CONFERENCE PROGRAM

Materials Challenges In Alternative & Renewable Energy

February 17-20, 2014 | Hilton Clearwater Beach Resort, Clearwater, Florida, USA

Organized by:

The American Ceramic Society
www.ceramics.org

Co-organized by:

ASM International
Everything Material
The Minerals Metals & Materials Society

Endorsed by:

MRS ENDORSED MEETING

www.ceramics.org/mcare2014

Welcome

Dear Colleagues and Friends,

Welcome to the Materials Challenges in Alternative & Renewable Energy Conference (MCARE 2014). 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 two premier materials organizations - The American Ceramic Society (ACerS) and ASM International, representing the disciplines of ceramics and materials, have joined forces to co-sponsor this meeting of global importance. In addition, we are pleased to have the endorsement of the Materials Research Society (MRS).

MCARE 2014 includes eight plenary 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 Hydrogen, Solar Fuels, Solar Power and Concentrators, Batteries and Energy Storage, Nanocomposites and Nanowires in conjunction with Materials for Photovoltaic and Photonic Technologies, Nuclear, and Other Energy Issues. MCARE 2014 will also host an International Workshop on Advanced Materials Challenges for Alternative and Renewable Energy Solutions to establish new networks between researchers and entrepreneurs to create new project consortia for collaborative efforts in the framework of the European Funding Program Horizon 2020.

Building a sustainable energy system represents one of the mega-challenges of our times that has triggered a quest for alternative energy solutions both in academia and industry. 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 challenges that need to be overcome to exploit new energy solutions. 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 Toyota Research Institute North America, A-Tech, and Henkel AG & Co. and the University of Cologne, Cologne, Germany. The conference Chairs gratefully acknowledge the support of the Advisory Program Co-Chairs, Dr. George Wicks and Dr. Jack Simon for their continuous support to the organization of MCARE 2014.

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

Thanks for your participation!

The 2014 Organizing Committee:

H.T. Lin
Oak Ridge National Laboratory

Sanjay Mathur
University of Cologne, Germany

Ragaiy Zidan
Savannah River National Laboratory

Table of Contents

Final Program

MEETING REGULATIONS

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Organizing Committee

Conference Co-Chairs
H.T. Lin, Oak Ridge National Laboratory
Sanjay Mathur, University of Cologne
Ragaiy Zidan, Savannah River National Laboratory

MCARE Founders and MCARE 2014 Advisory Program Co-Chairs
George Wicks
Jack Simon

Co-Organizing Societies

The American Ceramic Society
www.ceramics.org

ASM INTERNATIONAL®
The Materials Information Society

Endorsing Societies

MRS Materials Research Society

Schedule At A Glance

Sunday – February 16, 2014

Registration	4:30 – 6 p.m.	Grand Ballroom Foyer

Monday – February 17, 2014

Registration	7 a.m. – 6 p.m.	Grand Ballroom Foyer
Welcome & Plenary Session I	8:30 a.m. – 9:20 a.m.	Salon E
Coffee Break	9:20 a.m. – 9:40 a.m.	Grand Ballroom Foyer
Concurrent Technical Sessions	9:40 a.m. – 12:00 p.m.	Salons B-C, D, E
Networking Lunch	12:00 p.m. – 1:30 p.m.	Water's Edge Ballroom
Plenary Session II	1:30 p.m. – 2:10 p.m.	Salon E
European-USA Workshop	2:00 p.m. – 6 p.m.	Salon D
Concurrent Technical Sessions	2:20 p.m. – 5:40 p.m.	Salons B-C, E, G
Coffee Break	4 p.m. – 4:20 p.m.	Grand Ballroom Foyer
Welcome Reception	6 p.m. – 7:30 p.m.	Flamingo Deck

Tuesday – February 18, 2014

Registration	7 a.m. – 5:30 p.m.	Grand Ballroom Foyer
Plenary Session III	8:20 a.m. – 9:00 a.m.	Salon E
Coffee Break	9 a.m. – 9:20 a.m.	Grand Ballroom Foyer
Concurrent Technical Sessions	9:20 a.m. – Noon	Salons B-C, D, E, G
Networking Lunch	Noon – 1:30 p.m.	Water's Edge Ballroom
Plenary Session IV	1:30 p.m. – 2:10 p.m.	Salon E
Concurrent Technical Sessions	2:20 p.m. – 6:10 p.m.	Salons B-C, D, E, G
Coffee Break	4 p.m. – 4:20 p.m.	Grand Ballroom Foyer
Poster Set up	3:30 p.m. – 5 p.m.	Water's Edge Ballroom
Poster Session & Reception	6 p.m. – 8 p.m.	Water's Edge Ballroom

Wednesday – February 19, 2014

Registration	7:30 a.m. – 6 p.m.	Grand Ballroom Foyer
Plenary Session V	8:20 a.m. – 9:00 a.m.	Salon E
Coffee Break	9 a.m. – 9:20 a.m.	Grand Ballroom Foyer
Concurrent Technical Sessions	9:20 a.m. – Noon	Salons B-C, D, E, G
Networking Lunch	Noon – 1:30 p.m.	Water's Edge Ballroom
Plenary Session VI	1:30 p.m. – 2:10 p.m.	Salon E
Concurrent Technical Sessions	2:20 p.m. – 6 p.m.	Salons B-C, D, E, G
Coffee Break	4 p.m. – 4:20 p.m.	Grand Ballroom Foyer

Thursday – February 20, 2014

Registration	7:30 a.m. – Noon	Grand Ballroom Foyer
Plenary Session VII	8:20 a.m. – 9:00 a.m.	Salon E
Coffee Break	9 a.m. – 9:20 a.m.	Grand Ballroom Foyer
Concurrent Technical Sessions	9:20 a.m. – Noon	Salons D, E, G

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MCARE 2014 SYMPOSIA	Mon AM	Mon PM	Tues AM	Tues PM	Wed AM	Wed PM	Thur AM
Li-ion Batteries I	•						
Li-ion Batteries II		•					
Li-air and Flow Batteries			•				
Sodium-ion Batteries				•			
All Solid State Batteries					•		
Supercapacitors						•	
Li-S and Li-ion Batteries							•
Catalysis in Hydrogen Materials and Systems	•						
Hydrogen Technology and Novel Application		•					
Advances in Metal and Complex Hydrides			•				
Fundmentals Studies and Hydrogen Interactions with Nano-Materials I				•			
Science and Technology of Hydrogen Adsorption				•			
Nanocomposites and Nanowires Materials for Photovoltaic and Photonic Devices I			•				
Nanocomposites and Nanowires Materials for Photovoltaic and Photonic Devices II				•			
Nanocomposites and Nanowires Materials for Photovoltaic and Photonic Devices III					•		
Nanocomposites and Nanowires Materials for Photovoltaic and Photonic Devices IV						•	
Nanocomposites and Nanowires Materials for Photovoltaic and Photonic Devices V							•
Advanced Materials for Nuclear Energy	•						
Other Energy Technologies I					•		
Other Energy Technologies II						•	
Nanostructuring and Interfacial Aspects in Photoelectrochemical Water Splitting			•				
Photonic and Plasmonic Engineering of Water Splitting Photo Catalysts				•			
Doping of TiO_2 for Efficient Water Splitting				•			
Frontiers in Materials Development for Water Splitting Photocatalysts I					•		
Materials for Water Splitting: Hematite						•	
Materials for Water Splitting: Hematite & Multiferroics						•	
Frontiers in Materials Development for Water Splitting Photocatalysts II							•
Concentrated Solar Power		•					

2014 MCARE Plenary Speakers

M. Stanley Whittingham, SUNY Distinguished Professor,
State University of New York, Stony Brook, USA
Title: The $LiFePO_4$ Story: Theory, Experiment and Characterization

Whittingham received his BA and PhD in chemistry from Oxford University. In 1972, he joined Exxon Research and Engineering Company to initiate a program in alternative energy production and storage. He discovered there the role of intercalation in battery reactions, which resulted in the first commercial lithium rechargeable batteries. After 16 years in industry, he joined the Binghamton campus as a professor of chemistry to initiate an academic program in materials chemistry. His recent work focuses on the synthesis and characterization of novel microporous and nano-oxides and phosphates for possible electrochemical and sensor applications. He was elected a Fellow of the Materials Research Society in 2013. In 2010 he received the NERM award of the American Chemical Society for his contributions to chemistry, and in 2012 he received the Yeager Award of the International Battery Association for his lifetime contributions to battery research. He is presently Director of the Northeastern Center for Chemical Energy Storage, a DOE Energy Frontier Research Center, based at Stony Brook University. He is Vice-Chair, Board of Directors of the New York Battery and Energy Storage Technology Consortium.

D. Yogi Goswami, Director, Clean Energy Research Center,
University of South Florida, USA
Title: Recent Advances in Thermal Energy Storage for Solar Thermal Power

Goswami is a University Distinguished Professor, the John and Naida Ramil Professor in the Chemical Engineering Department and Director of the Clean Energy Research Center at the University of South Florida. He conducts fundamental and applied research on Solar Thermal Energy, Thermodynamics, Heat Transfer, HVAC, Photovoltaics, Hydrogen, and Fuel Cells. Dr. Goswami has served as an advisor and given testimonies on energy policy and the transition to renewable energy to the US Congress and the Government of India, as well as providing consultant expertise to the US Department of Energy, USAID, World Bank, NIST, among others. Goswami is the Editor-in-Chief of the Solar Energy journal, and Progress in Solar Energy. Within the field of RE he has published as author/editor 16 books, 16 book chapters, 6 conference proceedings and more than 300 refereed technical papers. He has delivered 51 keynote and plenary lectures at major international conferences. He holds 18 patents.

Silke Christiansen, Helmholtz-Zentrum für Materialien und Energie, Germany
Title: Silicon Nanowire based Thin Film Solar Cell Concepts on Glass for the >15% Era

Christiansen is the Director at Helmholtz-Center (Berlin) for Materials & Energy Institute of Nanoarchitectures for Energy Conversion and Group leader at the Max-Planck Institute for the Science of Light, of an Independent Scientific Research Group for Photonic Nanostructures (Erlangen). She has over 270 peer-reviewed journal articles, 12 patents, and has presented over 120 invited presentations at professional seminars and conferences. Some of Christiansen's current scientific interests include silicon thin film solar cells; solar cells and photonic devices based on nanostructures; nanostructuring using focused ion beam technology and electron beam lithography; and vapor deposition of semiconductors and dielectrics using chemical and physical vapour deposition methods including atomic layer deposition.

Bor Z. Jang, Co-founder and CEO,
Angstron Materials, Inc. and Nanotek Instruments, Inc., USA
Title: Graphene for Electrochemical Energy Storage

Jang, currently a professor of materials engineering at Wright State University, is also a co-founder and CEO, Nanotek Instruments, Inc. and Angstron Materials, Inc. Nanotek's business focus includes the development of nano materials and energy technologies. AMI, a spin-off from Nanotek, is widely considered a leader in the production of graphene materials. Dr. Jang received his MS (1979) and PhD (1982), both in Materials Science and Engineering from MIT. He is a former professor at Auburn University, former Chairman of the Department of Mechanical Engineering and Applied Mechanics at North Dakota State University, and former Dean of the College of Engineering and Computer Science at Wright State University. He was a Fulbright Scholar and Visiting Professor in Department of Materials Science and Metallurgy, University of Cambridge, England, UK. Jang is a pioneer in graphene science and technology, discovering single-layer pristine graphene in 2002. Dr. Jang is recognized as world's No. 1 graphene inventor (>150 graphene-related patents) according to a recent IP report on graphene. He is a co-inventor of 80+ patents on battery, fuel cell, and supercapacitor. He is an author or co-author for 150+ scientific papers, 240+ patent applications. Dr. Jang's areas of research interest include mass production of graphene materials, applications of graphene (particularly for energy storage), high energy batteries, high-power batteries, and supercapacitors.

No
Photo
Available

Taek-Soo Kim, Executive Director, Professor, Korea Institute for Rare Metal; Korea Institute of Industrial Technology; University Of Science & Technology
Title: Recycling & Materialization of Rare Earths with Energy

Kim in Material Science is driving for rare materials development in both science and industry. According to his carrier in the area from 2005, he contributed to establish Korea Institute for Rare Metals (KIRAM) with KITECH and government on 2010. Most of his publication of 120 scientific papers and 20 patents includes the rare metal related issues. Industrial activity is a strong point of his carrier, since he runs various industry care and developing program in KIRAM. He also contributes to global communities of rare metals by organizing Rare material committee since 2011 in conjunction with a series of International symposium on Rare Metals hold every year and also a type of bi-lateral workshop China, Japan, Germany, and etc. In order to educate the rare metals systematically, Department of Rare Metals was firstly installed in University of Science and Technology (UST), Korea.

Suklyun Hong, Director, Graphene Research Institute and
Dean, College of Natural Sciences, Sejong University
Title: Theoretical Study of Growth and Electronic Structure of Graphene and Graphene-based Nanostructures

Hong earned his B.S. ('88) and M.S. ('90) from Seoul National University in Korea. After then, he came to US and received his Ph.D. in Physics from University of Pennsylvania in 1995. He was Research Fellow at Georgia Institute of Technology during 1995-1997 and Research Associate at Oak Ridge National Laboratory during 1997-1999. In 1999, he joined in Department of Physics at Sejong University in Korea as a faculty member, where he is now Professor of Physics and Dean of College of Natural Sciences. Since 2010, he has been Director of Graphene Research Institute of Sejong University, which is the first government-funded institute of graphene research in Korea. His research area is theoretical condensed matter physics with an emphasis on electronic and structural properties of nanoscale low-dimensional materials such as graphene and carbon nanotubes. He has published more than 70 papers in professional journals.

Chikashi Nishimura, Hydrogen Materials Unit Director and Project Leader for Materials for Power Generation & Storage, National Institute for Materials Science (NIMS), Japan

Title: Non Palladium-based Alloy membranes for Hydrogen Separation and Production

Nishimura earned his Masters ('84) and PhD ('96) from WASEDA University, Japan. Previously he was the associate director of Eco-materials Center and the managing director of the Fuel Cell Materials Center at NIMS. He spent two years as a guest professor at Huazhong University of Science and Technology, China. His research fields include materials for hydrogen energy applications, including metallic membrane materials, hydrogen storage alloys; structural intermetallics, hydrogen embrittlement in metallic materials; and hydrogen behaviors in metallic materials.

Ned Stetson, Hydrogen Storage Program Manager,
Fuel Cell Technologies Office, DOE, USA

Title: Materials Development Synergies in Alternative and Renewable Energy Technologies

Stetson is the Hydrogen Storage Program Manager in the U.S. Department of Energy's Fuel Cell Technologies Office. Dr. Stetson has over 20 years of experience in hydrogen storage materials and technology development. For the U.S. DOE, Dr. Stetson manages the portfolio of hydrogen storage projects, that includes development of low cost carbon fiber composite overwrapped pressure vessels, hydrogen storage materials development and system engineering. Prior to joining the U.S. DOE, Dr. Stetson researched complex hydrides at the University of Geneva where one of his accomplishments was the synthesis and structure determination of BaReH9, the only reported compound with higher hydrogen to non-hydrogen atom ratio greater than that of methane. Dr. 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 – these efforts resulted in the commercialization of the Portable Ovonic™ Solid Hydrogen Storage canister product line. As part of the commercialization effort, Dr. Stetson led the safety certification efforts for the products, including obtaining approvals from key regulatory authorities such as the U.S. Department of Transportation. He has also been active with code and standard developing agencies, such as the Compressed Gas Association, Society of Automotive Engineers, International Code Council and the International Standards Organization, where he has acted as the convener of the working group developing the international standard for portable metal hydride hydrogen storage systems.

