. Mandell, Montana State University, USA

Recent fatigue data will be presented for resin infused laminates with systematic variations in glass fiber reinforcing fabric structure and resin type. Simple aligned strand reinforcement produces significantly improved fatigue resistance compared to commercial fabrics, for all resin systems tested. The backing strands present in fabrics serve as crack initiation sites, reducing fatigue resistance for polyester and, in most cases, vinyl ester resins. Epoxies are relatively insensitive to fabric structure for a wide range of commercial and specially prepared fabrics.

2:50 PM

(MCARE-141-2012) Study of Effects of Surface Coatings on Envrionmental Degradation of Wind Turbine Blades through Environmental Wind Tunnel

J. Gou*, D. Ritson, S. Murray, M. Doherty, C. Harrison, S. Rice, J. Kapat, University of Central Florida, USA

The structural properties of wind turbine blades are fundamental to the efficient extraction of power from wind. Ideal wind turbine blades are the combination of smooth surface which lead to aero-dynamical fluency and good mass distribution. For the weight consideration, glass fiber reinforced composites, carbon fiber reinforced composites or their hybrid composites are materials that mostly used for wind turbine blades. However, there are some problems in the use of these materials. The maintenance of such large size of composite blades becomes a big issue which calls for the research into environmental effects on the blade materials and structures. In the present work, an environmental wind tunnel was designed and built. An injection system was installed to inject salt water or sands into wind tunnel to simulate the operating environment of wind turbines in the desert or offshore areas. The injection nozzle configuration is adjustable to allow the changes in angle of attack and flow rate of salt water and sands. The test section is instrumented with a variety of sensors/techniques such as Pitot-static, Kiel and five-hole probes, thermal anemometers and smoke visualization. The effects of different surface coatings on the environmental degradation of wind turbine blades were studied through this environmental wind tunnel.

3:10 PM

(MCARE-142-2012) Lightning Strike Protection of Composite Wind Turbine Blades

J. Gou*, F. Liang, J. Kapat, University of Central Florida, USA

The nature of wind turbines consign themselves to be in vulnerable open-air environments. Areas of favorable locations for wind turbines usually coincide with areas of thunderstorm activity. With the rapid growth of wind power generation, comes the inevitability of the increase in lightning damage in wind energy systems. The present work developed a specialty paper made of carbon nanofibers and nickel nanostrands and explored potential replacement for existing lightning strike protection materials of wind turbine blades. The porous, flexible and nonwoven paper composed of both nanofibers and nickel nanostrands were first prepared by a paper-making process. They were then incorporated onto the surface of glass fiber reinforced polymer composites through resin transfer molding process. The lightning strike tests conducted on these composite panels showed that the lightning strike tolerance correlated to the surface conductivities of composite panels. The conductivity of the nanofiber/Nickel nanostrand paper was found to be as high as 34,100 S/m. During the lightning strike test, the nanofiber paper could provide safe conductive paths to prevent the underlying structural damage. The nanofiber paper functioned as sacrifice layer which was burnt out due to an enormous heat generated by lightning strike. The damaged surface on the composite panel can be easily repaired by simply applying a new layer of nanofiber paper.

3:50 PM

(MCARE-143-2012) Radar-wind farm interaction issues and mitigation via alternate wind turbine blade materials

J. J. McDonald, B. C. Brock, J. A. Paquette, S. E. Allen, K. W. Sorenson, E. D. Spoerke, J. Wheeler, D. A. Calkins, W. K. Miller, P. Clem*, Sandia National Laboratories, USA

In recent years, increasing deployment of large wind farms has become an issue of growing concern for the radar community. Expanding wind farms could impede radar operation for air traffic control (ATC), weather sensing, and other applications. Several approaches currently exist to minimize conflict between wind turbine and radar installations, including procedural adjustments, radar upgrades, and proper choice of low impact wind farm sites, but each has problems with limited effectiveness or prohibitive cost. An alternative approach is to alter turbine and blade design to reduce turbine RCS to the extent that turbines can be installed near existing radar installations. This presentation summarizes efforts to characterize and reduce the radar cross sections (RCS) of wind turbine blades, with particular emphasis on modification of blade design and materials. In this work, common blade materials have been characterized for RF electrical properties (complex permittivity and permeability) and a 3D electromagnetic model of the blades has been developed. We will discuss use of composite mixing rules to develop of novel blade materials with designed RF properties, previous literature approaches, and possible paths toward reduced radar interaction blade designs.

4:10 PM

(MCARE-144-2012) Novel Flexible Membrane for Structural Health Monitoring of Wind Turbine Blades – Feasibility Study

S. Laflamme*, R. L. Geiger, Iowa State University, USA; G. Kofod, M. Kollosche, Potsdam University, Germany; C. Sumit, R. Khrisna, Iowa State University, USA

Several sensing systems have been developed over the last decade for SHM of wind turbine blades, and some have shown promise at damage detection. However, there exists yet several challenges in establishing links between sensor signal, damage state (diagnosis), and residual life (prognosis) of a wind turbine blade. In order to create a complete SHM system capable of damage diagnosis, localization, and prognosis for wind turbine blades, the authors propose a novel sensing method capable of distributed sensing. The sensor is a flexible membrane composed of several soft capacitors arranged in a matrix, with the advantages of being robust, easy to install, inexpensive, capable of covering large surfaces, and involves relatively simple signal processing. By measuring changes in capacitance, it is possible to determine local strains on a structural member at pre-defined levels of precisions. To demonstrate the promise of the novel sensing system, a flexible membrane formed with a square matrix of 16 sensing patches covering a region of 0.5 x 0.5 meters is deployed on a cantilever subjected to a dynamic load. Test results show the great potential of the proposed sensing technology at damage diagnosis, localization, and prognosis of wind turbine blades.

4:30 PM

(MCARE-145-2012) Robotic and Multiaxial Testing for the Constitutive Characterization of Composites (Invited)

J. Michopoulos*, Naval Research Laboratory, USA; J. Hermanson, Forest Products Laboratory, USA; A. Iliopoulos, Resident at Naval Research Laboratory, USA

We present a methodology that utilizes robotically controlled mutliaxial testing combined with numerical optimization for the automated characterization of both the linear and non-linear (due to damage) constitutive response of composites. The optimization utilized solves the inverse problem associated with the estimation of the material parameters defining the constitutive model.

4:50 PM

(MCARE-146-2012) Spiral notch torsion test for fracture behavior evaluation of polymeric composite materials for wind turbine applications

J. Wang*, F. Ren, T. Tan, E. Lara-Curzio, Oak Ridge National Laboratory, USA; P. Agastra, J. Mandell, Montana State University, USA; W. Bertelsen, Gougeon Brothers, Inc., USA; C. LaFrance, Molded Fiber Glass Companies, USA

Improvement of the performance of wind turbines depends on enhancing the reliability of turbine blades, which requires more thorough knowledge of material properties. Wind turbines are subjected to complex, multiaxial stress states during operation. Thus, development of testing methods to characterize the fracture behavior of blade composite materials under mixed loading modes is essential to enable the qualification and use of these materials for the next generation wind turbines. In this project, a new testing method, the spiral notch torsion test (SNTT) was used to investigate the fracture behavior of glass/epoxy composites as well as pure resin materials. Using different sample geometries, mode I (opening mode) and mode III (tearing mode) loading conditions were obtained. Effects of fatigue and loading rate were also studied. Fracture surfaces were examined using optical and electron microscopy, while finite element analysis was used to calculate fracture toughness under different loading conditions.

Student Poster Contest and Design Contest

Room: Waters Edge Ballroom

(MCARE-P017-2012) Multi-layered (Y2O3)0.08(ZrO2)0.92 / (Sc2O3)0.1(CeO2)0.01(ZrO2)0.89 Electrolytes

Y. Chen*, N. Orlovskaya, University of Central Florida, USA

(Sc2O3)0.1(CeO2)0.01(ZrO2)0.89 (SCSZ) has superior ionic conductivity in the intermediate temperature range (700~800 °C) for the operation of solid oxide fuel cells (SOFCs), but it does not exhibit good phase stability and reliability in comparison with (Y2O3)0.08(ZrO2)0.92 (YSZ). In order to keep high ionic conductivity, good reliability and phase stability in the whole electrolyte at the same time, layered structure with YSZ outer layers and SCSZ inner layers were designed. Those YSZ/SCSZ electrolytes with 3, 4 and 6 layers design were manufactured via tape-casting, laminating and sintering. After sintering, the thickness of YSZ outer layers were kept constant at ~30 μm, the thickness of SCSZ inner layer varies from ~30 μm for a Y-SC-Y three layered electrolyte, ~60 μm for a Y-2SC-Y four layered electrolyte, and ~120 μm for a Y-4SC-Y six layered electrolyte. In the paper, the microstructure and phase structure of YSZ and SCSZ powders and sintered ceramics was studied by X-ray and neutron diffraction, Scanning and Transmission Electron Microscopy (SEM and TEM) and Secondary Ion Mass Spectroscopy (SIMS). Both microstructural features, crystal structures, such as lattice parameters, the chemical elements distribution in the layers were characterized.

(MCARE-P018-2012) Porous Media Burner Coupled with Thermoelectric Modules for Portable Power Generation

M. D. Robayo*, J. Hudson, E. Vinueza, J. Rodriguez, N. Orlovskaya, R. Chen, University of Central Florida, USA

Second generation prototype portable power generator that utilized matrix stabilized porous medium combustion is an advanced technique in which a solid porous ceramic matrix within the combustion chamber accumulates heat from the hot gaseous products and preheats incoming reactants. This heat recuperation allows the burning of ultra fuel-lean mixtures, which conserves energy. The heat generated by the porous burner can be harvested with thermoelectric devices for a reliable method of generating electricity for portable electronic devices by the burning of lean or otherwise noncombustible mixtures. This project has the ultimate goal of miniaturizing the generator for portability and improving flame visualization within the burner through a transparent casing or window.