Symposia

Hydrogen
Organizer: Ragaiy Zidan, Savannah River National Laboratory, USA

Solar Fuels
Organizers: J.R. Morante, Catalonia Institute for Energy Research, Spain; L. Vayssieres, Xian Jiao-Tong University, China; Dun-Wei Wang, Boston College, USA; Sanjay Mathur, University of Cologne, Germany; Menka Jain, University of Connecticut, USA; Volkmar Lüthen, Siemens, Germany; and Ravi Ravindra, New Jersey Institute of Technology, USA

Solar Power and Concentrators
Organizer: Dileep Singh, Argonne National Laboratory, USA

Batteries and Energy Storage
Organizers: Palani Balaya, National University of Singapore, Singapore; Sridhar Komarneni, Pennsylvania State University, USA; Robin von Hagen, University of Cologne, Germany; Arumugam Manthiram, University of Texas at Austin, USA; Madhavi Srinivasan, Nanyang Technical University, Singapore

Nanocomposites and Nanowires Materials for Photovoltaic and Photonic Technologies
Organizers: Yoon-Bong Hahn, Chonbuk University, Korea; S.R.P. Silva, University of Surrey, UK; Jordi Arbiol, ICREA and Institut de Ciencia de Materials de Barcelona, Spain; Qihua Xiong, Nanyang Technological University, Singapore

Nuclear
Organizers: Yutai Katoh, Oak Ridge National Laboratory, USA; Satoshi Konishi, Kyoto University, Japan

Other Energy Areas
Organizers: Sanjay Mathur, University of Cologne, Germany; H.T. Lin, Oak Ridge National Laboratory, USA

Joint EU-USA Workshop to Identify Collaborative Projects
Organizer: Sanjay Mathur, University of Cologne, Germany

Oral Presenters

Name	Date	Time	Room	Page Number
A				
Abraham, D.	17-Feb	10:20AM	Salon E	13
Adams, S.	20-Feb	10:40AM	Salon E	22
Alarcon-Llado, E.	19-Feb	10:00AM	Salon G	19
Alkali, A.	17-Feb	9:40AM	Salons B - C	13
Amaratunga, G.A.	18-Feb	9:20AM	Salon G	16
Anton, D.	19-Feb	3:00PM	Salons B - C	21
Arbiol, J.	18-Feb	3:00PM	Salon G	17
Augustynski, J.	18-Feb	9:20AM	Salon D	15
Autrey, T.	17-Feb	10:20AM	Salons B - C	13
B				
Barczuk, P.	18-Feb	5:00PM	Salon D	17
Barreca, D.	19-Feb	2:50PM	Salon D	20
Book, D.	18-Feb	10:00AM	Salons B - C	15
Brown-Shaklee, H.J.	19-Feb	5:20PM	Salon E	21
C				
Cahoon, J.	19-Feb	10:40AM	Salon G	19
Cao, J.	19-Feb	3:40PM	Salon E	20
Carlier, D.	18-Feb	5:00PM	Salon E	17
Ceh, M.	19-Feb	11:20AM	Salon G	19
Chaabane, N.	17-Feb	10:20AM	Salon D	13
Chahine, R.	18-Feb	4:50PM	Salons B - C	16
Chakrabarti, P.	18-Feb	5:40PM	Salon G	17
Christiansen, S.	17-Feb	1:35PM	Salon E	14
Corgnale, C.	17-Feb	5:20PM	Salons B - C	14
Cuentas-Gallegos, K.	19-Feb	4:20PM	Salon E	20
Curtiss, L.	18-Feb	9:20AM	Salon E	15
Cuskelly, D.	19-Feb	3:40PM	Salons B - C	21
D				
De Rango, P.	18-Feb	11:20AM	Salons B - C	15
Denton, M.	19-Feb	10:20AM	Salons B - C	19
Di Vona, M.	18-Feb	11:00AM	Salon E	15
Din, R.	17-Feb	11:20AM	Salons B - C	13
Doeff, M.	18-Feb	2:20PM	Salon E	17
Dolle, M.	19-Feb	10:00AM	Salon E	19
Dominko, R.	20-Feb	9:20AM	Salon E	22
Dong, C.	18-Feb	10:40AM	Salon D	15
F				
Fabrega, C.	18-Feb	4:20PM	Salon D	17
Filler, M.	20-Feb	9:20AM	Salon G	22
Fischer, T.	20-Feb	11:20AM	Salon D	22
Flox, C.	18-Feb	11:20AM	Salon E	15
Frantz, J.A.	20-Feb	10:40AM	Salon G	22
G				
Gaillard, J.B.	19-Feb	3:00PM	Salon E	20
Gao, L.	19-Feb	4:40PM	Salon E	21
Goenuellue, Y.	18-Feb	5:20PM	Salon D	17
Goswami, D.	17-Feb	8:45AM	Salon E	13
Gradecak, S.	18-Feb	2:20PM	Salon G	17
H				
Hamann, T.	19-Feb	2:10PM	Salon D	20
Han, S.	18-Feb	2:50PM	Salon D	16
Haverkort, J.	18-Feb	5:00PM	Salon G	17
Hong, S.	19-Feb	8:25AM	Salon E	18
I				
Idriss, H.	18-Feb	3:30PM	Salon D	16
J				
Jacques, H.	18-Feb	9:20AM	Salons B - C	15
Jang, B.Z.	18-Feb	8:25AM	Salon E	15
Jee, S.	19-Feb	11:20AM	Salon E	19
Jena, P.	18-Feb	2:10PM	Salons B - C	16
Jensen, C.M.	17-Feb	4:40PM	Salons B - C	14
Jensen, T.	18-Feb	10:40AM	Salons B - C	15
Jha, P.K.	18-Feb	3:40PM	Salon E	17
Johnson, D.C.	19-Feb	10:40AM	Salon E	19
Joya, K.	20-Feb	11:40AM	Salon D	22
K				
Kaouk, A.H.	19-Feb	2:40PM	Salons B - C	21
Kim, D.	19-Feb	5:20PM	Salon G	21
Kim, T.	18-Feb	1:35PM	Salon E	16
King, D.	17-Feb	11:00AM	Salon D	13
Knauth, P.C.	17-Feb	2:20PM	Salon E	14
Ko, M.	19-Feb	2:20PM	Salon G	21
Koel, B.E.	19-Feb	3:30PM	Salon D	20
Kubiak, P.S.	17-Feb	4:40PM	Salon G	14
Kunowsky, M.	18-Feb	5:30PM	Salons B - C	16
Kunowsky, M.	19-Feb	5:00PM	Salon E	21
L				
Lee, J.	19-Feb	10:20AM	Salon D	19
Lee, K.	18-Feb	11:20AM	Salon D	15
Lepcha, A.	20-Feb	10:40AM	Salon D	22
Liu, C.	18-Feb	4:20PM	Salon G	17
Liu, R.	18-Feb	2:10PM	Salon D	16
Lucht, B.	17-Feb	3:00PM	Salon E	14
M				
Ma, D.	18-Feb	11:20AM	Salon G	16
Maccato, C.	19-Feb	5:20PM	Salon D	20
Mahmoodi, T.	19-Feb	3:40PM	Salon G	21
Massasso, G.	17-Feb	11:20AM	Salon D	13
Mathur, S.	19-Feb	10:00AM	Salon D	19
Mayrhofer, L.	18-Feb	4:40PM	Salon D	17
Meng, S.	18-Feb	4:20PM	Salon E	17
Mettenboerger, A.	19-Feb	5:00PM	Salon D	20
Milne, S.J.	17-Feb	3:00PM	Salons B - C	14
Mohajeri, N.	17-Feb	4:20PM	Salons B - C	14
Mohd Yunos, N.	19-Feb	4:40PM	Salons B - C	21
Mohite, K.C.	20-Feb	11:20AM	Salon G	22
Mohtadi, R.	17-Feb	3:40PM	Salons B - C	14
Motyka, T.	17-Feb	3:20PM	Salons B - C	14
Mueller, R.	17-Feb	3:40PM	Salon E	14
Mukhopadhyay, A.	17-Feb	4:40PM	Salon E	15
N				
Nechache, R.	20-Feb	9:20AM	Salon D	22
Neti, S.	17-Feb	2:20PM	Salon G	14
Niederberger, M.	19-Feb	4:20PM	Salon D	20
Nishimura, C.	19-Feb	1:35PM	Salon E	20
O				
Osswald, S.	20-Feb	11:00AM	Salon E	22
Oyeleke, O.	19-Feb	5:00PM	Salon G	21
P				
Pfeifer, P.	18-Feb	5:50PM	Salons B - C	16
Post, E.	19-Feb	10:00AM	Salons B - C	19
Prochazka, J.	19-Feb	11:00AM	Salon E	19
Prochazka, J.	20-Feb	11:00AM	Salon D	22
Pundt, A.	18-Feb	3:50PM	Salons B - C	16
Q				
Quintero, F.J.	19-Feb	3:20PM	Salon E	20
R				
Ram, M.K.	19-Feb	11:40AM	Salon D	19
Ram, M.K.	19-Feb	5:40PM	Salon E	21
Rawson, A.J.	17-Feb	3:40PM	Salon G	14
Redel, E.	20-Feb	11:00AM	Salon G	22
Ren, Z.	20-Feb	10:00AM	Salon G	22
Rhee, S.	19-Feb	3:00PM	Salon G	21
Rho, W.	19-Feb	11:40AM	Salon G	19
Robayo, M.D.	19-Feb	10:40AM	Salons B - C	20
Robertson, R.	19-Feb	9:20AM	Salons B - C	19
Rojo, T.	18-Feb	3:00PM	Salon E	17

Presenting Author List

Oral Presenters

Name	Date	Time	Room	Page Number
Rokhvarger, A.	17-Feb	10:40AM	Salon D	13
Rokhvarger, A.	18-Feb	3:40PM	Salon G	17
Ronchetti, C.	19-Feb	11:20AM	Salons B - C	20

S

Name	Date	Time	Room	Page Number
Sauder, C.	17-Feb	9:40AM	Salon D	13
Scheicher, R.H.	18-Feb	4:30PM	Salons B - C	16
Selvamanickam, V.	17-Feb	5:00PM	Salon G	14
Sharma, N.	17-Feb	4:20PM	Salon E	15
Silva, S.P.	19-Feb	9:20AM	Salon G	19
Singh, D.	17-Feb	3:00PM	Salon G	14
Sisson, R.	20-Feb	11:20AM	Salon E	22
Solarska, R.	19-Feb	11:00AM	Salon D	19
Sopori, B.	17-Feb	4:20PM	Salon G	14
Stein, A.	19-Feb	9:20AM	Salon E	19
Stetson, N.	20-Feb	8:25AM	Salon E	21
Sun, J.	17-Feb	5:20PM	Salon E	15

T

Name	Date	Time	Room	Page Number
Takechi, K.	18-Feb	10:00AM	Salon E	15
Teprovich, J.A.	18-Feb	2:50PM	Salons B - C	16
Terracciano, A.C.	19-Feb	3:20PM	Salons B - C	21
Tirado, J.L.	17-Feb	11:00AM	Salon E	13
Tyagi, D.	17-Feb	11:00AM	Salons B - C	13

V

Name	Date	Time	Room	Page Number
Van der Ven, A.	17-Feb	9:40AM	Salon E	13
van Hassel, B.A.	17-Feb	2:20PM	Salons B - C	14
Vayssieres, L.	18-Feb	10:00AM	Salon D	15
Vidu, R.	19-Feb	11:00AM	Salons B - C	20
Vinu, A.	19-Feb	2:20PM	Salon E	20

W

Name	Date	Time	Room	Page Number
Wang, D.	17-Feb	11:40AM	Salon E	13
Wang, D.	19-Feb	9:20AM	Salon D	19
WANG, Y.	18-Feb	10:40AM	Salon E	15
Westin, G.	20-Feb	10:00AM	Salon D	22
Whittingham, S.	17-Feb	8:10AM	Salon E	13
Winarski, R.	17-Feb	5:00PM	Salon E	15
Winkler, P.	19-Feb	2:20PM	Salons B - C	21
Wu, N.	18-Feb	10:00AM	Salon G	16

X

Name	Date	Time	Room	Page Number
Xiao, J.	20-Feb	10:00AM	Salon E	22
Xie, K.	20-Feb	11:40AM	Salon E	22
Xue, C.	18-Feb	10:40AM	Salon G	16

Y

Name	Date	Time	Room	Page Number
Yakup, G.	19-Feb	11:20AM	Salon D	19

Z

Name	Date	Time	Room	Page Number
Zhang, P.	17-Feb	10:00AM	Salons B - C	13
Zhang, P.	18-Feb	11:40AM	Salon E	16
Zhao, W.	17-Feb	3:20PM	Salon G	14
Zhu, H.	19-Feb	4:20PM	Salon G	21
Zlotea, C.	18-Feb	3:10PM	Salons B - C	16
Zou, G.	19-Feb	4:20PM	Salons B - C	21

Poster Presenters

Name	Date	Time	Room	Page Number
Avellaneda, C.O.	18-Feb	6:00PM	Waters Edge Ballroom	18
Barman, M.	18-Feb	6:00PM	Waters Edge Ballroom	18
Barreca, D.	18-Feb	6:00PM	Waters Edge Ballroom	18
Bateni, A.	18-Feb	6:00PM	Waters Edge Ballroom	18
Beaman, B.T.	18-Feb	6:00PM	Waters Edge Ballroom	18
Buyanova, I.A.	18-Feb	6:00PM	Waters Edge Ballroom	18
Carreno, N.L.	18-Feb	6:00PM	Waters Edge Ballroom	18
Chen, Y.	18-Feb	6:00PM	Waters Edge Ballroom	17
Dangerfield, A.	18-Feb	6:00PM	Waters Edge Ballroom	17
Gou, Y.	18-Feb	6:00PM	Waters Edge Ballroom	18
Han, S.	18-Feb	6:00PM	Waters Edge Ballroom	18
Henderson, J.	18-Feb	6:00PM	Waters Edge Ballroom	18
Hughes, B.	18-Feb	6:00PM	Waters Edge Ballroom	18
Jian, K.	18-Feb	6:00PM	Waters Edge Ballroom	18
Ji Yea, L.	18-Feb	6:00PM	Waters Edge Ballroom	18
Jones, M.	18-Feb	6:00PM	Waters Edge Ballroom	17
Kaunisto, K.	18-Feb	6:00PM	Waters Edge Ballroom	18
Lebedeva, L.	18-Feb	6:00PM	Waters Edge Ballroom	18
Lee, Y.	18-Feb	6:00PM	Waters Edge Ballroom	18
Maccato, C.	18-Feb	6:00PM	Waters Edge Ballroom	18
Meda, L.	18-Feb	6:00PM	Waters Edge Ballroom	17
Rho, W.	18-Feb	6:00PM	Waters Edge Ballroom	18
Shao, C.	18-Feb	6:00PM	Waters Edge Ballroom	18
Sharma, S.	18-Feb	6:00PM	Waters Edge Ballroom	18
Shin, Y.	18-Feb	6:00PM	Waters Edge Ballroom	18
Sinha, R.	18-Feb	6:00PM	Waters Edge Ballroom	18
Song, X.	18-Feb	6:00PM	Waters Edge Ballroom	18
Wang, J.	18-Feb	6:00PM	Waters Edge Ballroom	18
Wang, Y.	18-Feb	6:00PM	Waters Edge Ballroom	18
Yang, H.	18-Feb	6:00PM	Waters Edge Ballroom	18

register now!

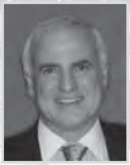
APRIL 7–9, 2014 | BALTIMORE, MD

Where Business and Manufacturing Meet Strategy

confirmed speakers

Andy Zynga, CEO, NineSigma, *Connecting with the Outside World to Advance Your Company's Technology and Product Innovation*

Katharine Frase, VP, CTO, Global Public Sector, IBM Corporation, *Technology Trends*



Al T. Lubrano, Chairman, NAM's Small to Medium Manufacturers, *Manufacturing Competitiveness: How We Can Improve It*

James P. Meil, VP, chief economist, Eaton, *Global Business Climate*

Frank O'Brien-Bernini, VP, chief sustainability officer, Owens Corning, *Manufacturing and Sustainability*

Eric Urruti, VP, research & technology development, SCHOTT NA, *Finding and Developing Engineering Talent*

Petra Mitchell, President and CEO, Catalyst Connection

Marty Curran, Executive vice president and chief innovation officer, Corning Incorporated

Anthony Nickens, Vice president energy & new business, Ceramatec, Inc.