(MCARE-P019-2012) Improving Electrostatic Energy Storage Density by Minimizing Voltage Tuning

K. Meyer*, Sandia National Laboratories, USA; Y. Jeon, Oregon State University, USA; H. Brown-Shaklee, Sandia National Laboratories, USA; D. Shahin, Missouri University of Science and Technology, USA; J. Ihlefeld, G. Brennecka, Sandia National Laboratories, USA

One of the most pressing challenges associated with integration of alternative energy sources is storage. Regardless of which flavor of high energy density primary storage is used, efficiency and performance can generally be improved with supplemental fast-response power units. Inexpensive ceramic capacitors could fill this role without the need for complex temperature-control systems required by ultracapacitors, but the use of high-permittivity ceramics for high-field applications is hindered by a decrease in permittivity with increasing applied electric field. Here, Bi(Sc,Zn,Ti,Mg)O3-modified BaTiO3 ceramics and thin films were studied to minimize such voltage tuning and improve temperature stability through control of the microstructure and cation distribution. Dense ceramics have been fabricated which maintain relative permittivity values greater than 1500 even at fields in excess of 100kV/cm, greatly surpassing the stored electrostatic energy of commercial high-voltage ceramic capacitors. Thin film versions of these complex compositions also show promise for low-voltage, high-field energy storage applications.

(MCARE-P020-2012) Nano facilitated charge transfer for an 11 electron redox couple for anodic charge storage: VB2

S. Licht, C. Hettige, J. Lau, J. Asercion, U. Cubeta*, George Washington University, USA

In today's society, there is a strong demand for a high capacity battery for use in a variety of applications including consumer electronics, industry, medical, military applications, and recently in hybrid and electric vehicles. The research for a long, uninterrupted power supply has focused on lithium-ion batteries, but a new material, zirconia stabilized vanadium diboride has recently been introduced as a potential high capacity anode, with a VB2-air battery being shown to have at least one order of magnitude higher than lithium-ion batteries. The storage of multiple electrons per molecule provides opportunities to greatly enhance electrochemical energy capacity. VB2 releases, via electrochemical oxidation, 11 electrons per molecule at a favorable, electrochemical potential. Coupled with an air cathode, this 4060 mAh/g intrinsic capacity anode, has energy capacity greater than that of gasoline. Nanochemical improvements of VB2 are probed to facilitate charge transfer and discharge voltage. Nanoparticle formation is accomplished with a planetary ball mill media (tungsten carbide) with hardness comparable to that of VB2 (8-9 Mohs2), the nano-VB2 improves VB2/air battery discharge voltage, while a retaining a high coulombic efficiency during discharge.

(MCARE-P021-2012) Assembly and Electrochemical Testing of Nano Silicon Lithium-Ion Batteries

L. Rueschhoff*, E. White, I. E. Anderson, S. W. Martin, Iowa State University, USA

Lithium-ion batteries are in great demand as an energy source for portable electronic and computing equipment due to their high energy density. They also offer higher operating voltages and lower self-discharge than most other types of batteries. Current commercially used lithium-ion cells using graphitic anodes have maximum capacities of 372mAh/g which is insufficient to satisfy current demand. Lithium alloys are a promising anode material as they can offer capacities upwards of ~4000 mAh/g.Silicon can alloy with lithium up to

Li4.1Si,corresponding to a capacity of 4212 mAh/g. However, this capacity is hard to reach due to the large volume change that occurs during the formation of various lithium silicon phases. Advancements have been made by producing silicon anode materials on the nanoscale which circumvents the volume expansion issue. This poster describes the process of making and testing lithium-ion coin cells made with nano silicon anodes. The problems with nano silicon anodes willbe discussed, as well as shown in collected data and calculations of the nano silicon cells.

(MCARE-P023-2012) The electrochemical enhancement of LiFePO4 by addition of surfactant via solid state method

J. Lee*, R. K. Singh, University of Florida, USA

Recently, Lithium iron phosphate (LFP) has been enormously attracted due to its eco-friendly, cheap, and thermally stable structural characteristics. Despite these many advantages, LFP exhibits a very poor cycle performance. Basically, particles can be easily agglomerated by sides of particles as they decrease to nano- sized particles. In an effort of solving this weakness, the effect of adding surfactant on electrochemical performance of LFP electrode during synthesis of LFP via solid state method will be studied without adding of carbon in this work. LFP with surfactant is expected to not only prevent particles from agglomeration but also improve the electrochemical cycle performance of electrode.

(MCARE-P024-2012) A Fast, Low-cost Aerobic Biodegradation Energy System

D. Yu*, H. Li, University of Nebraska-Lincoln, USA

With the continuous rise of energy prices, environment pollutions and waste generation rate worldwide, the needs of green renewable energy and alternative waste treatment solutions are getting desperate. The environmental- and ecological- friendly bio-degradation technology converting biomass waste to renewable energy and healthy bio-fertilizer could be a very important part of the solution. Also, the resources of biomass waste are economical, sufficient, and readily available throughout the world. However, the current biodegradation technology is still too slow to be applied prevalently and the vast thermal heat released during the aerobic bio-degradation is long-ignored and absolutely wasted. Thus, a novel aerobic bio-degradation energy system for reclaiming the massive thermal heat from biomass waste and delivering bio-fertilizer in a fast and cost-effective manner is developed in this study using industrial modular design method. It is demonstrated in the lab that the innovative energy system could accelerate the traditional aerobic degradation process by 10~15 times to release thermal heat (up to 140°F) at a rate of 15~20 W/lb of wet biomass waste after the reaction occurs less than 12 hours, and about 80% of thermal energy contained in the biomass waste could be recovered within 3 days.

(MCARE-P025-2012) PEC Properties of Nanostructured Hematite: Effect of Silicon Ion

P. Kumar*, P. Sharma, Dayalbagh Educational Institute, India; R. Shrivastav, S. Dass, Dayalbagh Educational Institute,Dayalbagh, India; V. R. Satsangi, Dayalbagh Educational Institute, India

Hydrogen generation from water splitting in photoelectrochemical (PEC) cells using solar energy is a renewable means of producing clean energy. In the present work two approaches: silicon doping and 100Mev Si8+ ion irradiation have been adapted to modify the properties of hematite thin films prepared by electrodeposition, for PEC generation of hydrogen. XRD, SEM, Raman, UV-Vis absorption spectroscopy characterization were carried out to observe the effect of Silicon ion on phase formation, particle size, surface morphology, absorption band edge of modified hematite thin films. Si ion irradiation was observed to highly influence the crystallinity of the material, with change in grain size. These films were used as photoelectrode in PEC cell and photoresponse were evaluated by getting current–voltage characteristic. Hematite thin films modified by both the methods showed significantly better photoresponse than that of pristine samples. Various parameters like crystallinity, resistivity, donor density, and flat band potential were analyze as factors crucially affecting the PEC performance of the samples. 100Mev Si8+ ion irradiated sample exhibited better photocurrent density of 2.5 mA/cm2 at 0.70 V/SCE, as compared to 1.90 mA/cm2 exhibited by Si doped sample at same potential. All the above mentioned results would be presented in the conference.

(MCARE-P026-2012) Portable Porous Media Burner for Thermoelectric Power Generation

E. Choi, A. DeWitt, T. Eman, J. Haglund*, N. Orlovskaya, R. H. Chen, University of Central Florida, USA

With the lack of a practical small-scale electric generator in the global marketplace, the versatility of portable electronic devices is stifled by the low power density and lifetime of today's batteries. Currently in progression, the goal of this research project is to develop a third generation prototype of a small-scale thermoelectric power generator for powering small-scale electronic devices. Using the thermoelectric effect to convert heat energy into electrical energy without the reliance on moving parts, thermoelectric generators offer a low-maintenance and reliable solution for generating electricity on a small-scale from heat. Thermally conductive porous materials have shown to enable extremely efficient combustion reactions. By using a porous matrix as a multimode heat transfer medium in a combustion chamber, supplementary heat from reaction products can be transferred to reactants, which allows leaner combustion, reduced pollutant emissions, and super-adiabatic flame temperatures. By focusing on space efficiency and materials optimization, the third prototype is expected to improve upon the second prototype by being lighter in weight (5-10 lb), smaller in size (400-600 in3 storage volume), and capable of delivering a larger power output (10-15 W).

(MCARE-P027-2012) Nano-scale Thermoelectrics for Enhanced Power Conversion Application

K. Wei*, G. S. Nolas, University of South Florida, USA

Thermoelectric (TE) devices make it possible to directly convert heat into electricity. The efficiency of TE devices is directly related to TE materials performance, therefore new, exotic, rare and costly materials are typically investigated. By affecting interfacial phonon scattering and introducing charge carrier filtering, nanostructured TE materials achieve enhanced TE performance over that of the bulk. This approach is applicable to existing low-cost TE materials. Coupled with low-cost processing techniques, this approach offers a new direction to low-cost TE power conversion technology. In our study, a variety of synthetic processes have been optimized to achieve phase purity, high yield and high crystalline quality materials for higher-quality and lower-cost materials. Potential applications include automotive waste-heat to electrical conversion, an application that is at the forefront of short term improvements in increasing the fuel efficiency of automobiles, and is thus of interest to the automotive industry as evidenced by our collaboration with General Motors, Inc., and Bosch, LLC.

(MCARE-P028-2012) Mineral Carbonation using Magnesium Oxide

K. Sushant*, Florida International University, USA

Fossil fuel accounts for the world's major energy supply and its use is anticipated to be continued throughout the 21st century. However, immense liability on its utilization led to various consequences. One of the major repercussions is vast emission of CO2 gas into the atmosphere. In this regard, mitigation routes for CO2 gas is of prime concern. In order to resolve this issue, mineral carbonation reaction has been considered. A chemical fixation of CO2 in the form of carbonate materials serves the permanent and safe method of disposal. Substantial heat is liberated while disposing CO2 in carbonate materials. We studied wet MgO reaction with CO2 which has shown a possibility to overcome the energy penalty as well as slow kinetics of mineral carbonation reactions. As well as, an analysis of efficiency penalty while integrating the fluidized bed reactor with post combustion coal fired power plant is under study.

(MCARE-P029-2012) Synthesis of nanocystalline AlMgB14 powders by solid state synthesis technique

Z. Xie*, N. Orlovskaya, University of Central Florida, USA

The AlMgB14 ternary boride is an important material with promising properties such as low density (2.46g/cm3) and high hardness values (Hv=33-35GPa). In this research work the different synthesis routes to produce nanocrystalline and single phase AlMgB14 powders were explored. The solid state synthesis with different raw materials was explored, where the heating of Al+Mg-B, AlB2+Mg+B; Al+MgB2+B, and AlB2-MgB2+B were done at 1200-1300oC for extended period of times. In addition to solid state synthesis, the mechanochemical synthesis of AlMgB14 using the same compositions of the initial raw powders were studied too. The synthesized powders were characterized by X-ray diffraction, Scanning Electron Microscopy (SEM) with energy dispersive X-ray spectroscopy (EDS), Transmission Electron Microscopy (TEM) and Secondary Ion Mass Spectroscopy (SIMS). Results show that the stoichiometrically mixed Al+Mg+B and AlB2+Mg+B powders are the best compositions for synthesis since the AlMgB14 phase yield is at maximum for such compositions and the formation of MgAl2O4 spinel is minimized. Also, amorphous boron performs better than crystalline boron in synthesis. The purity of initial raw materials is also of high importance.

(MCARE-P030-2012) Hierarchical TiO2 nanospheres fabricated by environmentally benign method for high efficiency photoanodes in DSSCs

M. V. Sunkara, B. Ramireddy*, P. Basak, CSIR-IICT, Hyderabad, India

Dye sensitised solar cells (DSSCs) are being envisaged as convenient and cost effective alternative for efficient harvesting of the abundant solar energy. The cornerstone of DSSC system is a mesoporous layer composed of semi-conducting material (TiO2, ZnO, SnO2) that are under intensive investigation as photoanodes. Over the years, the specification required to be met by these materials have evolved. Designer multifunctional nanostructured materials with improved light scattering, transparency, high surface area, faster electron mobilities could greatly enhance the efficiency of DSSCs. Further, synthetic methods adopted in exercising control on architecture should be ideally inexpensive, environmentally benign and easily scalable. Our present work deals with the synthesis of suitable photoanode with high surface area and tunable surface roughness for DSSCs. Rutile TiO2 spheres were synthesised in an environmentally viable route with tunable surface roughness and appreciable control on the morphology. XRD, SEM and TEM analysis reveals the nanostructures to be highly crystalline with primary particle sizes in the range of ~6-10 nm. These are observed to self-assemble into hierarchically aggregated secondary spherical structures of larger sizes. BET analysis confirms the comparatively higher surface area (168 m2/g), enabling added dye adsorption capacities.

(MCARE-P031-2012) Carbon-supported PtNi Nanoparticles Synthesized by Ultrasound for Oxygen Reduction Reaction in Fuel Cells

E. Lee*, SKKU Advanced Institute of Nanotechnology, Sungkyunkwan University, Republic of Korea; J. Jang, Center for Human Interface Nano Technology, Sungkyunkwan University, Republic of Korea; Y. Kwon, Department of Chemistry and BK21 School of Chemical Materials Science, Sungkyunkwan University, Republic of Korea

PEMFCs were remarkable candidate as promising power energy with high efficiency and cleanliness for application in transportation and in portable electronic devices. In order to commercialize the fuel cells, the several key challenges have to resolve. One of the key challenges for energy generation is to develop the cathode electrocatalyst for oxygen reduction. Previously, we reported that the ultrasound could reduce volatile metal precursors into nanoparticle electrocatalyst without stabilizer and capping reagent. This process is one of novel approach to obtain core-shell-like structured electrocatalyst in fuel cells. In this study, PtNi nanoparticle was prepared with Pt(acac)2 (acac = acetylacetonate) and Ni(hfac)2xH2O (hfac = hexafluoroacetylacetonate) by ultrasound-assisted polyol reduction method. Structural and morphological properties of electrocatalyst were characterized by X-ray Diffraction (XRD), Scanning Electron Microscopy-Energy Dispersive X-ray (SEM-EDX), Transmission Electron Microscopy (TEM). Based on physical characterization results, the particle size was in the range of 3~4 nm and Pt-rich composition was estimated. The electrocatalytic activity of catalyst for oxygen reduction reaction was measured by linear sweep voltammetry (LSV) with rotating disk electrode (RDE) which showed superior electrocatalytic activity than commercial Pt/C (E-TEK).

(MCARE-P032-2012) Charge Transfer Efficiency enhancement of Large Scale Graphene for Tri-iodide Reduction in Dye-Sensitized Solar Cells

S. Das*, Florida International University, USA; P. Sudhagar, Hanyang University, Republic of Korea; E. Ito, S. Lee, RIKEN-ASI, Japan; Y. Kang, Hanyang University, Republic of Korea; W. Choi, Florida International University, USA

Graphene, a newly discovered sp2 bonded 2D carbon material exhibits good mechanical, optical, thermal and charge transport properties. Large Scale graphene production and tailoring its charge transport properties for energy harvesting devices create enormous research possibilities for high efficiency solar cells. We report the fabrication and functionalization of large scale graphene and its electrocatalytic properties towards iodine reduction in the dye sensitized solar cell (DSSC). Graphene membrane was synthesized using chemical vapor deposition (CVD) and structural characterization was carried out using Raman spectroscopy, High Resolution Transmission Electron Microscopy (HRTEM) and Atomic Force Microscopy (AFM). Furthermore, the graphene film was doped with fluorine ions using CF4 reactive ion plasma as confirmed by XPS and UV-photoemission spectroscopy. We found the enhancement of catalytic activities of graphene for tri-iodide ions reduction with increasing plasma treatment time, which is attributed to an increase in graphene's edge-plane like electro-catalytically active sites for charge transfer. Furthermore, the catalytically active graphene was characterized as a DSSC counter electrode showing ~2.56% photon to electron conversion efficiency with ~11mAcm-2 current-density. We believe that the shift in work function in F- doped graphene is attributed to the shift in graphene redox potential which results in graphene electro catalytic activity enhancement.

(MCARE-P033-2012) Characterization of PECVD Thin Film Alumina for Electronic Passivation of Si Photovoltaics

L. R. Hubbard*, B. G. Potter, J. B. Kana-Kana, University of Arizona, USA

Recent interest in the development of Si photovoltaic architectures with p-type emitters has prompted the investigation of alternative passivation coating systems to enhance photocarrier extraction and improve overall energy conversion efficiency. In the present work, amorphous alumina films, grown using a high-throughput PECVD method onto p-type Si wafers, were subjected to a range of post-deposition isothermal annealing treatments to optimize thin film electronic passivation (EP)performance. Passivation behavior was monitored via minority carrier lifetime as measured using resonance-coupled photoconductive decay (RCPCD). Correlations between carrier lifetime and the Si- alumina interfacial character were examined using high resolution and scanning transmission electron microscopies coupled with energy dispersive spectroscopy (EDS). Annealing times of 4–6 minutes at 500C under a nitrogen atmosphere were found to produce the greatest enhancement in the minority carrier lifetime. The evolution of interfacial nanostructure as well as near-interface, oxygen stoichiometry have been associated with annealing-induced modifications in passivation performance.

The improvement in carrier lifetime was also correlated to an increase in the fixed space charge at the interface (capacitance-voltage (C V)), thus supporting a field-based mechanism for passivation in this system.

(MCARE-P034-2012) Silicon clathrates and their potential for photovoltaic applications

M. Blosser*, G. S. Nolas, University of South Florida, USA

The semiconductor Si is the most important semiconductor material for electronic devices. However, its relatively small and indirect band gap makes it inefficient for a variety of opto-electronic applications. A new class of materials, inorganic clathrates, has a rich variety of compositions and possesses interesting physical properties that are directly related to their structural and chemical properties. With the introduction of clathrates, one is able to perform "band gap engineering" by altering the geometry of the Si framework that forms the clathrate crystal structure in an attempt to alter its band gap. Recent theoretical predictions and experimental results have shown type-II silicon clathrates are in fact wide band gap materials. These materials therefore have enormous potential for renewable energy applications. We will be presenting an overview of the synthesis and characterization of Si clathrates, their interesting structure-property relationships, and why they are of great interest for photovoltaic applications.

(MCARE-P035-2012) The Use of Inexpensive All-Natural Organic Materials in Dye-Sensitized Solar Cells

J. Whitehead*, M. Shaw, J. Tannaci, California Lutheran University, USA

Given our planet's growing energy crisis, sustainable energy research is of vital importance. A seemingly limitless resource that should be utilized to its fullest extent is solar energy. The Dye-Sensitized Solar Cell (DSSC) is a photovoltaic cell which utilizes organic material to produce a small voltage, between 0.4V to 0.5V, in a process similar to photosynthesis. Our research explores the effects of using all-natural organic materials, specifically blackberries, blueberries, raspberries, and acai berries as sources of dye for DSSCs. The acai berries were specifically selected based on their high levels of anthocyanidins, pigment molecules which adhere well to the titanium dioxide nanostructure of the DSSC; as well as their increased absorbency as compared to other berries. To date, we have developed and commissioned a novel experimental apparatus including a digital data-acquisition capability. Furthermore, we have measured and compared the optical absorbance of the dyes to investigate how absorbance relates to electrical output. Finally, we have synthesized 12 cells from various berries, and demonstrated an electrical output of 0.3V to 0.5V from a white light source with an average intensity of 38,900 lux.