Lora Cooper-Rothen, CEO, Du-Co Ceramics Company

Wayne G. Butscher, Director, BioSTART and Lab Associates Program, BioTechnical Institute of Maryland, Inc.

R. Allen Kimel, Assistant professor, Pennsylvania State University

Greg Morris, Lead, strategy and business development for additive technologies, GE Aviation

Richard Norment, Executive director, National Council for Public-Private Partnerships

Dick K. Brow, Curators' Professor of Ceramic Engineering, Missouri University of Science & Technology

Steven Richey, Partner, Thompson Coburn LLP

topics covered

- Business climate overview
- Manufacturing and sustainability
- Finding and developing engineering talent
- Additive manufacturing technology
- Innovative partnerships and business models
- Innovation, intellectual property, and the America Invents Act
- Material sourcing challenges and strategies
- Navigating the current regulatory landscape
- Developing/Improving business practices
- Forming university, government and corporate partnerships to build a competitive workforce
- ACerS role in helping to develop technical talent

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submit abstracts by march 17th

3RD INTERNATIONAL CONFERENCE ON ELECTROSPINNING

August 4-7, 2014 | Westin San Francisco | San Francisco, CA

Electrospin 2014 is a biennial event created to provide a platform for researchers, engineers and students to exchange knowledge and advance the field of electrospinning, nanomaterials and their applications. The conference topics will address theory, all materials including polymers, metals and ceramics, applications in energy storage and harvesting, filtration, materials for sustainability, biomedical applications and more. Special focus will be given to the fast growing field of ceramic nanomaterials. Submit your abstract by March 17th to present.

Proposed Sessions:

- Advances in electrospinning theory and modeling
- Energy storage and harvesting with electrospun or sprayed materials
- Novel developments in electrospinning and other nano fiber fabrication technologies
- Ceramic and composite nanofibers
- Polymer nanofibers
- Biomedical applications of electrospun materials
- Filtration and textiles
- Electrospinning for green materials and sustainability

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Monday, February 17, 2014

Plenary Session I
Room: Salon E

8:00 AM

Opening Remarks, Sanjay Mathur

8:10 AM

(MCARE-PL1-2014) The $LiFePO_4$ Story: Theory, Experiment and Characterization
F. Omenya, N. Chernova, SUNY, USA; A. Abdellahi, G. Ceder, MIT, USA; S. Whittingham*, SUNY, USA

8:45 AM

(MCARE-PL2-2014) Recent Advances in Thermal Energy Storage for Solar Thermal Power
D. Yogi Goswami*, University of South Florida, USA

9:20 AM

Break

Hydrogen

Catalysis in Hydrogen Materials and Systems
Room: Salons B - C
Session Chairs: Claudia Zlotea, CNRS ICMPE; David Book, University of Birmingham

9:40 AM

(MCARE-160-2014) Hydrogen Separation & Purification Using Composite Palladium Membranes in a Catalytic Membrane Reactor
A. Alkali*, E. Gobina, Robert Gordon University, United Kingdom

10:00 AM

(MCARE-161-2014) Ni-SiO2 based Nanocomposite for Methane Dry Reforming Catalysis
P. Zhang*, X. Song, L. Gao, Shanghai Jiao Tong University, China

10:20 AM

(MCARE-162-2014) Reversible hydrogen activation in molecular complexes: approaches to catalysis and energy storage using amine boranes (Invited)
T. Autrey*, D. Camaioni, M. Bowden, A. Karkamkar, S. Whittemore, Pacific Northwest National Laboratory, USA

11:00 AM

(MCARE-163-2014) Role of Carbon support on Activity and Stability of Pt/C catalyst for Hydrogen production by S-I thermochemical cycle
D. Tyagi*, S. Varma, S. R. Bharadwaj, Bhabha Atomic Research Centre, India

11:20 AM

(MCARE-164-2014) Enhanced hydrogen storage performances of MgH2–NaAlH4 system catalyzed by TiO2 nanoparticles
R. Din*, Pakistan Institute of Nuclear Science and Technology Nilore Islamabad, Pakistan; Q. Xuanhui, University of Science and Technology Beijing, Hadian District, China

Batteries and Energy Storage

Li-ion Batteries I
Room: Salon E
Session Chairs: Palani Balaya, National University of Singapore; Donghai Wang, Penn State University

9:40 AM

(MCARE-065-2014) New electrochemical energy storage concepts (Invited)
A. Van der Ven*, University of California, Santa Barbara, USA

10:20 AM

(MCARE-066-2014) Diagnostic examination of high-energy Li-ion cells containing alumina-coated Li1.2Ni0.15Mn0.55Co0.1O2-based positive electrodes (Invited)
D. Abraham*, Argonne National Laboratory, USA

11:00 AM

(MCARE-067-2014) Nanostructured transition metal oxides prepared at moderate temperatures as Li- and Na-ion battery materials (Invited)
M. C. López, Universidad de Córdoba, Spain; G. F. Ortiz, Universidad de Córdoba, Spain; P. Lavela, Universidad de Córdoba, Spain; R. Alcántara, Universidad de Córdoba, Spain; J. L. Tirado*, Universidad de Córdoba, Spain

11:40 AM

(MCARE-068-2014) Integrating Si Nanoparticles to Structured Micro-sized Composites for Electrochemical Energy Storage (Invited)
D. Wang*, Penn State University, USA

Nuclear

Advanced Materials for Nuclear Energy
Room: Salon D
Session Chair: Yutai Katoh, Oak Ridge National Lab

9:40 AM

(MCARE-135-2014) Accident Tolerant Fuel cladding based on SiC/SiC composites for LWRs (Invited)
C. Sauder*, A. Michaux, J. Braun, P. Billaud, G. Loupias, CEA, France

10:20 AM

(MCARE-136-2014) Ion Beam Irradiated Silicon Carbide Composites
N. Chaabane*, M. Le Flem, T. Vandenberghe, CEA, France; C. Sandt, P. Dumas, Synchrotron-SOLEIL, France; Y. Serruys, CEA, France

10:40 AM

(MCARE-137-2014) Development of the full dense sintered MgAl2O4 ceramics for permanently safe containerization of nuclear solid waste
A. Rokhvarger*, E. Vaughn-Flam, Rokon Systems, Inc., USA

11:00 AM

(MCARE-138-2014) Plasma Arc Welding of ZrB_2 20 vol.% ZrC and $Zr^{11}B_2$
D. King*, J. Lonergan, G. Hilmas, W. Fahrenholtz, Missouri University of Science and Technology, USA

11:20 AM

(MCARE-139-2014) Entrapment of molecular iodine produced in nuclear industry with the Hofmann's clathrate Ni(pz)Ni(CN)4 where pz = pyrazine, and analogues
G. Massasso*, Y. Guari, J. Larionova, J. Long, J. Haines, G. Maurin, S. Devautour, Institut Charles Gerhardt, France; A. Grandjean, Institut de Chimie Séparative de Marcoule, France; B. Onida, Politecnico di Torino, Italy

Plenary Session II

Room: Salon E

1:30 PM

Introduction

1:35 PM

(MCARE-PL3-2014) Silicon Nanowire based Thin Film Solar Cell Concepts on Glass for the >15% Era

S. Christiansen*, Helmholtz-Zentrum für Materialien und Energie, Germany; S. Schmitt, S. Jaeckle, C. Tessarek, G. Sarau, M. Heilmann, M. Latzel, M. Goebelt, G. Shalev, M. Bashouti, A. Mahmoud, Max Planck Institute for the Science of Light, Germany; K. Hoeflich, Helmholtz-Zentrum für Materialien und Energie, Germany

Hydrogen

Hydrogen Technology and Novel Application

Room: Salons B - C

Session Chairs: Claudio Corgnale, Savannah River National Laboratory; Huot Jacques, UQTR

2:20 PM

(MCARE-153-2014) Engineering Technologies for Fluid Chemical Hydrogen Storage System (Invited)

B. A. van Hassel*, R. McGee, A. Murray, S. Zhang, United Technologies Research Center, USA

3:00 PM

(MCARE-154-2014) Improving the High-temperature Durability of CO2 Sorbents for H2 Production by Steam Reforming of Biomass

S. J. Milne*, M. Zhao, A. Brown, V. Dupont, University of Leeds, United Kingdom

3:20 PM

(MCARE-155-2014) Low-cost Metal Hydride-based Thermal Energy System for High Temperature Solar Power Plants (Invited)

T. Motyka*, C. Corgnale, B. Hardy, R. Zidan, J. Teprovich, B. Peters, SRNL, USA

3:40 PM

(MCARE-156-2014) Borohydrides Based Electrolytes for Rechargeable Magnesium Batteries (Invited)

R. Mohtadi*, F. Mizuno, T. S. Arthur, Toyota Research Institute of North America, USA; S. Hwang, California Institute of Technology, USA

4:20 PM

(MCARE-157-2014) Intellipigment™, Chemochromic Pigments for Hydrogen Leak Detection

N. Mohajeri*, HySense Technology, LLC, USA

4:40 PM

(MCARE-159-2014) Update on Hydrogen Storage Research and Development Activities in Hawaii (Invited)

D. Birkmire, M. Chong, E. Sadeghmoghaddam, University of Hawaii at Manoa, USA; D. Brayton, A. Narvaez, Hawaii Hydrogen Carriers, LLC, USA; C. M. Jensen*, University of Hawaii at Manoa, USA

5:20 PM

(MCARE-158-2014) Acceptability envelope for adsorption based hydrogen storage (Invited)

B. Hardy, C. Corgnale*, D. Tamburello, D. Anton, Savannah River National Laboratory, USA

Solar Power and Concentrators

Concentrated Solar Power

Room: Salon G

Session Chair: Dileep Singh, Argonne National Laboratory

2:20 PM

(MCARE-056-2014) Thermal Energy Storage at High Temperatures (Invited)

S. Neti*, Lehigh University, USA

3:00 PM

(MCARE-057-2014) Development of a High-Temperature High-Efficiency Thermal Energy Storage System for Concentrated Solar Power

D. Singh*, T. Kim, D. France, W. Yu, Argonne National Laboratory, USA; A. Gyekenyesi, M. Singh, Ohio Aerospace Institute, USA

3:20 PM

(MCARE-058-2014) Heat Transfer Characteristics of Graphite Foam-MgCl2 Thermal Energy Storage Systems for Concentrated Solar Power

W. Zhao*, Argonne National Laboratory, USA; D. M. France, University of Illinois at Chicago, USA; W. Yu, T. Kim, D. Singh, Argonne National Laboratory, USA

3:40 PM

(MCARE-059-2014) Miscibility Gap Alloys for High Energy Density and Thermal Conductivity Heat Storage

A. J. Rawson*, H. Sugo, E. Kisi, The University of Newcastle, Australia

4:00 PM

Break

4:20 PM

(MCARE-060-2014) PV Optics: Analytical Software for Optical Management and Light Trapping in Solar Cells and Modules (Invited)

B. Sopori*, National Renewable Energy Lab, USA; J. Mutitu, W. Shafarman, University of Delaware, USA

4:40 PM

(MCARE-062-2014) Chemical and Thermal Stability of Molten Nitrate Salts as High Temperature Fluids

P. S. Kubiak*, University of Central Florida, USA; N. Mohajeri, Florida Solar Energy Center, USA; O. S. Ahmed, Y. Sohn, University of Central Florida, USA

5:00 PM

(MCARE-064-2014) Thin film III-V photovoltaics on low-cost, flexible metal substrates using single-crystalline-like Germanium films

V. Selvamanickam*, P. Dutta, Y. Gao, Y. Yao, R. Wang, M. Rathi, E. Galtsyan, University of Houston, USA; P. Ahrenkiel, South Dakota School of Mines and Technology, USA; A. Mehrotra, A. Freundlich, University of Houston, USA

Batteries and Energy Storage

Li-ion Batteries II

Room: Salon E

Session Chairs: Robin von Hagen; Neeraj Sharma, The University of New South Wales (UNSW)

2:20 PM

(MCARE-087-2014) Towards lithium ion 3D microbatteries using TiO2 nanotubes (Invited)

P. C. Knauth*, T. Djenizian, Aix Marseille University-CNRS, France

3:00 PM

(MCARE-070-2014) Role of Solution Structure in Solid Electrolyte Interface (SEI) Formation on Graphite (Invited)

B. Lucht*, University of Rhode Island, USA

3:40 PM

(MCARE-071-2014) Graphene Oxide/M2+ Redox Reactions – A Pathway towards Graphene-based Electrode Materials

R. Mueller*, R. von Hagen, R. Raccis, S. Mathur, University of Cologne, Germany

4:00 PM

Break

4:20 PM

(MCARE-072-2014) Electrochemical-structural relationships probed by in-situ neutron and X-ray diffraction (Invited)
N. Sharma*, The University of New South Wales (UNSW), Australia

4:40 PM

(MCARE-073-2014) Stress associated with surface phenomenon in electrode materials for Li-ion Batteries (Invited)
A. Mukhopadhyay*, R. Kali, Indian Institute of Technology (IIT) Bombay, India; A. Tokranov, B. Sheldon, Brown University, USA; X. Xiao, General Motors R&D Centre, USA

5:00 PM

(MCARE-074-2014) Nanoscale X-ray Imaging of Advanced Battery Electrodes
R. Winarski*, B. Blaiszik, F. Brushett, L. Trahey, V. Rose, C. Johnson, Argonne National Laboratory, USA

5:20 PM

(MCARE-075-2014) Synthesis of α-Fe2O3 Nanoparticles from Fe(OH)3 Sol and the Hybrids with Reduced Graphene Oxide for Lithium Ion Batteries
J. Sun*, M. Du, C. Xu, Shanghai Institute of Ceramics, Chinese Academy of Science, China; L. Gao, School of Materials Science and Engineering, Shanghai Jiao Tong University, China

Tuesday, February 18, 2014

Plenary Session III

Room: Salon E

8:20 AM

Introduction

8:25 AM

(MCARE-PL4-2014) Graphene for Electrochemical Energy Storage
B. Z. Jang*, Angstron Materials, Inc. and Nanotek Instruments, Inc., USA

9:00 AM

Break

Hydrogen

Advances in Metal and Complex Hydrides

Room: Salons B - C

Session Chairs: Joseph Teprovich, Savannah River National Laboratory; Ralph Scheicher, Uppsala University

9:20 AM

(MCARE-172-2014) The formation reaction and the hydrogen storage properties of Mg2FeH6 (Invited)
A. Asselli, H. Jacques*, UQTR, Canada

10:00 AM

(MCARE-173-2014) Hydrogen storage in borohydride and Mg-based materials (Invited)
D. Book*, X. Yi, S. Guo, A. Walton, D. Reed, University of Birmingham, United Kingdom

10:40 AM

(MCARE-174-2014) Novel multi-purpose metal borohydrides (Invited)
T. Jensen*, Aarhus University, Denmark

11:20 AM

(MCARE-175-2014) Evolution of the physico-chemical properties of nanostructured MgH2 composites upon hydrogen cycles (Invited)
P. De Rango*, S. Nachev, D. Fruchart, CNRS, France; N. Skryabina, Perm State University, Russian Federation; P. Marty, Université Joseph Fourrier, France

Solar Fuels

Solar Fuels: Nanostructuring and Interfacial Aspects in Photoelectrochemical Water Splitting