Thursday, March 1, 2012

Hydrogen

Engineering and Modification of H-Storage Materials for Applications

Room: Ballroom E

Session Chairs: Jacques Huot, UQTR; Sabrina Sartori, IFE

8:00 AM

(MCARE-147-2012) Condensed Phase Hydrogen Storage Materials Requirements for Automotive Applications (Tutorial)

D. L. Anton*, Savannah River National Laboratory, USA

The Hydrogen Storage Engineering Center of Excellence is a US DoE initiative with objectives to develop the necessary tools required to predict performance of hydrogen storage systems, to achieve the DoE 2017 technical targets for automotive application and demonstrate sub-scale prototypes these systems to validate the models. The solid state media under consideration include (i) chemical hydrides which need to be regenerated off-board which are either exothermic or endothermic upon dehydrogenation, (ii) metal hydrides which are regenerable on board and endothermic and (iii) adsorbent systems which typically run at cryogenic temperatures and are on-board regenerable and endothermic. The Center has concluded initial design efforts resulting in identification of minimal media requirements and initial system design concepts. While no material currently under consideration meets all of the storage system targets, the majority are already met by all systems. Various design configurations will be presented for each material type, the modeled performance characteristics for each system shown, identification of current material shortcomings and specification of minimal materials characteristics identified. These results should be used to guide material development efforts towards those media which hold all of the characteristics necessary to make a function cost effective system.

8:40 AM

(MCARE-148-2012) Sorption and Heat Management Behavior of Complex Hydride-based Hydrogen Storage Tanks (Invited)

J. Bellosta von Colbe*, G. Lozano, J. Jepsen, T. Klassen, M. Dornheim, Helmholtz-Zentrum Geesthacht, Germany

This study was carried out in order to investigate the behavior of a weight-optimized hydrogen storage tank containing doped sodium alanate as active material. The tank was analyzed through the experimental measurement of hydrogen flow during absorption and desorption in combination with pressure and temperature measurement, leading to an evaluation of overall sorption kinetics and their relationship with the thermal characteristics of the tank. The results show that the energy liberated during hydrogen absorption is lower than previously assumed.

9:00 AM

(MCARE-149-2012) Development of High Capacity Portable Power Systems (Invited)

T. Motyka*, Savannah River National Laboratory, USA

The specific energy densities of today's best batteries vary from 150 Wh/kg for secondary Li batteries to less than 400 Wh/kg for primary Li batteries. The US DoD and commercial portable equipment manufacturers are requesting specific energy densities greater than 1000 Wh/kg – more than 2 to 3 times that of the best primary Li batteries today. Hydrogen with the highest energy density of any fuel at 33,000 Wh/kg (more than twice that of gasoline) has the greatest potential to meet this goal. Even when coupled with a fuel cell at 50% efficiency and a hydrogen storage material with 10 wt % hydrogen, a power system with > 1,000 wh/kg is doable. A team at SRNL has been working on the development of such a high energy density portable powered systems based on aluminum hydride or alane, a light-weight, high capacity solid-state hydrogen storage material. Results from the recently completed, 2-year SRNL project wil1 be discussed including the successful design, fabrication and operation of an alane-based hydrogen storage vessel and integration of the vessel with a 150 watt commercial fuel cell.

9:20 AM

(MCARE-150-2012) Metal Hydrides for Concentrated Solar Thermal Applications (Invited)

C. E. Buckley*, D. A. Sheppard, M. P. Paskevicius, Curtin University, Australia; D. N. Harries, University of Western Australia, Australia

Solar energy is the most abundant renewable energy resource that is available and therefore logically represents the most important renewable energy resource to be focused upon. The IEA roadmap for solar energy set a target of ca. 22% of global electricity production from solar energy by 2050, with 50% being produced from concentrating solar thermal power systems. Achieving this target will be possible only if the costs of producing electricity from solar energy are significantly reduced and cost effective energy storage technologies can be developed. A major challenge is to achieve continuous, low-variability power generation from renewable energy sources, for stand-alone applications or for integration with domestic power grids. Solar mirror collection fields can collect thermal energy during the day and run a heat engine to convert it into electricity, but cannot provide power at night. However, if some of the heat is used to remove hydrogen from a metal hydride, the reverse reaction where hydrogen absorbs back into the metal hydride can then occur at night, releasing heat for power generation. This allows solar energy to provide 24 hour power generation. By combining a high temperature metal hydride with a low temperature metal hydride a coupled pair reversible metal hydride thermochemical solar energy storage system is created. I will present results on the properties of suitable low temperature hydrides.

10:20 AM

(MCARE-151-2012) Novel metal hydrides for hydrogen storage (Tutorial)

T. R. Jensen*, Aarhus University, Denmark

Hydrogen is recognized as a potential and extremely interesting energy carrier system, which can facilitate efficient utilization of unevenly distributed renewable energy. A major challenge in a future 'hydrogen economy' is the development of a safe and efficient means of hydrogen storage, in particular for mobile applications. Here we report an overview of our recent results on four different experimental approaches (i) synthesis of novel materials, (ii) tailoring materials properties, (iii) nano-confinement of hydrides and chemical reactions and (iv) in situ powder X-ray diffraction for studies of hydrogen release and uptake reactions. We have recently explored mechano-chemical and solvent based methods for synthesis of new hydrides and have discovered new series of metal borohydrides M-M'-BH4, with dense or open structures and extreme structural flexibility, e.g. Mg(BH4)2.0.80H2, 17.4 wt% H2. We will illustrate that in situ powder X-ray diffraction is a unique, sensitive and informative technique for probing gas-solid reactions. We conclude, that the chemistry of hydrogen is divers and a lot still remain to be discovered with a hope to discover the magic hydride that may become the successor of gasoline.

10:40 AM

(MCARE-152-2012) Solving the hydrogen storage challenge using metal borohydrides (Invited)

L. H. Rude*, T. R. Jensen, Aarhus University, Denmark

Metal borohydrides are considered interesting materials for energy storage in mobile applications due to their high gravimetrical hydrogen content, e.g. $LiBH_4$ contains 18.5 wt% H_2. Unfortunately, utilization of borohydrides for practical applications is often limited by unfavorable kinetics and thermodynamic properties, i.e. $LiBH_4$ release hydrogen at $T > 410$ °C ($p(H_2) = 1$ bar). However, the metal borohydrides can be modified by anion substitution in order to change the stability of the materials. Anion substitution was performed by ball milling the MBH_4 (M = Li, Na, Ca) with the corresponding metal halide, MX (X = Cl, Br, I), obtaining solid solutions in a wide compositional range. The hydrogen release temperatures for the substituted borohydride material seem to be unchanged or slightly increased, however, hydrogen uptake appear to be facilitated by anion substitution. Furthermore, three novel anion substituted structures have been solved for the $Ca(BH_4)_2$-CaI_2 system. Fluoride substitution was performed by mixing MBH_4 with the corresponding MBF_4 resulting in significantly lowered decomposition temperatures of the metal borohydride material. For the $LiBH_4$-F and $Ca(BH_4)_2$-F systems the temperature of decomposition is decreased to below 200 °C, however, the weight losses indicate the gas consists of heavier molecules than H_2. The gas released from the $NaBH_4$-F system appear to mainly consists of hydrogen.

11:00 AM

(MCARE-153-2012) Materials development contributing to a distributed energy society (Invited)

C. Nishimura*, NIMS, Japan

The Great East Japan Earthquake and Tsunami and the accompanying nuclear power plant accident have spurred a radical review of energy supply strategy in Japan. One solution to this problem is the realization of a microgrid society, which combines distributed, small-scale power generation and networks. For this, it is extremely important to achieve even high performance in rechargeable batteries, fuel cells and similar technologies in addition to utilize natural energy sources such as solar power and wind power. National Institute for Materials Science, (NIMS) has started a five-year term project, Materials for Power Generation and Storage, from April 2011. In the project, research is being promoted under four subtopics, namely, (1) solid state lithium ion batteries, (2) high temperature non-humidified polymer electrolyte fuel cells, (3) catalysts and membranes for hydrogen production, and (4) thermoelectric materials for waste heat recovery. Here I introduce recent topics of materials development in our project.

11:20 AM

(MCARE-154-2012) Magnesium-based nanomaterials for hydrogen and energy storage (Invited)

V. Yartys*, Institute for Energy Technology, Norway

High densities of hydrogen in MgH2 boosted its studies as effective H and energy storage material. Faster H exchange and tailoring the thermodynamics of the Mg-H interactions are required to suit applications. Nanostructuring of the Mg-based systems and their catalysis by the rare earth metals and Ni proved to be effective in reaching these objectives. The applied nanostructuring techniques included Reactive Ball Milling in H2, Rapid Solidification, Equal Channel Angular Pressing and powder metallurgy processing. These techniques allowed to synthesise the nanostructured La-Mg and La(Mm)-Mg-Ni H storage alloys and to modify their hydrogen storage properties. Time resolved in situ synchrotron X-ray diffraction (50 bar H2), neutron powder diffraction (1000 bar D2) and TEM were used to characterise the mechanism and kinetics of the phase-structural transformations in the materials. RS was found to cause a significant grain refinement, formation of different allotropic modifications of the alloys, and even their amorphisation. The nanostructuring increased the hydrogenation rates and decreased the stabilities of the hydrides, in some cases dramatically, by several hundred K. For the ternary AB3/A2B7 La-Mg-Ni intermetallics magnesium strongly affected the crystal structures, H storage capacities, and thermodynamics of their hydrides allowing improved performance as electrodes in the rechargeable Ni-MH batteries.

11:40 AM

(MCARE-155-2012) Mechanical Processing as Materials Preparation Tool: Alternative Energy and Related Applications (Tutorial)

V. Balema*, Aldrich Materials Science, Sigma-Aldrich Corporation, USA

The presentation addresses an experimental approach, which proved to be indispensable for the Materials Science R&D — the preparation of molecular and ionic solids using mechanical processing in the form of ball milling or grinding. Common experimental approaches and applications of mechanochemical technique in different fields of Alternative Energy are reviewed. Possible scenarios of mechanically induced chemical transformations of metals, metal hydrides, metal salts and organic solids are discussed and representative examples of the most remarkable transformations are highlighted.

Geothermal

Geothermal Systems and Applications

Room: Ballroom G
Session Chairs: Jy-An Wang, Oak Ridge National Lab; Greg Stillman, U.S. Dept. of Energy

8:00 AM

(MCARE-157-2012) Development of High Temperature Tools and Materials for Geothermal Applications (Invited)

F. Maldonado, S. Lindblom, J. Henfling*, Sandia National Laboratories, USA

The mission of the Geothermal Technologies Program at Sandia National Laboratories is to support the vision of the DOE Geothermal

Technologies Program to make geothermal energy into a major source of clean, renewable domestic baseload electricity. Towards this end Sandia National Laboratories conducts research, development and demonstration projects to enable both Enhanced Geothermal Systems (EGS) and conventional hydrothermal systems to become a major contributor for electricity generation. The high temperature electronics program area within the geothermal department conducts basic research to expand the understanding of limitations with electronics, sensors, data acquisition systems and telemetry systems for drilling diagnostics and reservoir characterization. It includes both laboratory-based component testing and evaluation and systems-level testing of electronic tools in actual geothermal wells. The Sandia high temperature electronics program includes cross-cutting elements that are of interest to a variety of industries including automotive, aerospace, energy, and process industries. This paper highlights many of the electronics and material challenges encountered when designing high temperature downhole tools. Solutions and workarounds are also presented.

8:20 AM

(MCARE-159-2012) Development of High Temperature Silicon Carbide Electronics

A. Vert*, C. Chen, A. Emad, A. Patil, A. Kashyap, T. Zhang, D. Shaddock, GE Global Research, USA; W. Johnson, Auburn University, USA

Silicon carbide based devices, sensors and integrated circuits demonstrate promising results and offer a very attractive alternative for the replacement of silicon and silicon-on-insulator (SOI) in applications where high temperature reliable operation is required. The development of high temperature electronics and ceramic-based packaging capable to survive and operate in geothermal environments with temperatures up to 300°C is the main focus of this work. Functional silicon carbide analog and digital integrated circuits and ceramic based board assemblies have been demonstrated. This study reports on the results of high temperature electronics under development demonstrating feasibility of prolonged use in harsh environment applications.

8:40 AM

(MCARE-161-2012) Harsh Environment MEMS for Energy and Power Applications

A. P. Pisano*, University of California, Berkeley, USA

In this seminar, current research and future visions will be presented for extreme harsh environment, MEMS wireless sensors fabricated from silicon carbide and aluminum nitride. These sensors are being integrated with silicon carbide electronics and aluminum nitride energy harvesting devices to build the first instance of a single-chip, self-powered, wireless sensor system. The seminar will begin with a research motivation that examines the actual flows of energy (about 100 exajoules per year) through the United States. This energy flow is approximately 85% derived from the combustion of fossil fuel, and so the seminar proceeds to outline the options for a true high-temperature sensor system (600-1000 C). The seminar then will present a series of visions of sensors that can survive combustion environments, including some prototypes that have survived 600°C, 64,000 g shocks and a jet of dry steam. A number of thin film materials, suitable for fabrication via MEMS methods will be described as candidates for application to this sensor suite. Then, a number of sensors, both existing and under development, will be presented. Integration into silicon carbide electronics will be addressed, and new research results for the fabrication and testing of silicon carbide electronic devices (both active and passive) will be presented.

9:00 AM

(MCARE-163-2012) High-Temperature Circuit Boards for Use in Geothermal Well Monitoring Applications

M. Hooker*, J. Walsh, M. Lizotte, Composite Technology Development, Inc., USA

The mapping of geothermal resources involves the design and fabrication of sensor packages, including the electronic control modules, to quantify downhole conditions (temperature, pressure, seismic activity, etc.). Because of the extreme depths at which these measurements are performed, it is most desirable to perform the sensor signal processing downhole, and then transmit the information to the surface. The temperatures at these depths present a challenge for geothermal data logging because the multilayer circuit boards onto which the electronic modules are built were not specifically designed for use under these conditions. This presentation will describe the development of high-temperature circuit board materials designed for operation at temperatures up to 300 C. These boards are based on fiber-reinforced, high-temperature polymers so that the manufacturing processes are consistent with existing manufacturing processes. The thermal and mechanical properties of these materials, as well as progress towards the fabrication of test circuits, will be presented.

9:20 AM

(MCARE-165-2012) Characterization of Low Temperature Geothermal ORC Systems Employing Non-azeotropic Working Fluid Mixtures (Invited)

A. M. Mahmoud*, A. I. ElSherbini, J. Lee, D. Luo, United Technologies Research Center, USA

The utilization of low temperature geothermal resources can be significantly increased by employing non-azeotropic working fluid mixtures in ORC systems. These working fluid mixtures exhibit temperature glide during evaporation which minimizes pinch constraints in the evaporator. In this way, increased thermal energy can be extracted from a fixed flow geothermal well thereby yielding more power generation when compared to ORC systems employing pure fluids. A rigorous ORC cycle-level analysis was conducted in the current study and suggests several benefits and challenges associated with the use of non-azeotropic working fluid mixtures in ORC systems when compared to base-line R245fa systems. Through innovative system and component design, it was shown that a 30 % net power generation gain, at least, can be attained through the use of mixed working fluids. The current study also addresses the penalty associated with the design of heat exchangers utilizing non-azeotropic working fluid mixtures. In general, the degradation of refrigerant-side heat transfer is proportional to the magnitude of saturation temperature glide during the phase change process. An accurate estimation of the heat transfer degradation and the subsequent increase in the surface area required are essential in the design of ORC systems using these mixed working fluids.

9:40 AM

(MCARE-166-2012) Metal-Organic Heat Carrier Nanofluids for Geothermal Systems (Invited)

P. McGrail*, P. K. Thallapally, J. Blanchard, S. Nune, J. Jenks, PNNL, USA

Nanofluids offer unique potential to improve efficiency of binary power plant systems without major modifications to equipment or operating conditions of the cycle. Previous nanofluids suffer from a large mismatch in particle density versus fluid density, mass/volume displacement of working fluid, and need for surfactant stabilizers, all of which tend to degrade overall performance of the system more than can be compensated by the improvement in heat transfer properties. Our approach aims to fundamentally eliminate these problems by developing metal-organic heat carriers (MOHCs), nanophase materials that interact at the molecular level with working fluids. MOHC nanofluids offer the potential to boost heat carrying capacity per kg, increase effective latent heat of vaporization, and maintain or potentially exceed the molar density of the liquid phase state of the pure working fluid. In this paper, adsorption and calorimetric results will be presented for several different prototype MOHC materials and a number of straight chain and polycyclic alkane working fluids. Permanently stable nanofluids have been demonstrated at 1 wt% loading in hexane and methanol. Capillary tube experiments prove for the first time that complete vapor-liquid phase transitions occur with MOHC nanofluids without nanoparticle deposition provided Re numbers remain at 250 or higher in the heat exchanger.

10:20 AM

(MCARE-168-2012) Quantum Dots for Use as Tracers in Geothermal Reservoirs

P. Rose*, Energy and Geoscience Institute at the University of Utah, USA; D. Riasetto, J. Siy, M. Bartl, University of Utah, USA; M. Mella, K. Leecaster, Energy and Geoscience Institute at the University of Utah, USA

The objective of this study was to characterize semiconductor colloidal quantum dots for use as tracers in geothermal reservoirs. To this end, we developed a low-temperature (50-130 °C) organometallic nucleation- and crystallization-based synthesis route for the fabrication of high-quality CdSe/CdS nanocrystals with a narrow size distribution and tunable (size-dependent) electronic and optical properties. While the inorganic semiconducting nanocrystal core delivers tunable emission colors (ranging from the visible to the NIR range), the surface chemistry of colloidal quantum dots can be independently adjusted by the choice of ligands to optimize their interaction with the geothermal reservoir rock, which possesses a negative surface charge. If anionic ligands are used, the quantum dots will resist sorption onto the fractured rock surfaces and therefore flow uninhibited through the geothermal reservoir. If weakly cationic ligands are used then the quantum dot tracers can be made to sorb reversibly and thereby serve (in combination with numerical simualtion models) to constrain fracture surface area, which is an important parameter in the design and function of an engineered geothermal system. Laboratory experiments were conducted in order to verify the predicted performance of the quantum dots under conditions that simulate a hydrothermal environment.

10:40 AM

(MCARE-170-2012) Self-degradable Cementitious Sealing Materials

T. Sugama*, T. Butcher, Brookhaven National Laboratory, USA

Objective is to develop temporary cementitious fracture sealing materials possessing self-degradable properties in Enhanced Geothermal System (EGS). The ideal sealer's self-degradation occurs when sealer heated at temperatures of ≥200°C comes in contact with water. The study centers on formulating sodium silicate-activated slag/Class C or F fly ash blend cements and investigating the ability of sodium carboxymethyl cellulose (CMC) as thermal degradable additive to promote the disintegration of sealer. We developed self-degradable slag /C or F fly ash blend cements to meet the following criteria including an initial setting time ≥60min at 85°C, compressive strength >2000 psi for 200°C autoclaved specimen, and a self-disintegration. The calcium silicate hydrate and tobermorite crystal phases, and geopolymer as amorphous phase were identified as hydrothermal reaction products responsible for developing compressive strength. Sodium hydroxide derived from hydrolysis of sodium silicate activator not only initiated the pozzolanic reaction of slag and fly ash, but also played a vital role in generating in-situ exothermic heat that significantly contributed to promoting self-degradation of cementitious sealers. The source of this exothermic heat was interactions between sodium hydroxide and gaseous reactants generated from thermal decomposition of CMC additive in an aqueous medium.

11:00 AM

(MCARE-172-2012) High Temperature, High Pressure Devices for Zonal Isolation in Geothermal Wells

J. Barker*, R. Taylor, P. Fabian, Composite Technology Development, Inc., USA

Geothermal energy offers the potential for an abundant, renewable source of power. A key barrier to the success of enhanced geothermal system (EGS) development is proper zonal isolation which will enable increased fracture stimulation for increased efficiency and other well development operations such as lost circulation material or as flow control devices. Current state-of-the-art technology cannot withstand high pressure applications at temperatures exceeding 175 °C, with the primary barrier being the poor stability of elastomeric seals in zonal isolation devices. This paper details the technology being developed by CTD to create novel high temperature, high pressure (HTHP) zonal isolation device technology. CTD's Porous Expansive Seal (PES) is a flow-delivered seal that can be used in a variety of well geometries. The porous seal utilizes high temperature porous silicone materials to expand on demand downhole and create pressure by restricting fluid flow. A porous seal concept has numerous advantages including the ability to react high pressure loads from isolation pressures into the wellbore formation over a significant surface area. The expansive nature of the PES system in addition to being delivered in small pieces allows the seal to fill highly variable well geometries such as large breakout sections or smaller loss zones, and reduce unwanted formation stress concentrations.