Room: Salon D

Session Chairs: Hicham Idriss, SABIC; Ru-Shi Liu, National Taiwan University

9:20 AM

(MCARE-027-2014) To what extent the nanostructuring of metal oxide photo-electrodes affects their water splitting efficiency? (Invited)
J. Augustynski*, R. Solarska, P. Barczuk, K. Bienkowski, University of Warsaw, Poland

10:00 AM

(MCARE-028-2014) Advances in quantum confinement effects and interfacial electronic structure for solar water splitting (Invited)
L. Vayssieres*, Xian Jiaotong University, China

10:40 AM

(MCARE-029-2014) In-situ soft x-ray spectroscopy study of mesoscale interfacial phenomena in solar fuel generation (Invited)
J. Guo, Lawrence Berkeley Natl Lab, USA ; C. Dong*, National Synchrotron Radiation Research Center, Taiwan

11:20 AM

(MCARE-030-2014) Self-Powered Flexible Electronic Systems (Invited)
K. Lee*, Korea Advanced Institute of Science and Technology, Republic of Korea

Batteries and Energy Storage

Li-air and Flow Batteries

Room: Salon E

Session Chairs: Madhavi Srinivasan, Nanyang Technical University; Yuxi WANG, TUM CREATE

9:20 AM

(MCARE-076-2014) Insights into Discharge and Charge Chemistries in Li-O2 Batteries from Theory and Experiment (Invited)
L. Curtiss*, K. Amine, Argonne National Laboratory, USA

10:00 AM

(MCARE-077-2014) Recent Development of Lithium Air Battery using Ionic Liquid Based Electrolyte (Invited)
K. Takechi*, Toyota Central R&D Labs., Inc., Japan

10:40 AM

(MCARE-078-2014) A Novel Refuelable Lithium Battery based on Anodic Lithium Solvated Electrons Solution (Invited)
Y. WANG*, TUM CREATE, Singapore; R. Yazami, K. Tan, Nanyang Technological University, Singapore

11:00 AM

(MCARE-079-2014) Anion-conducting ionomer membranes for redox flow batteries
M. Di Vona*, Univ. Rome Tor Vergata, Italy; P. C. Knauth, Aix Marseille University-CNRS, France

11:20 AM

(MCARE-080-2014) Nano-structured carbon-based electrodes materials for high-performance vanadium redox battery
C. Flox*, C. Fabrega, M. Skoumal, T. Andreu, J. R. Morante, Catalonian Institute for Energy Research, Spain

11:40 AM

(MCARE-081-2014) Organic-inorganic hybrid anion conducting materials for alkaline fuel cell

P. Zhang*, K. Miyajima, Noritake Co., Limited, Japan; T. Yamaguchi, Tokyo Institute of Technology, Japan; A. Gopinathan M., Noritake Co., Limited, Japan

Nanocomposites and Nanowires Materials for Photovoltaic and Photonic Technologies

Nanocomposites and Nanowires Materials for Photovoltaic and Photonic Devices I

Room: Salon G

Session Chairs: S. Ravi Silva, University of Surrey; Can Xue, Nanyang Technological University

9:20 AM

(MCARE-108-2014) Nanotube and nanowire photonics for photovoltaic devices

G. A. Amaratunga*, H. Butt, T. Butler, R. Rajashekaran, H. Zhou, P. Hiralal, Q. Dai, T. D. Wilkinson, University of Cambridge, United Kingdom

10:00 AM

(MCARE-109-2014) Plasmonic Metal-Semiconductor Nanostructures for Solar Energy Conversion (Invited)

N. Wu*, West Virginia University, USA

10:40 AM

(MCARE-110-2014) Metal-TiO2 Composite Nanofibers for Plasmon-Enhanced Solar-to-Hydrogen Conversion (Invited)

C. Xue*, Z. Zhang, Nanyang Technological University, Singapore

11:20 AM

(MCARE-111-2014) Designing Plasmonic Nanostructures and Quantum Dots for Solar Cell Applications (Invited)

D. Ma*, INRS, Uni Quebec, Canada

Plenary Session IV

Room: Salon E

1:30 PM

Introduction

1:35 PM

(MCARE-PL5-2014) Recycling and materialization of rare earths with energy sustainability

H. Chae, H. Choi, S. Kim, B. Kim, T. Kim*, Korea Institute of Industrial Technology, Republic of Korea

Hydrogen

Fundamentals Studies and Hydrogen Interactions with Nano-Materials

Room: Salons B - C

Session Chairs: Bart van Hassel, United Technologies Research Center; Rana Mohtadi, Toyota Research Institute of North America

2:10 PM

(MCARE-168-2014) Nano Materials for Hydrogen Storage (Invited)

P. Jena*, Virginia Commonwealth University, USA

2:50 PM

(MCARE-169-2014) Elucidation of Hydride Interaction with Carbon Nanostructures and the Formation of Novel Nanocomposites for Energy and Storage Devices (Invited)

J. A. Teprovich*, H. Colon-Mercado, B. Peters, R. Zidan, Savannah River National Laboratory, USA

3:10 PM

(MCARE-170-2014) Nanoconfined hydrides for hydrogen storage and electrochemical conversion (Invited)

C. Zlotea*, Y. Oumellal, S. Bastide, C. Cachet-Vivier, CNRS ICMPE UPEC, France; C. Matei Ghimbeu, C. Vix-Guterl, CNRS IS2M, France; M. Latroche, CNRS ICMPE UPEC, France

3:50 PM

(MCARE-171-2014) Measure hydrogen distribution in nano-sized metals: hydrogen microscopy techniques (Invited)

A. Pundt*, University of Goettingen, Germany

4:30 PM

(MCARE-172-2014) Effect of uniaxial strain on the site occupancy of hydrogen in vanadium: density-functional calculations (Invited)

R. Johansson, R. Ahuja, O. Eriksson, B. Hjörvarsson, R. H. Scheicher*, Uppsala University, Sweden

Science and Technology of Hydrogen Adsorption

Room: Salons B - C

Session Chairs: Patricia De Rango, CNRS; Theodore Motyka, SRNL

4:50 PM

(MCARE-167-2014) Tutorial on Sorption Storage (Invited)

R. Chahine*, P. Bénard, D. Cossement, R. Zacharia, J. Xiao, Hydrogen Research Institute, Canada

5:30 PM

(MCARE-165-2014) Dense Carbon Monoliths for High Pressure Gas Adsorption

M. Kunowsky*, J. Marco-Lozar, F. Suárez-García, Universidad de Alicante, Spain; J. Carruthers, ATMI, Adsorbent & Gas Technology, USA; ÁNGEL. Linares-Solano, Universidad de Alicante, Spain

5:50 PM

(MCARE-166-2014) Hydrogen densities greater than liquid hydrogen at 77 K in engineered carbon nanospaces

P. Pfeifer*, University of Missouri, USA; A. Gillespie, University of Missouri, USA; E. Dohnke, University of Missouri, USA; Y. Soo, University of Missouri, USA

Solar Fuels

Solar Fuels: Photonic and Plasmonic Engineering of Water Splitting Photo Catalysts

Room: Salon D

Session Chairs: Leonhard Mayrhofer, Fraunhofer IWM; Jan Augustynski, University of Warsaw

2:10 PM

(MCARE-031-2014) Plasmon-enhanced Upconversion Nanoparticles in Photoelectrochemical Water Splitting (Invited)

R. Liu*, C. Chen, C. Chen, National Taiwan University, Taiwan; S. Hu, National Taiwan Normal University, Taiwan

2:50 PM

(MCARE-032-2014) Local structural and chemical property changes of Pt and Pd nanoparticles during catalysis (Invited)

S. Han*, E. Jeong, C. Park, I. Hwang, Z. Jin, J. Park, Chonbuk National University, Republic of Korea

3:30 PM

(MCARE-033-2014) Hydrogen production from water; the effect of photonic and plasmonic properties (Invited)

V. Jovic, University of Auckland, New Zealand; K. Wahab, O. Maher, SABIC-CRI, Saudi Arabia; G. Waterhouse, University of Auckland, New Zealand; J. Llorca, UPC, Spain; H. Idriss*, SABIC-CRI, Saudi Arabia

4:10 PM

Break

Solar Fuels: Doping of TiO2 for Efficient Water Splitting

Room: Salon D

Session Chairs: Lionel Vayssieres, Xian Jiaotong University; Sang-Wook Han, Chonbuk National University

4:20 PM

(MCARE-034-2014) Tuning the Fermi Level and the Kinetics of Surface States of TiO2 Nanorods by Means of Ammonia Treatments

C. Fabrega*, D. Monllor-Satoca, S. Ampudia, A. Parra, T. Andreu, J. Morante, IREC, Spain

4:40 PM

(MCARE-035-2014) Engineering the electronic properties of titania by doping. An ab-initio approach

L. Mayrhofer*, M. Moseler, Fraunhofer IWM, Germany

5:00 PM

(MCARE-036-2014) Co-doping as a tool to increase photo-electrochemical activity of TiO2 photo-anodes

P. Barczuk*, K. Bienkowski, J. Augustynski, University of Warsaw, Poland

5:20 PM

(MCARE-037-2014) Effects of nano- structuring on TiO2 based photocatalytic materials

Y. Goenuellue*, S. Mathur, University of Cologne, Germany; B. Saruhan-Brings, German Aerospace Center, Germany

Batteries and Energy Storage

Sodium-ion Batteries

Room: Salon E

Session Chairs: Sridhar Komarneni, Pennsylvania State University; Dany Carlier, ICMCB-CNRS

2:20 PM

(MCARE-082-2014) Titanate Anodes for Sodium Ion Batteries (Invited)

M. Doeff*, M. Shirpour, Lawrence Berkeley National Laboratory, USA

3:00 PM

(MCARE-083-2014) Advanced materials for low cost Na- ion batteries (Invited)

T. Rojo*, University of the Basque Country, Spain

3:40 PM

(MCARE-084-2014) Na2S-P2S5 based solid electrolytes for sodium-ion batteries at room temperature as a renewable source

P. K. Jha*, Thapar University, Patiala, India

4:00 PM

Break

4:20 PM

(MCARE-085-2014) Designing and investigating novel electrode materials for rechargeable Na-ion batteries with high energy and low cost (Invited)

S. Meng*, J. Xu, C. Ma, University of California San Diego, USA

5:00 PM

(MCARE-086-2014) Sodium Layered oxides as positive electrode material for Na-batteries (Invited)

D. Carlier*, M. Guignard, B. Mortemard de Boisse, R. Berthelot, ICMCB-CNRS, France; J. Cheng, C. Pan, NTUST, Taiwan; M. Yoncheva, R. Stoyanova, Bulgarian Academy of Sciences, Bulgaria; A. Wattiaux, ICMCB-CNRS, France; B. Hwang, NTUST, Taiwan; C. Delmas, ICMCB-CNRS, France

Nanocomposites and Nanowires Materials for Photovoltaic and Photonic Technologies

Nanocomposites and Nanowires Materials for Photovoltaic and Photonic Devices II

Room: Salon G

Session Chairs: James Cahoon, University of North Carolina at Chapel Hill; Jordi Arbiol, ICREA and Institut de Ciencia de Materials de Barcelona

2:20 PM

(MCARE-112-2014) Semiconductor nanowires for energy harvesting and conversion (Invited)

S. Gradecak*, MIT, USA

3:00 PM

(MCARE-113-2014) Self-Assembled 0D, 1D and 2D Quantum Structures in-a-Nanowire: energy, light and sensing applications (Invited)

J. Arbiol*, ICREA and Institut de Ciencia de Materials de Barcelona, Spain

3:40 PM

(MCARE-114-2014) Nanofabrication of the superconductive YBa2Cu3O7–x (YBCO) macro-ceramics and electric round wire

A. Rokhvarger*, L. Chigirinsky, Retired, USA

4:00 PM

Break

4:20 PM

(MCARE-115-2014) Nanowire-based structure integration for artificial photosynthesis (Invited)

C. Liu*, N. P. Dasgupta, J. Tang, P. Yang, UC Berkeley, USA

5:00 PM

(MCARE-116-2014) An 11.1% efficiency nanowire solar cell (Invited)

J. Haverkort*, Y. Cui, J. Wang, S. Plissard, A. Cavalli, L. Gao, A. Standing, Eindhoven University of Technology, Netherlands; M. Verheijen, Philips innovation Services, Netherlands; E. Bakkers, Delft University of Technology, Netherlands

5:40 PM

(MCARE-117-2014) Characterization of Piezoelectric Nanogenerators Based on ZnO Nanostructures for Self-powering Nanodevices

C. Periasamy, MNNIT-Allahabad, India; P. Sreenath, Indian Institute of Technology (BHU), Varanasi, India, India, Indian Institute of Technology (BHU), Varanasi, India, IndiaSociety Integrated Technology Applied Research), Bangalore, India; P. Chakrabarti*, Indian Institute of Technology (BHU), Varanasi, India, India

Poster Session

Room: Waters Edge Ballroom

6:00 PM

(MCARE-P001-2014) Improving properties of 0.4Li2MnO3-0.6LiNi1/3Co1/3Mn1/3O2 Cathode Materials with Coating LiNi0.5Mn1.5O4

Y. Chen*, K. Xie, Y. Pan, Z. Chen, National University of Defense Technology, China

(MCARE-P002-2014) Electrochemical Cycle Life Improvement in RuO2 Nanoplate Architectures

L. Meda*, A. Navulla, Xavier University of LA, USA

(MCARE-P003-2014) Metal Organic Chemical Vapor Deposition of α-Fe2O3 nanoparticles and their Electrochemical Properties

A. Dangerfield*, A. Navulla, L. Meda, Xavier University of Louisiana, USA

(MCARE-P004-2014) Direct Growth of High-Capacity Manganese Oxide via Chemical Vapor Deposition

M. Jones*, Xavier University of Louisiana, USA

(MCARE-P005-2014) β-Fe2O3 Nanomaterials by Chemical Vapor Deposition for Innovative Li-Battery Anodes
C. Maccato*, G. Carraro, Padova University, Italy; D. Barreca, CNR-IENI and INSTM, Padova University, Italy; M. Cruz-Yusta, Universidad de Córdoba, Spain; A. Gasparotto, Padova University, Italy; J. Morales, Universidad de Córdoba, Spain; C. Sada, Padova University, Italy; L. Sanchez, Universidad de Córdoba, Spain

(MCARE-P006-2014) CuxO-TiO2 (x = 1, 2) Nanomaterials by CVD: Promising Anodes for Thin Film Lithium Batteries
D. Barreca*, IENI-CNR and INSTM - Padova University, Italy; G. Carraro, A. Gasparotto, C. Maccato, Padova University and INSTM, Italy; M. Cruz-Yusta, J. Gomez-Camer, Universidad de Córdoba, Spain; C. Sada, Padova University, Italy; J. Morales, Padova University and INSTM, Italy; L. Sanchez, Universidad de Córdoba, Spain

(MCARE-P007-2014) Facile synthesis of nitrogen-doped graphene-ultrathin MnO2 sheets composites and their electrochemical performances
X. Song*, P. Zhang, L. Gao, School of Materials Science and Engineering, Shanghai Jiao Tong University, China

(MCARE-P008-2014) Carbon coated layered LiNi0.44Mn0.31Co0.25O2 cathode materials with enhanced electrochemical performance
M. Barman*, S. Mitra, Indian Institute of Technology Bombay, India

(MCARE-P009-2014) Electrochemical properties of CNT-SnO2-Li4ti5O12 anode for lithium ion battery with hihg capacity
L. Ji Yea*, J. SeungHyn, L. SeokHee, L. KangSoo, W. SungPil, L. YouNa, Y. Young Soo, Gachon university, Republic of Korea

(MCARE-P010-2014) The revisit of potential of optical fiber modification as solar concentrator/transportation
J. Wang*, NSYSU, Taiwan

(MCARE-P011-2014) Synthesis and characterization of preceramic copolymers from ferrocenylsilane by living anionic polymerization to prepare SiC ceramics
Y. Gou*, H. Wang, T. Mao, X. Tong, National University of Defense Technology, China