Hydropower

Hydropower Coatings

Room: Ballroom D

Session Chairs: Bernadette Hernandez-Sanchez, Sandia National Laboratories; Paul Savage, Brigham Young University

8:00 AM

(MCARE-175-2012) Rapid Biological Laboratory Assays for Evaluating the Performance of Antifouling Coatings and Materials Used to Construct Marine Hydrokinetic Devices (Invited)

S. J. Stafslien*, J. Daniels, J. Bahr, B. Chisholm, North Dakota State University, USA

The colonization of organisms on surfaces immersed in the marine environment, known as biofouling, can result in a number of undesirable and detrimental consequences. In the case of marine hydrokinetic (MHK) technologies, the accumulation of marine fouling can dramatically affect their overall performance, efficiency and operational lifetime. Efforts are currently underway to develop and identify new coatings and materials that can potentially be used to mitigate the occurrence of biofouling on these devices. In this regard, a suite of rapid biological laboratory assays have been utilized to quickly screen the performance of new antifouling marine coating and material technologies. A variety of marine fouling organisms, including bacteria, microalgae and adult barnacles, are maintained year round and employed in the rapid laboratory assays to assess their broad spectrum performance. Several components of the biological screening workflow have been automated through the use of commercially available and custom-built robotic equipment and instrumentation. Correlations have been established between the rapid biological laboratory assays and ocean immersion testing, demonstrating the efficacy of the biological laboratory screening workflow to aid in the development of new antifouling technologies used to construct MHK devices.

8:20 AM

(MCARE-176-2012) Immobilization of Non-Peptide Mimics of Antimicrobial Peptides on Surfaces to Prevent Bacterial Biofilm Formation

P. B. Savage*, J. Snarr, Y. Li, X. Gu, L. Gao, Brigham Young University, USA

Antimicrobial peptides (AMPs) play a central role in the innate immune function of most higher organisms, and the ubiquity of AMPs and their broad-antimicrobial activities argue that they are one of Nature's primary means of controlling microbial growth. However, use of AMPs to control bacterial growth on artificial surfaces presents problems including the high costs associated with preparing peptides on a large scale and the susceptibility of AMPs to common proteases. We have developed non-peptide mimics of AMPs, termed ceragenins, that were designed to replicate the amphiphilic morphology of AMPs. The ceragenins are readily prepared on a large scale and are not substrates for proteases. They actively kill bacteria, including established biofilms, and they can be immobilized on surfaces to prevent bacterial adhesion. A variety of chemistries can be used to attach ceragenins including siloxane chemistry, radical polymerization, and "click" reactions. Ceragenin densities on a surface can be controlled and densities of over 1015 molecules per square centimeter have been generated. The relationship between ceragenin density and bacterial biofilm prevention properties has been investigated. Results from these studies and descriptions of immobilization techniques will be presented.

8:40 AM

(MCARE-177-2012) Biofouling Resistant Coatings Based on Zwitterions and Ceragenins for Marine Hydrokinetic Devices

M. Hibbs*, Sandia National Laboratories, USA; P. B. Savage, Brigham Young University, USA; L. Vanderwal, J. Daniels, S. Stafslien, North Dakota State University, USA; B. Hernandez-Sanchez, Sandia National Laboratories, USA

Marine Hydrokinetic (MHK) Technology harnesses the ocean's energy to produce renewable electricity. To accelerate the commercialization of MHK, advances in the prevention of biofouling are required. Sandia and its partners are engaged in research to develop biofouling-resistant coatings that do not release toxins. One coating being developed is based on tethering ceragenins to a surface. Ceragenins are non-peptide mimics of antimicrobial peptides and are intended to disrupt the basic fouling sequence by preventing bacterial colonization. Other coatings are based on zwitterionic molecules which are known to be resistant to nonspecific protein and bacteria adsorption. Both coatings have been prepared and applied to metal substrates for biofouling evaluation against marine bacteria and microalgae. Results show the coatings perform similar to commercial standards in biofouling tests and are superior in easing the removal of foulants, particularly the microalgae. Analysis indicates that the surface density of ceragenins and zwitterions can be increased greatly and this is the current thrust of the project. Sandia National Laboratories is a multi-program laboratory managed and operated by Sandia Corporation, a wholly owned subsidiary of Lockheed Martin Corporation, for the U.S. Department of Energy's National Nuclear Security Administration under contract DE-AC04-94AL85000.

9:00 AM

(MCARE-178-2012) Sulfonium-Based Antibiofouling Coatings

S. M. Dirk*, M. B. Denton, M. F. Kirk, S. J. Altman, Sandia National Laboratories, USA; S. J. Stafslien, North Dakota State University, USA; B. A. Hernandez-Sanchez, Sandia National Laboratories, USA

Marine Hydrokinetic (MHK) technologies harness the energy of water as it moves and are vital in providing clean and sustainable energy. Biofouling presents a problem for MHKs as organisms cling to their surfaces, resulting in a decrease in efficiency. Coatings that ensure easy removal of organisms or prevent adhesion would ensure MHKs operate at optimal efficiency over time. A large amount of research has focused on ammonium salts, as coatings for anti-biofouling applications. Ammonium salts that contain a long chain aliphatic moiety can penetrate the microbial cell wall leading to lysis of the cell. Our work has focused on the development of an alternative type of surfactant. We have been exploring the use of a sulfonium based polymers which should have similar antimicrobial and antibacterial properties to quaternary ammonium salts. The sulfonium is linked at the benzylic position of a poly(phenylene ethylene) precursor polymer. The polymer can be transformed to a conjugated polymer with heat or UV light. Coatings prepared using this polymer should have a releasable aspect to them. As the conjugated polymer forms the attached biofilm should be lifted away from the surface. Initial results will be discussed. Sandia is a multi-program laboratory operated by Sandia Corporation, a Lockheed Martin Company, for the United States Department of Energy's National Nuclear Security Administration under contract DE-AC04-94AL85000

9:20 AM

(MCARE-179-2012) Nanobased Coatings For The Prevention Of Corrosion And Biofouling For Marine Hydrokinetic Energy

B. A. Hernandez-Sanchez*, S. Altman, M. Kirk, S. Dirk, R. Rasberry, D. Enos, Sandia National Laboratories, USA; S. J. Stafslien, North Dakota State University, USA

Advances in coatings, to prevent biofouling and corrosion, are needed to support marine hydrokinetic (MHK) device operation, performance, and reliability. MHK devices are being developed to produce renewable energy from ocean waves, tides, and thermal gradients. Due to the promise of enhanced protection, nanobased coatings are being pursued to determine performance—which is critical before they can be accepted by the MHK industry. To investigate fundamental properties, self-assembled monolayers and nanocomposites of: Ag, ZnFe2O4, CNT, CeO2, SiO2 were explored. The nanoparticles were prepared through either a solution precipitation or solvothermal route. Corrosion resistance was characterized from electrochemical impedance spectroscopy while High-Throughput and CDC reactor techniques were used to determine biofouling prevention. Results were compared to commercially available coatings. Sandia National Laboratories is a multi-program laboratory operated by Sandia Corporation, a wholly owned subsidiary of Lockheed Martin company, for the U.S. Department of Energy's National Nuclear Security Administration under contract DE-AC04-94AL85000.

10:00 AM

(MCARE-180-2012) Efficacy Testing Of Biofouling Resistant Materials For Marine Hydrokinetic Technology

S. J. Altman*, Sandia National Laboratories, USA; L. K. McGrath, LMATA Government Services LLC, USA; M. F. Kirk, Sandia National Laboratories, USA; S. J. Stafslien, North Dakota State University, USA; M. Hibbs, S. M. Dirk, K. N. Cicotte, Sandia National Laboratories, USA; M. Nagarajan, Owens Corning Science and Technology, LLC, USA; B. A. Hernandez-Sanchez, Sandia National Laboratories, USA

The ability of foul-resistant coatings to prevent biological fouling on the surfaces of Marine Hydrokinetic (MHK) energy devices was tested. MHK Technology harnesses the ocean's energy to produce renewable electricity. Biofouling makes marine and MHK devices less efficient because it increases surface roughness and drag and the frequency of maintenance. To accelerate the commercialization of MHK, advances in the prevention or reduction of biofouling is required. Sixteen different commercially available and experimental coatings were tested. Coatings were tested on different materials relevant to MHK devices. Materials were tested in a CDC biofilm growth reactor using a modified standard method (ASTM, E 2562-07) and a 'spinjet' apparatus to test fouling-release coatings. Good release properties were observed on the fouling-release coatings. Four of the coatings tested demonstrated the ability to decrease biofouling, with reductions ranging from 57% to 85%. It appears that one coating leached into the reactor solution and affected cell attachment and growth on both coated and control coupons (on average a2.8 log reduction in cell density). The tests did not demonstrate the magnitude of reduction in biofouling this project aims to achieve.