(MCARE-P012-2014) Surfactant Free Nanocomposites as Highly Active Catalysts for the Hydrolytic Dehydrogenation Hydrogen from Ammonia Borane
C. Shao*, H. Wang, J. Wang, National University of Defense Technology, China

(MCARE-P013-2014) Improving Hydrogen Properties of Magnesium Borohydride with M(NH2)(2)(M=Na,Li,Mg)
A. Bateni*, M. Somer, Koc University, Turkey

(MCARE-P014-2014) Influence of support on catalytic (from Ni and Fe functionalized reduce graphene oxide catalysts) in the steam reforming of ethanol for hydrogen production
N. L. Carreno*, G. R. Dewantier, C. O. Avellaneda, C. F. Correa, Universidae Federal de Pelotas, Brazil; H. V. Fajardo, Federal University of Ouro Preto, Brazil; A. Valentini, Federal University of Ceara, Brazil; R. Rhodes, R. S. Silva, University of Surrey, United Kingdom; L. S. de Mello Carreno, Universidae Federal de Pelotas, Brazil

(MCARE-P015-2014) Growth of TiO2 nanosheets on SiC nanofibers for promising nanocomposite photoelectrodes
Y. Wang*, B. Wang, Science and Technology on Advanced Ceramic Fibers and Composites Laboratory, College of Aerospace Science and Engineering, National University of Defense and Technology, China

(MCARE-P016-2014) GaNP Nanowires – a Novel Material System for Solar Cell Applications
A. Dobrovolsky, Linkoping University, Sweden; Y. J. Kuang, S. Sukrittanon, C. W. Tu, University of California, USA; W. M. Chen, I. A. Buyanova*, Linkoping University, Sweden

(MCARE-P017-2014) Efficient counter electrode based on pyrenecarboxylic acid-grafted reduced graphene oxide in dye-sensitized solar cells
W. Rho*, T. Mahmoudi, H. Yang, Y. Hahn, Chonbuk National University, Republic of Korea

(MCARE-P018-2014) Bulk heterojunction (BHJ) hybrid solar cells with nanoimprinted ZnO layer
H. Yang*, W. Rho, V. Muhammad, Y. Hahn, Chonbuk National University, Republic of Korea

(MCARE-P019-2014) Study & Characterization of Semiconductor Nanowires as Sensing Interfaces for Electrochemical Biosensor Applications
R. Sinha*, R. Roop Kumar, S. Sundaram, BITS Pilani Dubai Campus, United Arab Emirates

(MCARE-P020-2014) The Influence of Dopants on the Defect Structure and Sinterability of Actinide and Rare-earth Oxides
J. Henderson*, Netzsch Instruments, USA

(MCARE-P021-2014) Evolution and Controlling of Defects during the Preparation of Continuous High-temperature Resistant SiC(Al) Fibers
K. Jian*, Y. Song, Y. Wang, H. Wang, National University of Defense Technology, China

(MCARE-P022-2014) Structure of zirconium alloy consolidated by high voltage electric discharge consolidation
E. Grigoryev, L. Lebedeva*, E. Olevsky, NRNU "MEPhI", Russian Federation; E. Olevsky, San Diego State University, USA

(MCARE-P023-2014) Novel biogas purification design utilizing Botryococcus braunii as a method of carbon capture
Y. Shin*, J. Albanese, M. Chen, J. Chiao, L. Cho, H. Huang, P. Puppala, B. Lin, M. Meyerson, A. Sekaran, D. Wang, C. Zhou, M. Yu, University of Maryland, College Park, USA

(MCARE-P024-2014) Catalytically enhanced combustion in porous media utilizing thermoelectric devices for power conversion
B. T. Beaman*, M. D. Robayo, A. Terracciano, B. Hughes, N. Orlovskaya, R. Chen, University of Central Florida, USA

(MCARE-P025-2014) Syngas Combustion in Porous Media: Creation of an Experimental Porous Combustor
B. Hughes*, A. C. Terracciano, B. Beaman, M. D. Robayo, N. Orlovskaya, S. S. Vasu, University of Central Florida, USA

(MCARE-P026-2014) Charge transfer dynamics in perylene diimide-C60/poly(3-hexylthiophene) blend films studied by transient absorption
K. Kaunisto*, P. Vivo, M. Niemi, R. Dubey, T. Ruoko, N. Tkachenko, H. Lemmetyinen, Tampere University of Technology, Finland

(MCARE-P027-2014) Reduction of CO2 by nanocrystals of metal-organic framework photocatalyst
Y. Lee*, J. Kang, Korea Advanced Institute of Science and Engineering, Republic of Korea

(MCARE-P028-2014) Local structural, optical, and electrical properties of ion-implanted ZnO nanorods
S. Han*, Z. Jin, C. Park, E. Jeong, I. Hwang, Chonbuk National University, Republic of Korea

(MCARE-P029-2014) FTO/CuO/Graphite as counter electrode in DSSC
C. O. Avellaneda*, E. Portugal, T. Sampaio, E. Santos, Universidade Federal de Pelotas, Brazil; A. Gundel, W. H. Flores, Universidade Federal do Pampa, Brazil; N. Carreño, Universidade Federal de Pelotas, Brazil

(MCARE-P030-2014) Narrowband infrared emitter for Energy Harvesting Applications
S. Sharma*, E. Stefanakos, D. Y. Goswami, J. Zhou, University of South Florida, USA

Wednesday, February 19, 2014

Plenary Session V

Room: Salon E

8:20 AM

Introduction

8:25 AM

(MCARE-PL6-2014) Theoretical Study of Growth and Electronic Structure of Graphene and Graphene-based Nanostructures
S. Hong*, Sejong University, Republic of Korea

9:00 AM

Break

Solar Fuels

Solar Fuels: Frontiers in Materials Development for Water Splitting Photocatalysts I

Room: Salon D

Session Chairs: Thomas Hamann, Michigan State University; Davide Barreca, IENI-CNR and INSTM - Padova University

9:20 AM

(MCARE-038-2014) Materials aspects of solar water splitting (Invited)

D. Wang*, Boston College, USA

10:00 AM

(MCARE-039-2014) Development of Precursor Chemistry for Metal Oxide Thin Films and Nanostructures (Invited)

S. Mathur*, T. Fischer, L. Brueckmann, J. Schläfer, G. Fornalczyk, J. Leduc, L. Appel, University of Cologne, Germany

10:20 AM

(MCARE-040-2014) Design of photoelectrodes for efficient solar water spliitting (Invited)

J. Lee*, Ulsan National Institute of Sci & Tech (UNIST), Republic of Korea

11:00 AM

(MCARE-041-2014) Enhancement of sensitivity and charge carrier collection in mixed metal oxides photo-anodes employed for photo-electrochemical water splitting

R. Solarska*, K. Bienkowski, M. Sarnowska, J. Augustynski, University of Warsaw, Poland

11:20 AM

(MCARE-042-2014) The synthesis of Ti alloying DLS coating for the application of bipolar plates in fuel cell (Invited)

D. Jung, N. Lee, K. Moon, KITECH, Republic of Korea; G. Yakup*, S. Mathur, University of Cologne, Germany

11:40 AM

(MCARE-043-2014) Nano-hybrid Structured Regioregular Polyhexylthiophenes Blend Films for Photoelectrochemical Applications

M. K. Ram*, P. Basnayaka, P. Villalba, E. Stefanakos, A. Kumar, University of South Florida, USA

Batteries and Energy Storage

All Solid State Batteries

Room: Salon E

Session Chairs: Mickael Dolle, University of Montreal; Derek Johnson, Prieto Battery, Inc

9:20 AM

(MCARE-069-2014) Porous and Nanostructured Electrodes for Energy Storage Devices (Invited)

A. Stein*, A. Vu, N. Petkovich, B. Wilson, Y. Fang, Y. Qian, University of Minnesota, USA

10:00 AM

(MCARE-088-2014) Materials Challenges to Develop Reliable "All-Solid-State" Batteries (Invited)

L. Castro, CEMES/CNRS, France; A. Kubanska, MADIREL/CNRS, France; R. Bouchet, LEPMI/CNRS/INPG, France; C. Jordy, SAFT, France; L. Tortet, MADIREL/CNRS, France; V. Viallet, V. Seznec, LRCS/CNRS, France; G. Caillon, SAFT, France; M. Dolle*, University of Montreal, Canada

10:40 AM

(MCARE-089-2014) Three-Dimensional Solid-State Lithium-ion Cell Fabrication with Integrated Electrodes (Invited)

D. C. Johnson*, Prieto Battery, Inc, USA; A. L. Prieto, Colorado State University, USA

11:00 AM

(MCARE-090-2014) 3D-New Lithium Battery Technology Platform

J. Prochazka*, HE3DA, Czech Republic

11:20 AM

(MCARE-091-2014) Stability Increase of Cathode Materials by NASICON structured electrolyte for all-solid-state batteries

S. Jee*, S. Lee, K. Lee, S. Woo, Y. Lee, J. Lee, Y. Yoon, Gachon Univeristy, Republic of Korea

Nanocomposites and Nanowires Materials for Photovoltaic and Photonic Technologies

Nanocomposites and Nanowires Materials for Photovoltaic and Photonic Devices III

Room: Salon G

Session Chairs: Esther Alarcon-Llado, EPFL; Yoon-Bong Hahn, Chonbuk National University

9:20 AM

(MCARE-118-2014) 4G Hybrid Organic Solar Cells for Energy Harvesting: Inorganics-in–Organics

S. P. Silva*, K. Jayawardena, L. J. Rozanski, C. A. Mills, M. J. Beliatis, G. R. Dabera, University of Surrey, United Kingdom

10:00 AM

(MCARE-119-2014) Semiconductor nanowires for next generation photovoltaics (Invited)

E. Alarcon-Llado*, A. Fontcuberta i Morral, EPFL, Switzerland

10:40 AM

(MCARE-120-2014) Designing Sub-Wavelength Silicon Nanowires for Photovoltaics: Synthesis, Measurement, and Modeling (Invited)

C. Pinion, J. Christesen, X. Zhang, J. Cahoon*, University of North Carolina at Chapel Hill, USA

11:20 AM

(MCARE-121-2014) The use of TiO_2 nanotubes arrays for photoanodes in dye-sensitized solar cells

L. Suhadolnik, Jozef Stefan Institute, Slovenia; I. Jerman, National Institute of Chemistry, Slovenia; A. Kujan, Cinkarna Celje, d.d. Inc., Slovenia; M. Krivic, K. Zagar, M. Ceh*, Jozef Stefan Institute, Slovenia

11:40 AM

(MCARE-122-2014) Hollow-flowered ZnO as scattering layer for improving energy conversion efficiency in dye-sensitized solar cells

W. Rho*, M. Vaseem, D. Jung, Y. Hahn, Chonbuk National University, Republic of Korea

Other Energy Issues

Other Energy Technologies I

Room: Salons B - C

Session Chairs: Rachael Robertson, Melbourne University; Ali Kaouk, AK Mathur, Institute for Inorganic and Material Sciences

9:20 AM

(MCARE-140-2014) Life in the freezer - leadership, water and energy challenges in Antarctica (Invited)

R. Robertson*, Melbourne University, Australia

10:00 AM

(MCARE-141-2014) Pyrolysis of Rush Grass and Wood investigated by TG-GC-MS

E. Post*, NETZSCH Geraetebau GmbH, Germany; B. Fidler, NETZSCH Instruments NA, LLC, USA

10:20 AM

(MCARE-142-2014) Switchable Antibiofouling Coatings

M. Denton*, M. Kirtk, Sandia National Laboratories, USA; S. Stafslien, North Dakota State University, USA; B. Hernandez-Sanchez, S. Dirk, Sandia National Laboratories, USA

10:40 AM

(MCARE-143-2014) Thermoelectric power generation coupled with perovskite catalyst enhanced combustion in porous media
M. D. Robayo*, B. Beaman, B. Delose, N. Orlovskaya, R. Chen, University of Central Florida, USA

11:00 AM

(MCARE-144-2014) On the Electrodeposition of Antimony and Cobalt in Citrate Solutions
R. Vidu*, University of California Davis, USA; R. Vidu, NanoRIS, USA; D. V. Quach, P. Stroeve, University of California Davis, USA

11:20 AM

(MCARE-145-2014) Parameter Calibration for Glass Strength Prediction Model Considering the Influence of Environment
C. Ronchetti*, Roma Tre University, Italy

Plenary Session VI

Room: Salon E

1:30 PM

Introduction

1:35 PM

(MCARE-PL7-2014) Non Palladium-based Alloy membranes for Hydrogen Separation and Production
C. Nishimura*, National Institute for Materials Science, Japan

Solar Fuels

Solar Fuels: Materials for Water Splitting: Hematite

Room: Salon D

Session Chairs: Gunnar Westin, Uppsala University; Ashok Kumar, University of South Florida

2:10 PM

(MCARE-044-2014) Photocatalytic Water Oxidation with Hematite Films (Invited)
T. Hamann*, O. Zandi, Michigan State University, USA

2:50 PM

(MCARE-045-2014) Tailored Fabrication of Fluorine-Doped Fe2O3 Nanomaterials via PE-CVD: Synthesis, Characterization and Photo-Activated Performances (Invited)
D. Barreca*, IENI-CNR and INSTM - Padova University, Italy; G. Carraro, Padova University, Italy; A. Gasparotto, IENI-CNR and INSTM - Padova University, Italy; C. Maccato, C. Sada, Padova University, Italy; S. Mathur, A. Mettenborger, Cologne University, Germany; O. Lebedev, Laboratoire CRISMAT, CNRS-ENSICAEN, France; S. Turner, G. Van Tendeloo, EMAT, Antwerp University, Belgium

3:30 PM

(MCARE-046-2014) Photoelectrochemistry and Surface Science of Composite Hematite Photoelectrodes (Invited)
B. E. Koel*, P. Zhao, C. X. Kronawitter, Princeton University, USA

4:10 PM

Break

Solar Fuels: Materials for Water Splitting: Hematite & Multiferroics

Room: Salon D

Session Chairs: Bruce Koel, Princeton University; Renata Solarska, University of Warsaw

4:20 PM

(MCARE-047-2014) Nonaqueous sol-gel chemistry: From nanoparticles to particle-based aerogels, films and metal foams (Invited)
M. Niederberger*, ETH Zurich, Switzerland

5:00 PM

(MCARE-048-2014) Plasma Deposition and Modification of Semiconducting Thin Films for Photoelectrochemical Hydrogen Production
A. Mettenboerger*, S. Mathur, University of Cologne, Germany

5:20 PM

(MCARE-049-2014) Novel Fe2O3 Nanostructures: From Synthesis to Photo-assisted H2 Production (Invited)
C. Maccato*, Padova University, Italy; D. Barreca, CNR-IENI and INSTM, Padova University, Italy; A. Gasparotto, G. Carraro, Padova University, Italy; P. Fornasiero, V. Gombac, ICCOM-CNR - INSTM, Trieste University, Italy; O. Lebedev, Laboratoire CRISMAT, CNRS-ENSICAEN, France; T. Montini, ICCOM-CNR - INSTM, Trieste University, Italy; S. Turner, G. Van Tendeloo, EMAT, Antwerp University, Belgium

Batteries and Energy Storage

Supercapacitors

Room: Salon E

Session Chairs: Karina Cuentas-Gallegos, Universidad Nacional Autónoma de México; Amartya Mukhopadhyay, Indian Institute of Technology (IIT) Bombay

2:20 PM

(MCARE-093-2014) Nanoporous Carbon Based Materials for Energy Storage Application (Invited)
A. Vinu*, The University of Queensland, Australia

3:00 PM

(MCARE-094-2014) High Performance Supercapacitors Using Graphene Nanoribbons
J. B. Gaillard*, H. Colon-Mercado, Savannah River National Laboratory, USA; R. Czerw, NanoTechLabs, Inc., USA