10:20 AM

(MCARE-181-2012) Evaluating the Environmental Risks of Biofouling Resistant Coatings for Marine and Hydrokinetic Technologies (Invited)

M. S. Greeley*, D. F. Glass-Mattie, M. S. Bevelhimer, Oak Ridge National Laboratory, USA

Crucial to the success of the marine and hydrokinetic (MHK) energy industry is the development of materials and coatings highly resistant to corrosion, biofouling, and fatigue, while remaining affordable, easy to manufacture, and with low toxicity to the environment. Devices utilized in the aquatic environment must be coated with an anti-biofouling agent to protect exposed areas from the attachment, growth, and colonization of aquatic organisms that can interfere with normal operation. Traditional anti-biofouling coatings contain toxic biocides such as tributyl tin, copper, or zinc demonstrated to accumulate in aquatic environs causing significant environmental and regulatory concerns. Newer anti-biofouling coatings, specifically formulated to be more environmentally-friendly while retaining efficacy, incorporate substances such as peroxides, growth repellents, pepper extracts, or various antimicrobial compounds to deter biofouling organisms, or can be self-polishing, silicone-based, or nanomaterial-based paints that create a "slick" surface that inhibits adherence and facilitates removal of any biofouling organisms that do adhere. We review the current state of knowledge of the environmental risks of anti-biofouling coatings and describe ongoing studies at the Oak Ridge National Laboratory (ORNL) into the aquatic toxicity of a variety of new and innovative coatings.

Materials Availability

Materials Availability for Alternative Energy

Room: Ballroom F
Session Chairs: Mike Tupper, Composites Technology Development; Gary Fischman, Future Strategy Solutions

8:00 AM

(MCARE-182-2012) Heterogeneous Functional Materials for Energy Storage and Conversion Systems

K. Reifsnider*, Q. Liu, F. Rabbi, U. South Carolina, USA

Batteries, fuel cells, solar cells and many other energy storage and conversion devices require multiphase functional materials that change the chemical or mechanical state of fuels, etc. The design of these heterogeneous materials is a modern grand challenge. The present paper will discuss this problem in general, and in particular, focus on dielectric material properties in the context of charge and energy storage.

8:20 AM

(MCARE-183-2012) The role of raw materials in current and emerging energy technologies

B. Achzet*, University of Augsburg, Germany

Our future energy system is highly dependent on specific metals and their provided functionalities. The availability for many of these strategic metals is highly uncertain and poses an enormous risk for the stability of our energy system. In order to handle these uncertainties several consideration levels are necessary in order to understand the complexity of raw material availability and to plan sustainable and raw material efficient products.

8:40 AM

(MCARE-184-2012) Catalyzing Alternative & Renewable Energy Research

M. Schneider*, A. Schnyder, Chemspeed Technologies AG, Switzerland

Save and Solar - process improvement, mobility, sustainability and electricity generation are pivotal fields of interest in energy research nowadays. Enhanced development of better membranes, more efficient fuel cell catalysts, biomass treatment and tailor-made conversion, hydrogen storage, lighter batteries with increased energy density, and organic photovoltaics have been boosted over the past few years by Chemspeed's high-throughput and high-output solutions. This presentation covers a selection of case studies in these fields in order to highlight the beneficial use in synthesis, process research, formulation, application and testing.

9:00 AM

(MCARE-185-2012) Preparation of Organic-modified Ceria Nanocrystals with Hydrothermal Treatment

K. Kobayashi*, M. Haneda, M. Ozawa, Nagoya Institute of Technology, Japan

Morphology control of ceria nanocrystals has attracted strong attention in both the academic and the industrial circles due to their wide-ranging application such as electrolyte materials for solid oxide fuel cells, solar cells and catalysts for environmental detoxification. For preparation of ceria nanocrystals, simple and environmentally benign routes have been required. In this study, synthesis of ceria nanocrystals has been attempted using an organic-modified precipitation method combined with a hydrothermal treatment. Cerium solution was first mixed with organic stabilizing agents to form ceria precursors. Ammonia solution was then added to the mixed solution for the precipitation of organic-modified ceria nanoparticles, followed by the hydrothermal treatment at 423-473 K. Produced organic-modified ceria nanocrystals were well dispersed in a nonpolar solvent and were hardly agglomerated. Effect of the synthetic temperature and amount of ammonia solution on the size and shape of ceria nanocrystals was investigated in detail by transmission electron microscope (TEM) observation, Raman spectroscopy and X-ray diffraction (XRD) measurement. Results obtained by the independent measurements were well consistent with each other, indicating that the nanocrystal size strongly depended on temperature of the hydrothermal treatment and that the shape was affected by the amount of ammonia solution.

9:20 AM

(MCARE-186-2012) Synthesis of Pt doped Cr2O3/Bi2O3 Hybrid photocatalysts for Hydrogen Production from Water Splitting under Visible Light Irradiation

J. Wu*, Feng Chia University, Taiwan

This study was focused on the preparation of modified bismuth oxide photocatalysts, including Ru, Cr, and Pt doped Bi2O3, using sonochemically and photodeposition assisted method to enhance their photocatalytic activity. The crystalline phase composition and surface structure of Bi2O3 photocatalysts were examined using SEM, TEM, XRD, UV-visible spectroscopy, and XPS. The photocatalytic performance of the Bi2O3 composites were evaluated with the addition of sacrificial reagent in the reactant solution. According to the experimental results, visible-light-driven photocatalysis for water splitting with the addition of 0.03 M H2C2O4 as sacrificing agents shows that Cr2O3/Pt/RuO2:Bi2O3 catalyst could effectively increase the amount of hydrogen evolution, which is around 17.2 μmol/g-h. A plausible formation mechanisms of modified bismuth oxide and reaction mechanisms of photocatalytic water splitting have been proposed in this paper.

9:40 AM

(MCARE-187-2012) Effect of spray solution flow rate on the physical properties of In2S3 grown by spray

Z. Seboui, N. Jebbari, K. T. Najoua*, Université de Tunis El Manar, Tunisia

In2S3 thin films have been successfully prepared on glass substrates using Spray pyrolysis technique. Characterization of the films was carried out by X-Ray diffraction (XRD), scanning electron microscopy (SEM) and by spectrophotometry. In this work, we study the effect of the flow rate on the physical properties of In2S3 thin films. X-ray diffraction pattern of indium sulfide thin layers reveals a polycrystalline of cubic structure with (400) preferential orientation. Optical analysis by means of transmission T(λ) and reflection R(λ) measurements allow to determine the direct band gap energy value in the order of 2.68 eV. The In2S3 thin films grown by spray pyrolysis have a big potential use as a window material for photovoltaic devices such as Au/CuInS2/In2S3/SnO2:F in which CuInS2 is used as an absorber material and SnO2:F as an ohmic contact.

10:20 AM

(MCARE-188-2012) Investigation on ammonium phosphate mixed heteropolyacid and SiO2/polymer composite membranes

U. Thanganathan*, Okayama University, Japan

Fuel cells, in general, are attractive because they provide an innovative alternative to current power sources with higher efficiencies, renewable fuels, and a lower environmental cost. The objective of the present investigation was to study the influence hybrid composite membrane as an electrolyte, and to perform an economical assessment of the utilization of proton exchange membrane fuel cells (PEMFCs) with less expensive electrolyte. This class of electrolyte is giving rise to improved cell performances and cell stabilities for PEM fuel cells operating at room temperature. The maximum power and current density was attained at low temperature with relative humidity. These results were discussed and presented in this work.

10:40 AM

(MCARE-189-2012) Mechanical and Physical Properties of Carbon S-Phase on Stainless Steel, Produced by Carbon Supersaturation

R. Hunger*, Bodycote Hardiff GmbH, Germany

While the excellent corrosion resistance of austenitic stainless steels has resulted in wide commercial application of these materials, poor tribological behaviour, especially low abrasive/adhesive wear resistance and a tendency for fretting, has prevented the use of these materials in applications where both corrosion and wear resistance are required. For more than 20 years, the Kolsterising process has offered a solution to the industry; enhanced wear properties and unaltered corrosion resistance. Suitable for austenitic and duplex stainless steels and nickel base alloys, this thermo-chemical diffusion process enriches the austenitic surface with carbon, forming a carbon supersaturated layer or carbon S-phase while avoiding the carbide precipitation that causes sensitization. This paper compares the properties of treated and untreated austenitic stainless steels. Results show improvement in wear resistance and fatigue life with Kolsterising, while corrosion resistance is unaffected.

Hydrogen

Analytical Methods and Characterization of Novel Hydrogen Storage Systems

Room: Ballroom E
Session Chairs: Thomas Gennett, NREL; Claudia Zlotea, CNRS ICMPE

1:30 PM

(MCARE-190-2012) The anelastic spectroscopy in the research on the hydrogen storage materials (Tutorial)

R. Cantelli*, Sapienza University of Rome, Italy; A. Paolone, O. Palumbo, CNR-ISC, Italy

Anelastic spectroscopy supplies the measurement of the complex elastic modulus, $M(\omega)= M'(\omega)+ jM''(\omega)$, where: i) the real part is the dynamic elastic modulus, which is very sensitive to the phase transformations and the time evolution of the chemical reactions; ii) the imaginary part gives the coefficient of elastic energy dissipation, which directly measures the jumping times and the other motion parameters of mobile species. Experimentally, anelastic spectroscopy is measured by applying extremely small external stresses to the sample which shift the energy levels of the mobile entities (atoms, lattice defects, polarons, etc.) by fractions of meV and by measuring their diffusion parameters while they are redistributing themselves among the perturbed levels by thermal activation. It will be shown that the application of this spectroscopy, which is complementary to NMR and n-scattering, to hydrogen storage materials provides essential information sometimes not obtainable by other techniques. In alanates, the first evidence was reported of H-vacancy formation in the AlH6-x units during the tetrahydride to hexahydride decomposition and of their fast dynamics; in addition, a model was proposed for the atomistic mechanism of decomposition and the role of the Ti catalyst. In ammonia borane the dynamics of the rotations and torsions of the NH3-BH3 groups were studied.

2:10 PM

(MCARE-191-2012) Lifecycle analysis of a hydrogen storage material: formation, structure, and thermal decomposition mechanisms of Al(BH4)3 - TEDA adducts

R. Lascola*, D. A. Knight, R. Zidan, Savannah River National Laboratory, USA

We have synthesized the 1:1 and 1:2 adducts of aluminum borohydride (Al(BH4)3) and the Lewis base triethylenediamine (TEDA). Thermogravimetric analysis shows that both adducts are more stable with respect to thermal decomposition than Al(BH4)3. Structural characterization by Raman spectroscopy and x-ray analysis indicates that stabilization occurs through the donation of electron density through N-Al dative bonds, leading to a more ionic character of the borohydride subunit. Uniquely, the borohydrides displaced by TEDA form dative bonds with the second N lone pair of TEDA, preserving the hydrogen storage capacity of the material. Ex situ analysis of the breakdown products allows a determination of the decomposition mechanism and provides insight towards the decomposition of the parent Al(BH4)3. These results suggest new routes for synthesis, separation, and stabilization of the high hydrogen storage capacity material Al(BH4)3.

2:30 PM

(MCARE-192-2012) Hydrogen Storage Characterization via Raman Spectroscopy

P. A. Ward*, R. N. Compton, University of Tennessee, USA

Storing hydrogen safely and efficiently is one of the most significant roadblocks for the realization of a hydrogen economy. Characterization of porous hydrogen storage materials is typically carried out with several different techniques, which require multiple instruments for analysis. Raman spectroscopy can be used to obtain useful information which would otherwise require multiple techniques. Sorption behavior can be detected by the formation of new vibrational modes (chemisorption) or by perturbations of the Q branch of free hydrogen for strong Van der Waals interactions. For materials in which binding causes a perturbation of the Q branch, the ratio of intensity of the free hydrogen to bound hydrogen at different temperatures can be used to acquire binding energies. Also, the intensity of the Q-branch of free hydrogen can be measured at multiple temperatures to determine if the material adsorbs hydrogen. Furthermore, site specific information may be obtained if the interaction is strong enough to perturb known vibrational mode of the material by comparison with quantum mechanical calculations.

2:50 PM

(MCARE-193-2012) Relaxation processes and structural changes in LiH and NaH doped fullerene for hydrogen storage (Invited)

A. Paolone*, F. Vico, CNR & Sapienza university of Rome, Italy; F. Teocoli, Sapienza University of Rome, Italy; S. Sanna, CNR & Sapienza university of Rome, Italy; O. Palumbo, CNR-ISC, Italy; R. Cantelli, CNR & Sapienza university of Rome, Italy; D. Knight, J. A. Teprovich, R. Zidan, Savannah River National Laboratory, USA

Undoped fullerene was widely studied in the past. The occurrence of a structural phase transition was revealed around 260 K from a high temperature rotationally disordered phase to a low temperature ordered structure. In the ordered phase, a relaxation process ascribed to the rotation of the C60 balls between two different configurations was detected by means of ultrasound spectroscopy. Quite recently it has been shown that LiH and NaH doped fullerene can reversibly store about 2.5 and 4.9 wt% hydrogen. Our anelastic spectroscopy measurements indicate that LiH and NaH remain dispersed in fullerene. The same experiments show that both the structural phase transition and the relaxation process due to the dynamics of the C60 units, which are clearly visible in the as prepared samples, are suppressed after hydrogen discharging and recharging. Those measurements provide evidence that the structure of doped C60 is strongly modified by hydrogenation.

3:10 PM

(MCARE-194-2012) Synthesis of SOFC electrolytes using e-beam deposition technique

D. Milcius*, Lithuanian Energy Institute, Lithuania; G. Laukaitis, K. Bockute, D. Virbukas, University of Technology, Lithuania

Today it is widely accepted that lowering the operating temperature of SOFCs in the range of 600 – 700 °C is preferable for several reasons: lowering of the operating temperature can provide higher thermodynamic efficiency, higher Nernstian voltages, enhanced durability of cell performance, and the usage of cheaper stainless steel interconnects and compliant temperature gaskets. One of the ways for lowering the cost and increasing the performance is to use as much as possible thinner electrolyte layers (by now it is 2-3 μm of range). Moreover, the electrolyte should be made not porous on the porous substrates. Different types of electrolyte materials could be used such as lanthanum gallate ceramic including lanthanum strontium gallium magnesium, bismuth yttrium oxide, barium cerate, strontium cerate, zirconium oxide or cerium oxide stabilized by rare earth oxides and etc. In the present study, different types of electrolyte thin membranes (oxygen ions and proton conductive) were deposited using e-beam deposition technique. The influence of deposition parameters, substrate temperature and post annealing at high temperatures on membrane microstructure, crystallite size, electrical properties and homogeneity were studied. The presented results are based on doped cerium oxide, zirconium oxide and lanthanum oxide thin film used as electrolytes in fuel cells investigation.

3:50 PM

(MCARE-195-2012) Best Practices in Characterizing Today's Most Advanced Hydrogen Storage Materials (Tutorial)

K. J. Gross*, H2 Technology Consulting LLC, USA

The wide variety of materials being proposed for hydrogen storage today present a number of different challenges to the researcher from an analytical characterization perspective. These include both evaluating the true performance of the materials for real-world applications as well as understanding the underlying fundamental mechanisms controlling the materials properties. An overview will be presented on the best practices for state-of-the-art characterization of thermodynamic and kinetic properties of hydrogen storage materials. Challenges to accurate measurements on particular types of materials or conditions will also be discussed.

4:10 PM

(MCARE-196-2012) Thermodynamics and Kinetics of Complex Borohydride and Amide Hydrogen Storage Materials (Invited)

A. Goudy*, H. Yang, S. Sabitu, A. Ibikunle, T. Durojaiye, S. Orefuwa, Delaware State University, USA

In this study the hydrogen storage characteristics of several new destabilized borohydride systems were determined. The mixtures included: Mg(BH4)2/Ca(BH4)2; Mg(BH4)2/CaH2/3NaH; and Mg(BH4)2/CaH2; systems as well as a bimetallic hydride MnLi(BH4)3. TPD analyses showed that the desorption temperature of Mg(BH4)2 can be lowered by ball milling it with these additives. The PCT isotherm of the resulting mixtures displayed well-defined plateau regions. These systems, however, are only partially reversible. TPD analysis also showed that a bimetallic material, MnLi(BH4)3 can release hydrogen in the range of 130 oC but the process is irreversible. Lithium amide / magnesium hydride mixtures with initial molar compositions of (LiNH2 + MgH2) and (2LiNH2 + MgH2) were also studied with and without the presence of 3.3 mol% potassium hydride dopant. TPD analyses showed that the KH doped samples had lower onset temperatures than their corresponding pristine samples. The de-hydriding kinetics of the doped and pristine mixtures was compared using a constant pressure driving force. The (LiNH2 + MgH2) mixture desorbed hydrogen faster than the (2LiNH2 + MgH2) mixture. The addition of KH dopant was found to significantly increase hydrogen desorption from the (2LiNH2 + MgH2) mixture, however it had almost no effect on the desorption rates from the (LiNH2 + MgH2) mixture.

4:30 PM

(MCARE-197-2012) Scandium-based Laves Phases for Hydrogen Storage (Invited)

M. Sahlberg*, Uppsala University, Sweden

Demands for zero greenhouse-gas emission vehicles have sharpened with today's increased focus on global warming. Hydrogen storage is a key technology for the implementation of hydrogen powered vehicles. Metal hydrides can claim higher energy densities than alternative hydrogen storage materials, but a remaining challenge is to find a metal hydride which satisfies all current demands on practical usability. The main problems are the weight of the material and the reaction energy between the metal and hydrogen. Many rare-earth based alloys have been investigated as hydrogen storage materials. However, they all suffer from a low gravimetric storage capacity. In this study, Scandium, the lightest of the rare-earth elements, has been explored from a hydrogen storage point of view. Various scandium-containing compounds and their hydrides have been investigated. The compounds were synthesized in sealed tantalum tubes or by arc melting, and investigated by in situ synchrotron radiation X-ray powder diffraction (SR-XRD), neutron powder diffraction, isothermal measurements, thermal desorption spectroscopy and electron microscopy. Samples of composition Sc1-xAx(Ni1-yBy)2 (A=Zr & B=Al, Co) were investigated for 0< x,y <1. All samples absorb large amounts of hydrogen reversibly and some even at room temperature. It is shown that both the amount of absorbed hydrogen and the reaction temperature depends strongly on the x and y ratio.

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(MCARE-198-2012) Practical low-pressure hydrogen storage from nanoscale processing of complex and chemical hydrides

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The synthesis of polymer-hydride composites through solution processing and electrospinning can provide a lightweight, flexible and safe hydrogen storage material that releases hydrogen at ambient pressure and temperatures below 100°C. At Cella Energy, a spin-out from the UK's Rutherford Appleton Laboratory, we are developing materials optimised for applications such as fuel cell portable power units, hydrogen cars and low-emission fuels. Encapsulating hydride particles with a thin polymer shell can prolong their shelf-life and safety by shielding them from air and moisture. Incorporating the hydride in a nanoscaffold lowers the hydrogen release temperature and speeds up its delivery to the application, making currently impractical hydrogen storage materials a real commercial option. Our patented method creates nanoporosity in a one-step process by electrospinning two near-miscible solutions through a concentric nozzle, forcing a phase separation followed by solidification via rapid solvent evaporation. The resulting 1-2 micron fibres or spun particles act as a scaffold for the hydride, improving hydrogen release kinetics and reducing emission of impurities. We describe the methods we have developed to select these complex solutions and optimise their miscibility, viscosity and conductivity for electrospinning, and we also explain how their properties create the nanostructure.

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(MCARE-199-2012) NMR Tool for Characterization of Materials for Hydrogen Storage Application (Tutorial)

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Nuclear Magnetic Resonance (NMR) spectroscopy is a non-destructive and quantitiatve analytical tool for characterization of structures and dynamics of chemical species in all states. Thanks to numerous advancements in detection methods and therefore analysis capability for last several decades, NMR has become a powerful and essential tool of choice and is widely utilized in studies of advanced functional materials. Structure and phase changes during hydrogenation/dehydrogenation chemical reactions of many hydrides, especially metal borohydrides, are complex and challenging to study by conventional crystallographic tools since intermediates and end products often form as amorphous phases. Due to high accessibility in probing local chemical bonds and geometries, NMR has been playing a key role in leading the characterization. In this tutorial, basic NMR principles and NMR methods are introduced and several examples of their application in studies of hydrogen storage materials, complex metal hydrides in particular, are presented.

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*** Denotes Presenter**

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