3:20 PM

(MCARE-095-2014) Effect of the number of rings on the capacitance of bamboo-type titania nanotube arrays prepared by alternating voltage anodizing
F. J. Quintero*, P. J. Arias, J. D. Reyes, J. Agreda, H. Zea, National University of Colombia, Colombia

3:40 PM

(MCARE-096-2014) Mesoporous graphene synthesized by sacrificial template approach for electrochemical capacitor applications
J. Cao*, J. Xu, Z. Chen, Changzhou University, China

4:00 PM

Break

4:20 PM

(MCARE-097-2014) Surface Modification of Carbon Materials for Improved Capacitance (Invited)
K. Cuentas-Gallegos*, D. A. Baeza-Rostro, E. Fuentes-Quezada, Universidad Nacional Autónoma de México, Mexico; D. Pacheco-Catalán, J. M. Baas-López, Centro de Investigación Científica de Yucatán A.C., Mexico

4:40 PM

(MCARE-098-2014) Self-assembled porous α-Fe2O3 mesocrystals-graphene hybrid nanostructures for Enhanced electrochemical capacitor

L. Gao*, X. Song, P. Zhang, S. Yang, School of Materials Science and Engineering, Shanghai Jiao Tong University, China

5:00 PM

(MCARE-099-2014) Carbon Monoliths for EDLC Electrodes with Outstanding Volumetric Capacitances

M. Kunowsky*, University of Alicante, Spain; A. Garcia-Gomez, V. Barranco, J. Rojo, Instituto de Ciencia de Materiales de Madrid, CSIC, Spain; J. Carruthers, ATMI, Adsorbent & Gas Technology, USA; ÁNGEL. Linares-Solano, University of Alicante, Spain

5:20 PM

(MCARE-100-2014) High Reliability Ceramic Capacitors based on Temperature and Voltage-Stable Relaxor Dielectrics for High Operating Temperature Inverter Applications

G. Brennecka, H. J. Brown-Shaklee*, Sandia National Laboratories, USA; N. Raengthon, Oregon State University, USA; M. A. Blea, Sandia National Laboratories, USA; D. P. Cann, Oregon State University, USA

5:40 PM

(MCARE-101-2014) Novel Approach of Increasing Capacitance by Coating Polyvinylidene Fluoride Langmuir-Schaefer Film on Graphene-Polyaniline Nanocomposite Electrode for Supercapacitor Applications

M. K. Ram*, P. Bolisetty, A. Takhi, Y. Goswami, E. Stefanakos, A. Kumar, University of South Florida, USA

Nanocomposites and Nanowires Materials for Photovoltaic and Photonic Technologies

Nanocomposites and Nanowires Materials for Photovoltaic and Photonic Devices IV

Room: Salon G

Session Chairs: Dongling Ma, INRS, Uni Quebec; Shi-Woo Rhee, POSTECH

2:20 PM

(MCARE-123-2014) Nanocomposite Hybrids Photoelectrodes for the High Efficiency Flexible Dye-Sensitized Solar Cells

M. Ko*, Korea Institute of Science and Technology (KIST), Republic of Korea

3:00 PM

(MCARE-124-2014) Amorphous and Graphitic Carbon Nanoparticles for Energy Conversion: New Kids on the Carbon Block (Invited)

W. Kwon, S. Rhee*, POSTECH, Republic of Korea

3:40 PM

(MCARE-127-2014) graphene base solar cell by incorporation new organic aromatic functionalized graphene oxide as charge transfer amplificator

T. Mahmoodi*, W. Rho, Y. Hahn, Chonbuk National University, Republic of Korea

4:00 PM

Break

4:20 PM

(MCARE-126-2014) Graphene-based Sensors and Solar Cells (Invited)

H. Zhu*, Tsinghua University, China

5:00 PM

(MCARE-128-2014) Comparative Study of the Output of Amorphous Silicon Photovoltaic Solar Cells when Receiving Direct and Diffused Radiations

M. O. Olatinwo, O. Oyeleke*, O. H. David, Federal Polytechnic Offa, Kwara State,Nigeria, Nigeria

5:20 PM

(MCARE-129-2014) Application of nitrogen-doped TiO2 Films for Inverted Polymer Solar Cells

D. Kim*, H. Kim, H. Cho, Chonnam National University, Republic of Korea

Other Energy Issues

Other Energy Technologies II

Room: Salons B - C

Session Chairs: Michele Denton, Sandia National Laboratories; Dylan Cuskelly, University of Newcastle

2:20 PM

(MCARE-146-2014) Positioning to Win Government Research, Development, and Demonstration Funding

P. Winkler*, Government Contracting Specialists, LLC, USA

2:40 PM

(MCARE-147-2014) Low Temperature Hydrogen Free Large Scale Graphene Growth Using Plasma-Enhanced Chemical Vapor Deposition for Energy Applications

A. H. Kaouk*, T. Singh, S. Mathur, Institute of Inorganic and Material Chemistry, Germany

3:00 PM

(MCARE-148-2014) Modeling of thermal treatment of raw briquet in the course of foam glass production

D. Anton*, SPbGASU, Russian Federation

3:20 PM

(MCARE-149-2014) Numerical Study of Heterogeneous H-O-C-N-S Syngas Combustion System with a Porous Ceramic Media

A. C. Terracciano*, B. Hughes, N. Orlovskaya, S. S. Vasu, University of Central Florida, USA

3:40 PM

(MCARE-150-2014) MAX Phase Synthesis Via Reduction Reactions

D. Cuskelly*, University of Newcastle, Australia

4:00 PM

Break

4:20 PM

(MCARE-151-2014) Carbon Nanotubes Integrated with Superconducting NbC

G. Zou*, Soochow University, China

4:40 PM

(MCARE-152-2014) High Temperature Reactions of Agricultural Wastes as Material Resources for EAF Steelmaking

N. Mohd Yunos*, A. Ismail, M. Idris, University Malaysia Perlis, Malaysia

Thursday, February 20, 2014

Plenary Session VII

Room: Salon E

8:20 AM

Introduction

8:25 AM

(MCARE-PL8-2014) Materials Development Synergies in Alternative and Renewable Energy Technologies

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

9:00 AM

Break

Solar Fuels

Solar Fuels: Frontiers in Materials Development for Water Splitting Photocatalysts II

Room: Salon D

Session Chairs: Markus Niederberger, ETH Zurich; Riad Nechache, INRS-EMT

9:20 AM

(MCARE-050-2014) Photovoltaic proprieties and Photocatalytic activity of Multiferroics-based systems (Invited)
R. Nechache*, S. Li, F. Rosei, INRS-EMT, Canada

10:00 AM

(MCARE-051-2014) Solution synthesis routes to advanced materials (Invited)
G. Westin*, Uppsala University, Sweden

10:40 AM

(MCARE-052-2014) Atomic Layer Deposition Modified Electrospun Nanofibers for Energy Conversion
A. Lepcha*, T. Singh, S. Mathur, University of Cologne, Germany

11:00 AM

(MCARE-053-2014) Production, Applications and Toxicology of nano TiO2 (Invited)
J. Prochazka*, HE3DA, Czech Republic

11:20 AM

(MCARE-054-2014) In-Situ investigations on CVD grown photo catalysts for photoelectrochemical water splitting
T. Fischer*, S. Mathur, University of Cologne, Germany

11:40 AM

(MCARE-055-2014) Electrocatalysts for Water Splitting and Solar Fuel
K. Joya*, Leiden University, Netherlands

Batteries and Energy Storage

Li-S and Li-ion Batteries

Room: Salon E

Session Chairs: Stefan Adams, National University of Singapore; Sebastian Osswald, Naval Postgraduate School

9:20 AM

(MCARE-102-2014) Insight into Li-S batteries using analytical tools in operando mode (Invited)
M. Patel, National Institute of Chemistry, Slovenia; I. Arčon, CO-NOT, Slovenia; G. Aquilanti, Elettra-Sincrotrone Trieste S.C.p.A., Italy; R. Dominko*, National Institute of Chemistry, Slovenia

10:00 AM

(MCARE-103-2014) Lithium Sulfur Batteries: Fundamental Understanding Towards Practical Application (Invited)
J. Xiao*, J. Zheng, D. Lv, T. Lozano, J. Liu, Pacific Northwest National Laboratory, USA

10:40 AM

(MCARE-104-2014) High energy density batteries using thiophosphate solid electrolytes (Invited)
S. Adams*, National University of Singapore, Singapore

11:00 AM

(MCARE-105-2014) Thermodynamics and Kinetics of Semi Solid Flow Cells (Invited)
S. Osswald*, Naval Postgraduate School, USA

11:20 AM

(MCARE-106-2014) Fabrication of TiO2/graphene in core-shell structure as advanced anode materials
Y. Yao, R. Sisson*, Worcester Polytechnic Institute, USA; Q. Xu, Z. Xia, University of North Texas, USA; Y. Cen, J. Liang, Worcester Polytechnic Institute, USA

11:40 AM

(MCARE-107-2014) High capacity Li2MnSiO4/C nanocomposite prepared by a resorcinol-formaldehyde assisted sol-gel method
K. Xie*, Y. Pan, College of Aerospace Science and Engineering, National University of Defense Technology, China

Nanocomposites and Nanowires Materials for Photovoltaic and Photonic Technologies

Nanocomposites and Nanowires Materials for Photovoltaic and Photonic Devices V

Room: Salon G

Session Chairs: Michael Filler, Georgia Institute of Technology; Zhifeng Ren, University of Houston

9:20 AM

(MCARE-130-2014) Vapor-Liquid-Solid Synthesis as a Route to Manipulate Energy Flow at the Nanoscale (Invited)
N. Shin, M. Filler*, Georgia Institute of Technology, USA

10:00 AM

(MCARE-131-2014) Nanostructures for High Efficient Photovoltaic Solar Cells and Flexible Transparent Electrode (Invited)
Z. Ren*, University of Houston, USA

10:40 AM

(MCARE-132-2014) Iron Pyrite Films with Passivated Surface States for Photovoltaic Applications
J. A. Frantz*, C. C. Baker, S. C. Erwin, N. D. Bassim, S. B. Qadri, J. D. Myers, J. A. Freitas, E. R. Glaser, J. S. Sanghera, Naval Research Laboratory, USA

11:00 AM

(MCARE-133-2014) Photonic Metal Oxide Nanomaterials for Energy Related Applications & Solar Fuels
E. Redel*, KIT (Karlsruhe Insitute of Technology), Germany

11:20 AM

(MCARE-134-2014) Nitrogen doped TiO2 and Eosin-Y dye for Dye sensitized solar cell (Invited)
K. C. Mohite*, University of pune, India; M. T. Sarode, Mahatma Phule Arts, Science and Commerce College, India; B. B. Kale, Centre for Materials for Electronics Technology (C-MET), India

Monday, February 17, 2014

Plenary Session I

Room: Salon E

8:10 AM

(MCARE-PL1-2014) The $LiFePO_4$ Story: Theory, Experiment and Characterization

F. Omenya, N. Chernova, SUNY, USA; A. Abdellahi, G. Ceder, MIT, USA; S. Whittingham*, SUNY, USA

The olivine cathode, LiFePO4, presents a quandary. It is a very good electronic insulator and thought to react by a two-phase mechanism, yet has one of the highest power capabilities of any cathode material. NECCES therefore chose it as a model compound to understand the ultimate limitations of intercalation electrodes. A theoretical model was developed that could explain the high rates, based on a metastable single phase. Ex-situ and in-situ tools were employed to determine the kinetic vs thermodynamic pathways. Vanadium was chosen as an aliovalent substituent, because it has a very different neutron scattering factor to iron. Vanadium substitution was found to increase the single-phase regions and the rate capability consistent with a single-phase mechanism. When V+Fe>1>Li, the iron resides on the Li site forming clusters, e.g. sarcopside, keeping the diffusion tunnels open. This "simple" material is now understood, and this understanding will allow us to design new batteries.

8:45 AM

(MCARE-PL2-2014) Recent Advances in Thermal Energy Storage for Solar Thermal Power

D. Goswami*, University of South Florida, USA

Abstract not available

Hydrogen

Catalysis in Hydrogen Materials and Systems

Room: Salons B - C

Session Chairs: Claudia Zlotea, CNRS ICMPE; David Book, University of Birmingham

9:40 AM

(MCARE-160-2014) Hydrogen Separation & Purification Using Composite Palladium Membranes in a Catalytic Membrane Reactor

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

A 6 um palladium composite membrane was prepared on alumina support using a modified electroless plating method. In this method, the sensitization step was skipped and only the activation step was carried out on the support. However, the pH of the plating solution was adjusted to stimulate the adsorption of the palladium metal ions on the substrate surface. This method also drastically reduced the plating time and avoided the threats of Sn (11) impurities. When the membrane was investigated for both single and mixed gas hydrogen permeation and separation, it showed high hydrogen flux. The hydrogen flux for the gas mixture (H2= 50%, CO= 28%, CH4= 8%, N2= 4%) was significantly lower than that of the single gas owing to the presence of CO in the mixed gas which inhibits hydrogen permeation through the membrane. The temperature dependence on hydrogen permeation through the membrane was fitted with an Arrhenius plot to determine the activation energy Ea. The hydrogen transport through the membrane was also investigated to determine the rate controlling processes.

10:00 AM

(MCARE-161-2014) Ni-SiO2 based Nanocomposite for Methane Dry Reforming Catalysis

P. Zhang*, X. Song, L. Gao, Shanghai Jiao Tong University, China

Reforming of natural gas into syngas is becoming more and more attractive for the production of hydrogen and further synthesis fuels due to the benchmark development of shale gas exploitation techniques. The Ni based alloy composite nanostructures supported on SiO2 showed superior performance in methane dry reforming catalysis including a high CH4 conversion, high H2/CO ratio (0.9), resistance to coke formation and particle sintering, as well as the ability to restrain the side reactions. The morphologies of the composite nanostructures can be tuned through synthetic conditions. The strong interaction between metal and support is ascribed to the superior performance of the catalysts.

10:20 AM

(MCARE-162-2014) Reversible hydrogen activation in molecular complexes: approaches to catalysis and energy storage using amine boranes (Invited)

T. Autrey*, D. Camaioni, M. Bowden, A. Karkamkar, S. Whittemore, Pacific Northwest National Laboratory, USA

Novel approaches for activating hydrogen are needed to increase efficiency and decrease costs in energy-intensive industrial processes. Amine boranes have the potential to provide unique solutions to two seemingly different applications: (i) catalytic hydrogenation, critical to many industrial processes, ranging from upgrading crude oil to ammonia synthesis, and (ii) hydrogen storage, a potentially critical solution to storing energy from intermittent renewable sources such as wind and solar. In this presentation the relationship between hydrogen storage and catalysis is discussed. The work starts with the pedagogical example of ammonia borane and ammonium borohydride in hydrogen storage and extends to more complex amine borane structures that provide the ability to tune thermodynamics. We describe a combination of experimental and computational approaches to gain insight into structure and reactivity of non-metal molecular complexes composed of Lewis acid Lewis base functionality to understand the mechanism of heterolytic activation of molecular hydrogen.

11:00 AM

(MCARE-163-2014) Role of Carbon support on Activity and Stability of Pt/C catalyst for Hydrogen production by S-I thermochemical cycle

D. Tyagi*, S. Varma, S. R. Bharadwaj, Bhabha Atomic Research Centre, India

Hydrogen can be the energy carrier of future if it is produced in large scale and in environment friendly way. S-I thermochemical cycle is one of the promising method to produce H2 from water. HI decomposition is an integral part of S-I cycle. We have synthesized Pt catalysts supported on different carbon supports and evaluated them for HI decomposition reaction. Pt/C catalysts were prepared by the following two methods (i) Direct impregnation of carbon support (activated carbon and colloidal graphite) (ii) Hard templating method using mesoporous silica templates (SBA-15 and MCM-41). These catalysts were named as Pt/AC, Pt/Gr, Pt/SBA-C and Pt/MCM-C. The catalysts were used for liquid phase HI decomposition reaction. Catalysts were characterized by XRD, SEM, Raman and N2 adsorption. The used catalysts were analyzed for their integrity and their stability against platinum leaching was determined by analyzing the eluent after the reaction by ICP-OES. The % conversion values for Pt/AC, Pt/Gr, Pt/SBA-C and Pt/MCM-C were found to be 13.2 %, 17.8 %, 15.2 % and 16.2% respectively which is significantly higher than blank value of 3.1 %. The concentrations of Pt in (µg/l) were 39.7, 38.8, 18.8 and 39.8 respectively. The Pt/C catalysts were found to be active for HI decomposition reaction. The mesoporous ones were found to be more stable against platinum leaching.

11:20 AM

(MCARE-164-2014) Enhanced hydrogen storage performances of MgH2–NaAlH4 system catalyzed by TiO2 nanoparticles

R. Din*, Pakistan Institute of Nuclear Science and Technology Nilore Islamabad, Pakistan; Q. Xuanhui, University of Science and Technology Beijing, Hadian District, China

MgH2–NaAlH4 composite is considered a prospective reactive hydride composite (RHC) for hydrogen storage applications due to its low cost, good chemical stability, high hydrogen capacity, and potential recyclability. Present work presents more precise clarification of sorption properties, indicating the most probable dehydrogenation pathway for each of the various stoichiometries (1:2, 1:1, and 2:1) in this composite. It is concluded that stoichiometry has influence on reaction kinetics and high-temperature reaction progression. Moreover, impact of TiO2 nanoparticles on reaction mechanism and hydrogen sorption properties of MgH2–NaAlH4 system is also investigated. The results have indicated that TiO2 nanoparticles are active in ameliorating the dehydriding/rehydriding kinetics and reducing the dehydrogenation temperature. The doped sample has displayed substantially reduced activation energies for NaAlH4, Na3AlH6, MgH2, and NaH relevant decompositions. TiO2 doping has also markedly enhanced reversible capacity of binary composites. XRD, XPS, and FESEM-EDS analyses have demonstrated that finely dispersed oxygen-deficient titanium species, formed during first desorption and migrated to bulk during cycling, might contribute to kinetic improvement by serving as active sites to facilitate hydrogen diffusion both during dehydrogenation/ rehydrogenation.

Batteries and Energy Storage

Li-ion Batteries I

Room: Salon E

Session Chairs: Palani Balaya, National University of Singapore; Donghai Wang, Penn State University

9:40 AM

(MCARE-065-2014) New electrochemical energy storage concepts (Invited)

A. Van der Ven*, University of California, Santa Barbara, USA

Electrochemical energy storage relies on the breaking and reforming of chemical bonds to store and recover energy. This is achieved by the decomposition of a stable compound, MX, into more elemental components, M and X, that in their separated form have a higher free energy than the original compound. The reverse reaction, M+X→MX, releases the stored energy. Very specific geometric and kinetic constraints need to be imposed on these reactions in order to convert the chemical free energy change, ΔG, into useful electrical work. First-principles computational methods have proven invaluable in elucidating and predicting a wide variety of thermodynamic and kinetic properties of electrode and electrolyte materials. In this talk I will describe how these tools can be used to explore and design new electrochemical energy storage concepts and devices.

10:20 AM

(MCARE-066-2014) Diagnostic examination of high-energy Li-ion cells containing alumina-coated Li1.2Ni0.15Mn0.55Co0.1O2-based positive electrodes (Invited)

D. Abraham*, Argonne National Laboratory, USA

Layered Li-rich transition metal oxides are high energy storage materials and currently considered for advanced transportation applications. But significant capacity loss and impedance rise is observed when these materials are repeatedly cycled or held at high voltages against graphitic negative electrodes in electrochemical full-cells. In this presentation, we investigate one particular system, containing Li1.2Ni0.15Mn0.55Co0.1O2-based positive electrodes, and show how capacity loss and impedance rise can be reduced by modification of the positive electrode. This modification is done in several ways that include the following: i) coating alumina onto composite electrodes via atomic layer deposition (ALD); ii) by blending commercially available Al2O3 powder with the other electrode constituents; (iii) by preparing electrodes from oxide particles coated with alumina by a sonochemical process. Full-cells containing the alumina-coated particles and positive electrodes, cycled between 2.2-4.6V, show better capacity retention and lower impedance rise than the baseline electrodes. In this presentation we'll correlate the electrochemical data with materials analysis data (X-ray photoelectron spectroscopy, secondary ion mass spectrometry) to determine reasons for the improved performance of the alumina-coated samples.

11:00 AM

(MCARE-067-2014) Nanostructured transition metal oxides prepared at moderate temperatures as Li- and Na-ion battery materials (Invited)

M. C. López, Universidad de Córdoba, Spain; G. F. Ortiz, Universidad de Córdoba, Spain; P. Lavela, Universidad de Córdoba, Spain; R. Alcántara, Universidad de Córdoba, Spain; J. L. Tirado*, Universidad de Córdoba, Spain

A recently developed procedure of electrodeposition followed by mild thermal treatment, is used to prepare advanced oxide electrodes for Li- and Na-ion batteries. Starting from Fe^{2+} and Ni^{2+} solutions, the resulting thin films annealed at 450 °C for 2h contain a nanocomposite of NiO and Fe_2O_3 on the current collector that can be directly used as conversion electrodes without needing binder or conducting additives. Lithium test cells show an unusually high first cycle reversibility (>740 mA h g^{-1}) and low cell polarization during cycling. Synergic effects due to the presence of both transition metal elements as well as a high interfacial surface resulting from the nano-crystalline character are the origin of the enhanced performance. In sodium cells, maximum first-discharge capacities of ca. and 870 mA h g^{-1} are achieved, which decrease to ca. 400 mA h g^{-1} after ten cycles. Post-mortem analyses of used electrodes by XPS and ^{57}Fe Mössbauer spectroscopy are used to study the changes in the oxidation state of the transition elements upon cycling, which agree with a reversible conversion reaction. The kinetic response is studied in galvanostatic and potentiostatic experiments, which showed an additional pseudocapacitive contribution to the total capacity particularly for high cycling rates, thus allowing an improved rate performance.

11:40 AM

(MCARE-068-2014) Integrating Si Nanoparticles to Structured Micro-sized Composites for Electrochemical Energy Storage (Invited)

D. Wang*, Penn State University, USA

Silicon has been considered as a promising anode for next generation lithium-ion batteries because of its natural abundance, environmental friendliness, and most importantly, low discharge potential and the high theoretical capacity. Practical application of Si anodes has thus far been mainly hindered by the enormous volume change and instability of solid electrolyte interphase (SEI), both of which therefore lead to fast capacity fading. Nano-sized Si has been widely reported to show good cycling stability due to its tolerance of volume changes. In order to utilize the good cycling performances of the nano-sized Si, it is desired to assemble them into macroscopic bulk materials to obtain increased mass loading and packing density for practical anode applications. In this presentation, we will present new approaches to integrate nano-sized Si nanoparticles into macroscopic Si composites while maintaining the excellent performance with good conductivity, cycling stability and high capacity. We will also present advances of SiOx coating on the Si composites in formation of stable SEI to obtain anodes with superior cycling stability.

The finding will help to design new structured materials for high-volume-change anodes to be used in advanced Li-ion batteries.

Nuclear

Advanced Materials for Nuclear Energy

Room: Salon D
Session Chair: Yutai Katoh, Oak Ridge National Lab

9:40 AM

(MCARE-135-2014) Accident Tolerant Fuel cladding based on SiC/SiC composites for LWRs (Invited)

C. Sauder*, A. Michaux, J. Braun, P. Billaud, G. Loupias, CEA, France

In the case of a loss of cooling water (LOCA), the temperature can increase over 800°C, resulting in rapid oxidation of the zirconium alloy cladding material. The purpose of this work is to assess a cladding effective in service conditions, able to resist to high temperature oxidation in steam and to sustain dimension stability in order to avoid these risks. A heat-resistant cladding based on silicon carbide (SiC/SiC) composites materials has been developped in CEA. Such a solution, should enable the cladding to reach very high temperatures (> 1400°C) without significant oxidation or hydrogen production. The dimensional stability of the material also ensures a coolable and then reliable core geometry. The "sandwich" design patented by CEA includes a metal layer, which ensures leaktightness, inserted between two layers of SiC/SiC composites that provide overall mechanical resistance. The preliminary oxidation tests at 1200-1400°C in moisture atmosphere have highlighted the superiority of the SiC/SiC material at 1200°C. Tensile test after oxidation confirmed the very good behavior of the composite. To access the in-service like behavior of this innovative cladding, oxidation in autoclaves has been conducted for 5 months (T= 360°C and P=180 bars) on various SiC/SiC composites and high purity CVD SiC samples. Mechanical results demonstrated the good resistance of SiC/SiC composites ater such oxidation.

10:20 AM

(MCARE-136-2014) Ion Beam Irradiated Silicon Carbide Composites

N. Chaabane*, M. Le Flem, T. Vandenberghe, CEA, France; C. Sandt, P. Dumas, Synchrotron-SOLEIL, France; Y. Serruys, CEA, France

Silicon carbides (SiC) are considered as one of the promising candidates for some nuclear applications. In this work, three SiC/SiC grades involving the same Chemical Vapor Infiltrated (CVI) SiC matrix but various types of fibers (Tyranno S, Tyranno SA3 and Hi-Nicalon type S), were irradiated with 12 MeV Au ions up to 0.05 and 1 dpa both at RT and 800°C. The irradiation-induced microstructural evolution of SiC matrix and fibers has been investigated by combining SEM, Raman spectroscopy on the irradiated surface and by TEM along the beam penetration. Step height differences among the SiC matrix and the TS fibers were observed for the irradiated composites at 1 dpa and both temperatures. This step height is quantitatively evaluated through AFM measurements and is ~350 nm after irradiation at RT. At 800°C the step height is ~140 nm. This dimensional change suggests different behaviors of SiC matrix and TS fibers under irradiation. TS fiber shrinkage together with slight expansion of the matrix was already observed for ion irradiation at RT, related to full amorphization, as shown from TEM observations. The formation of such amorphous layer is consistent with Raman results. However, this effect is enhanced by a decreased swelling of SiC matrix at higher irradiation temperature suggesting irradiation defect annealing, which is consistent with Raman data that show a slightly disordered material with increasing temperature.

10:40 AM

(MCARE-137-2014) Development of the full dense sintered MgAl2O4 ceramics for permanently safe containerization of nuclear solid waste

A. Rokhvarger*, E. Vaughn-Flam, Rokon Systems, Inc., USA

We developed nano-technology of fully dense sintered alumina-magnesium MgOxAl2O3 spinel ceramics (no additives), which are permanent chemical, water, and thermal resistant and impenetrable for radon gas emanating from nuclear materials. Ultimate structural resistance of Rokon' ceramics under radiation was approved by BNL specialists using testing in a nuclear reactor. We are also developed: the microwave assisting nanotechnology and a special kiln for cost-effective firing of extruded large-sized and thick walled ceramic container vessels; the microwave assisting nanotechnology and an apparatus for seamlessly joining of ceramic vessels and their lids to close loaded containers; multi-layer construction of the dry casks (DC) consisting of a) the inner cylindrical ceramic container and b) outer shells of the multi-layer canister package providing radiation shielding and mechanical protection; and method and technique for onsite loading, closing, assembling and permanently safe disposing of Rokon DC at the nuclear power plant backyard.

11:00 AM

(MCARE-138-2014) Plasma Arc Welding of ZrB_2 20 vol.% ZrC and $Zr^{11}B_2$

D. King*, J. Lonergan, G. Hilmas, W. Fahrenholtz, Missouri University of Science and Technology, USA

Plasma arc welding was used to join coupons of ZrB_2 containing 20 vol.% ZrC (ZrB_2-20ZrC), and melt $Zr^{11}B_2$ specimens. ZrB_2-20ZrC powders were hot-pressed to produce dense billets at a temperature of 1980°C with phenolic resin as a sintering aid. $Zr^{11}B_2$ billets were formed using reaction hot-pressing of ZrH_2 and ^{11}B powders at a temperature of 2100°C. To combat oxidation and thermal shock, welding was carried out under an inert argon atmosphere in a sealed furnace designed to preheat the samples prior to welding. Melt pools from the $Zr^{11}B_2$ specimens were analyzed using SIMS to determine isotope ratios before and after melting. Thermal diffusivity of the samples was measured from room temperature to 2000°C and was used to calculated thermal conductivities for both ZrB_2-20ZrC and $Zr^{11}B_2$. At room temperature, thermal conductivities of 68 and 137 W/mK were measured for ZrB_2-20ZrC and $Zr^{11}B_2$, while thermal conductivity was seen to drop to 62 and 84 W/mK at 2000°C. With a high thermal conductivity, strengths reported to be ~220 MPa at temperatures above 1600°C, and the ability to be arc welded (with additions of ZrC), ZrB_2 may be a versatile material for cladding applications in nuclear reactors.

11:20 AM

(MCARE-139-2014) Entrapment of molecular iodine produced in nuclear industry with the Hofmann's clathrate Ni(pz)Ni(CN)4 where pz = pyrazine, and analogues

G. Massasso*, Y. Guari, J. Larionova, J. Long, J. Haines, G. Maurin, S. Devautour, Institut Charles Gerhardt, France; A. Grandjean, Institut de Chimie Séparative de Marcoule, France; B. Onida, Politecnico di Torino, Italy

Coordination polymers with formula M'(L)M''(CN)4 (where M and M'' are transition metals and L is an organic molecule), also known as Hofmann's clathrates and previously investigated for spin transition properties and hydrogen storage at low temperature are studied as decontaminant materials for the entrapment of molecular radioactive iodine deriving from effluents and outgases of nuclear industry. The clathrate Ni(pz)Ni(CN)4 is kept in dynamic contact with solutions of I2 in cyclohexane at different concentrations, until equilibrium conditions are reached. X-ray diffraction shows a swelling effect on the clathrate tetragonal lattice after iodine is introduced in the structure. As elemental analysis indicates, the maximal capture of entrapped iodine results to be 1 mol of I2 per mole of clathrate; the same result is obtained by molecular modeling by using lattice parameters detected via Rietveld refinement on XRD spectra after entrapment. FT-IR spectroscopy shows shifts in the bands of pyrazine indicating a preferential interaction between iodine and the aromatic rings. Moreover, Raman and UV-VIS spectroscopies show both the presence of molecular iodine and the formation of iodides. The entrapped iodine can be retained up to 150 °C as TGA indicates. Data support the use this family of compounds for the entrapment of the nuclear iodine.

Plenary Session II

Room: Salon E

1:35 PM

(MCARE-PL3-2014) Silicon Nanowire based Thin Film Solar Cell Concepts on Glass for the >15% Era

S. Christiansen*, Helmholtz-Zentrum für Materialien und Energie, Germany; S. Schmitt, S. Jaeckle, C. Tessarek, G. Sarau, M. Heilmann, M. Latzel, M. Goebelt, G. Shalev, M. Bashouti, A. Mahmoud, Max Planck Institute for the Science of Light, Germany; K. Hoeflich, Helmholtz-Zentrum für Materialien und Energie, Germany

Aligned silicon nanowire (SiNW) arrays for the efficiencies >15% - era are fabricated on multi-crystalline Si layers on glass using reactive ion etching with lithographic large area nano-patterning using densely packed polystyrene (PS) spheres. Diameter, length, density and shape of SiNWs can be tuned for highest absorptions (close to 90%) and as small as possible surface areas, since surfaces are prone to carrier recombination. Various SiNW cell concepts are: (i) a hybrid organic/inorganic cell with SiNWs absorber and a hole conducting polymer (PEDOT:PSS - encapsulation procedures for long term stability suggested); (ii) a semiconductor-insulator-semiconductor (SIS) cell with SiNW absorber, oxide (few Å Al2O3 by atomic layer deposition-ALD)) tunneling barriers for charge carrier separation and a transparent conductive oxide (TCO – here: Al:ZnO, by ALD). Initial thin film solar cell prototypes reached open-circuit voltages of > 630 mV, short-circuit current densities of even ~ 30 mA/cm2 and efficiencies >13%. Analytics to improve materials / cells are: (i) electron beam induced current (EBIC) - charge carrier distributions; (ii) electron backscatter diffraction (EBSD) - structural quality of the multi-crystalline Si layer; (iii) integrating sphere measurements, external quantum efficiency - optical properties and (iv) 4-point nano-probing of individual NWs - electrical properties. Novel electrodes (e.g. graphene, silver nanowire webs) to further improve the cells are shown.

Hydrogen

Hydrogen Technology and Novel Application

Room: Salons B - C

Session Chairs: Claudio Corgnale, Savannah River National Laboratory; Huot Jacques, UQTR

2:20 PM

(MCARE-153-2014) Engineering Technologies for Fluid Chemical Hydrogen Storage System (Invited)

B. A. van Hassel*, R. McGee, A. Murray, S. Zhang, United Technologies Research Center, USA

Fluid forms of chemical hydrogen storage materials require a gas/liquid separation between the evolved H2 gas and the fluid phase that contains the reacted chemical hydrogen storage material. The United Technologies Research Center (UTRC) evaluated the performance of a particular gas/liquid separator (GLS) design over a wide range of temperature, pressure and mass flow rate with a silicone oil as surrogate for the fluid chemical hydrogen storage material and nitrogen gas as surrogate for hydrogen gas. The temperature was shown to have a large effect on the efficiency of the gas/liquid separator, prompting the need to cool down the two-phase mixture before separation. The experimental results show a critical N2 gas flow rate above which the efficiency of the separation drops below 99.99%. An optical high-pressure side glass assembly was installed downstream of the GLS in order to measure the droplet size distribution of the liquid that carried over with a laser droplet size analyzer. The difference in droplet size between the results of a Computational Fluid Dynamics (CFD) model and the experimental results was explained by the formation of a liquid film inside the vortex finder of the gas/liquid separator.

3:00 PM

(MCARE-154-2014) Improving the High-temperature Durability of CO2 Sorbents for H2 Production by Steam Reforming of Biomass

S. J. Milne*, M. Zhao, A. Brown, V. Dupont, University of Leeds, United Kingdom

In principle, the efficiency of H2 production by steam reforming of biomass can be improved by the near-instantaneous removal of the CO2 by-product at reaction temperatures of ~ 600 °C using a sorbent such as CaO. After capturing the CO2, the sorbent needs to be regenerated by calcination at higher temperatures ≥ 800 °C ready for the next cycle, but CO2 sorption capacity diminishes due to particle sintering and loss of porosity. Because of this sorbent durability problem, the period for efficient H2 production falls which severely restricts the implementation of this promising technology. This paper presents examples of approaches, based on ceramic science principles, to inhibit sorbent densification and so enhance multicycle CO2 uptake under different carbonation-calcination conditions pertinent to sorbent enhanced steam reforming with chemical looping. The mode of operation of modified Ca-based and Na-based sorbents is examined with the aid of scanning and transmission electron microscopy to interpret mulicycle thermogravimetric analysis data

3:20 PM

(MCARE-155-2014) Low-cost Metal Hydride-based Thermal Energy System for High Temperature Solar Power Plants (Invited)

T. Motyka*, C. Corgnale, B. Hardy, R. Zidan, J. Teprovich, B. Peters, SRNL, USA

The major improvement areas for solar plants thermal energy storage (TES) systems are in lowering their costs, increasing their volumetric energy density and increasing their temperature of operation to improve the concentrating solar power plant overall efficiency. Metal hydride TES systems, which couple a high temperature material storage tank with a low temperature material storage tank, have the ability to enable all of these improvements. The paper will show the results of the activities carried out at Savannah River National Laboratory for the DOE's SunShot program. Some potential candidate metal hydride materials have been evaluated and screened against the targets from the SunShot program, relative to cost, volumetric density and working temperatures. Results show that some high temperature Mg-family based materials as well as Ca-hydride and Na-hydride show potential to achieve the cost target of 15$/kWhth. Among the low temperature candidate materials, sodium aluminum hydride material seems to have the best potential to make the system capable to achieve the low cost target. Selected material pairs have also been simulated in the coupled bed configuration, to check their real compatibility and the actual behavior. Results from the screenign analyses and the simulation will be presented.

3:40 PM

(MCARE-156-2014) Borohydrides Based Electrolytes for Rechargeable Magnesium Batteries (Invited)

R. Mohtadi*, F. Mizuno, T. S. Arthur, Toyota Research Institute of North America, USA; S. Hwang, California Institute of Technology, USA

Rechargeable magnesium batteries have been attracting attention as compared to lithium, magnesium offers higher energy density (3833 vs. 2046 mAh/cc), cheaper cost and non-dendritic deposition. Several high performance electrolytes were proposed for magnesium batteries; however they caused corrosion of the battery metallic components. Recently, we proposed novel non corrosive magnesium borohydride based electrolytes. These electrolytes represented the first relatively ionic salts compatible with magnesium metal and therefore, understanding these on a fundamental level would aid the design of future electrolytes. Here, we will show results obtained from systematic spectroscopic and electrochemical studies conducted to help pave the path towards designing future borohydrides based electrolytes for rechargeable magnesium batteries.

4:20 PM

(MCARE-157-2014) Intellipigment™, Chemochromic Pigments for Hydrogen Leak Detection

N. Mohajeri*, HySense Technology, LLC, USA

Hydrogen is one of the most important energy resources in current and future national energy portfolio and creating a safe environment for its producers and utilizers is of utmost importance. Presently, the large majority of hydrogen detection has been focused on the development of electronic sensors. Electronic sensors have several drawbacks including loss of sensitivity in the field due to the environmental effects, costs, and problems associated with power required on-site. Thus an alternative cost-effective, high specific chemochromic (visual) leak detector can greatly enhance the market acceptance and expansion of these valuable energy sources. In this presentation, the features of Intellipigment™, a new line of chemochromic pigment product for hydrogen leak detection and produced by HySense Technology, LLC are discussed.

4:40 PM

(MCARE-159-2014) Update on Hydrogen Storage Research and Development Activities in Hawaii (Invited)

D. Birkmire, M. Chong, E. Sadeghmoghaddam, University of Hawaii at Manoa, USA; D. Brayton, A. Narvaez, Hawaii Hydrogen Carriers, LLC, USA; C. M. Jensen*, University of Hawaii at Manoa, USA

A wide variety of hydrogen storage projects are currently underway at the Department of Chemistry of the University of Hawaii (UH) and Hawaii Hydrogen Carriers, LLC (HHC). The fundamental research efforts at UH are currently focused on: 1) the reversible dehydrogenation of borohydrides to boranes; and 2) probing hydrogen-substrate interactions that have isosteric heats of absorption that are intermediate between classic physic-sorption and chemi-sorption. We have shown that magnesium borohydride, $Mg(BH_4)_2$ at 200 °C results in the selective formation of $Mg(B_3H_8)_2$ and that this process can be rapid reversed at conditions as mild as 100 °C and 40 atm H_2. More recently we have found that a modification of the reaction conditions that allows hydrogen cycling between $Mg(BH_4)_2$ and $Mg(B_{10}H_{10})$ thus increasing the hydrogen storage capacity from 2.7 to >7 wt %. The second effort at UH originated from studies palladium-doped, boron containing graphene (BCX) and high surface area, templated carbon by high-pressure solid state 1H NMR. We observed a significant population of hydrogen that is bound to the substrates at room temperature. Our results compliment a steadily increasing set of gas sorption isotherm data that this is meta-sorbed hydrogen, that is hydrogen whose binding energies are intermediate between physic-sorption or chemi-sorption.

5:20 PM

(MCARE-158-2014) Acceptability envelope for adsorption based hydrogen storage (Invited)

B. Hardy, C. Corgnale*, D. Tamburello, D. Anton, Savannah River National Laboratory, USA

Media based H2 storage systems undergo complex, coupled physical processes, making the use of numerical models essential for design and evaluation. Model development requires a significant expenditure of time. Thus, an efficient tool is needed to identify system designs that are likely to meet requirements, prior to conducting detailed evaluations. This work focuses on adsorbent based H2 storage systems. A methodology was developed to assess the ability of an adsorbent system to meet the targets. The analysis is based on a transient model, including mass and energy balances, along with material thermodynamics and gas state equations. The tool can be used to identify the required range of operating conditions, material properties and heat transfer design parameters needed to meet selected targets. The range of acceptable parameters forms a multi-dimensional volume (envelope). The behavior of the adsorption system is described under different conditions. The model is applied in two ways: 1) the chemical and physical characteristics of the most promising of the existing adsorbents are used as baseline data of the analysis to assess the performance of such systems and comparing different materials; 2) the DOE technical targets are considered to determine the required range of ideal adsorbent (i.e. being able to achieve the targets) parameters, which are not known a priori. The results will be presented and discussed.

Solar Power and Concentrators

Concentrated Solar Power

Room: Salon G
Session Chair: Dileep Singh, Argonne National Laboratory

2:20 PM

(MCARE-056-2014) Thermal Energy Storage at High Temperatures (Invited)

S. Neti*, Lehigh University, USA

Renewable energy use is receiving a lot of attention due to a desire to decrease fossil fuel use. By their very nature renewable energy sources are dilute (~1kW/m2) and intermittent in their availability limited to usually about 2,000 hours in a year. Methodologies for the storage of energy are essential for the successful implementation of renewable energy power systems to match demand patterns. Commercial implementations of solar thermal storage systems have relied primarily on sensible heat and a few of the applications that have used phase change materials (PCM) have been at low temperatures. Thermal storage technologies that use encapsulated phase change materials (EPCM) for large-scale (~1,800 MWhth) energy storage at high exergy conditions (220°C to 900°C) are the current focus of discussion. $NaNO_3$, eutectics of $NaNO_3$-KNO_3 and NaCl-$MgCl_2$, $MgCl_2$, NaCl, Zinc, Aluminum and some Oxides have been identified as suitable PCM with stainless steel, carbon steel and ceramics for encapsulation. Issues considered include material properties; heat transfer and energy transfer limitations and related solutions. A cost analysis of these EPCM storage systems indicates that thermoclines for thermal energy storage systems operating around 400°C that use stainless steel encapsulation can be implemented with investments of about $21/kWhth. High temperature TES will require ceramic encapsulation that could use Oxides as PCM.

3:00 PM

(MCARE-057-2014) Development of a High-Temperature High-Efficiency Thermal Energy Storage System for Concentrated Solar Power

D. Singh*, T. Kim, D. France, W. Yu, Argonne National Laboratory, USA; A. Gyekenyesi, M. Singh, Ohio Aerospace Institute, USA

The focus of the presentation is on the development of a high efficiency thermal energy storage (TES) system. As part of this work, we plan to impregnate ultra-high thermal conductivity, low-density graphite foams with a phase change material (PCM) salt, thereby, offering a combined system with conductivities significantly greater than the salt alone. To investigate the effect of the graphite foam, a thermal analysis was conducted of the proposed latent heat thermal energy storage. Based on this analysis it was determined that the solidification thickness/front increased by over a factor of 10 as the effective PCM thermal conductivity increased from 0.3 W/mK (no foam) to 85 W/mK by the addition of the graphite foam. As part of the materials development effort, graphite foam samples were received from a commercial vendor and characterized. Results on the detailed characterizations of the foam samples will be presented, including porosity measurements, coefficient of thermal expansion, mechanical properties and oxidation behavior. Further, use of protective coatings on the graphite foams to prevent oxidation will be discussed.

3:20 PM

(MCARE-058-2014) Heat Transfer Characteristics of Graphite Foam-MgCl2 Thermal Energy Storage Systems for Concentrated Solar Power

W. Zhao*, Argonne National Laboratory, USA; D. M. France, University of Illinois at Chicago, USA; W. Yu, T. Kim, D. Singh, Argonne National Laboratory, USA

Three-dimensional heat transfer analysis was conducted for latent heat thermal energy storage systems in concentrated solar power plants using the commercial software COMSOL. The graphite foam-MgCl2 combination was chosen as the thermal energy storage medium. The objective of the heat transfer simulations was to understand the heat transfer performance of the graphite foam-MgCl2 combination to optimize the design of the latent heat thermal energy storage systems. Because MgCl2 has a very low thermal conductivity of less than 1 W/mK, the graphite foam acts as an additional heat conduction path and remarkably improves the effective thermal conductivity of the graphite foam-MgCl2 combination. Furthermore, the effective thermal conductivity of the infiltrated graphite foam (graphite foam-MgCl2 combination) has a heterogeneous nature based on the current measurements and calculations. It has a higher thermal conductivity in one direction and only half of that in the other two directions. This characteristic of the infiltrated graphite foam was one of the main considerations in the simulations. The melting front in the phase change material during the thermal energy storage process was determined through the heat transfer simulations. The results can be used to optimize the arrangement of the heat transfer fluid pipes in the thermal energy storage tank.

3:40 PM

(MCARE-059-2014) Miscibility Gap Alloys for High Energy Density and Thermal Conductivity Heat Storage

A. J. Rawson*, H. Sugo, E. Kisi, The University of Newcastle, Australia

Miscibility Gap Alloys are combinations of two immiscible materials where a high thermal conductivity matrix contains a low melting point inclusion. Upon phase transition the latent inclusions accept a great amount of energy which may act as thermal inertia for a range of systems. The alloys have many benefits over current state of the art thermal storage systems such as high thermal conductivity, latent heat of fusion and matter density yielding high energy density materials with fast charge/discharge rates. We have developed a range of alloys with phase transitions from <250°C to 1400°C and chemical and thermal stability. The alloys have up to two orders of magnitude greater conductivity than molten salts and paraffin waxes. Energy densities are comparable to the state of the art thermal storage media and the structurally robust alloys may be directly coupled to a working fluid in a thermal cycle. An overview of current research will cover characterising thermal properties, analysing thermal fatigue and developing novel applications. Through Lattice Monte Carlo and Finite Element methods the alloy effective properties are characterised and maximised. Cycled loading investigation will reveal the lifetime performance of the alloys. Applications in Renewable Power and Refrigeration Cycles, Industrial Processes and other areas will be identified.

4:20 PM

(MCARE-060-2014) PV Optics: Analytical Software for Optical Management and Light Trapping in Solar Cells and Modules (Invited)

B. Sopori*, National Renewable Energy Lab, USA; J. Mutitu, W. Shafarman, University of Delaware, USA

The current favored path to lower the cost of photovoltaic (PV) energy is to develop technologies compatible with commercial production of higher efficiency (> 20%) solar cells. This approach requires advanced cell designs as well as simplified fabrication steps. Typically, light management involves: (i) minimizing of reflection (and maximizing transmission) at the front surface for the spectral range useable by the cell, (ii) a device structure that maximizes absorption in regions that contribute to the current in the device, and (iii) minimizing parasitic absorption in regions that do not directly contribute to the device current. An advanced solar cell may have optical structure involving several absorbing layers (or multi-junctions), non-planar interfaces that can lead to light trapping and concomitant enhanced absorption, reflection and antireflection coatings, and metallic regions that carry the current (but also cause optical losses). This paper will give a general review of the considerations for efficient optical management in cells and modules, concepts of light trapping/photon recycling and their application in various types of solar cells for enhancing light absorption. Then, we will discuss some results of PV Optics aimed at optimizing cell configurations for c-Si, a-Si multi-junctions, and for CIGS.

4:40 PM

(MCARE-062-2014) Chemical and Thermal Stability of Molten Nitrate Salts as High Temperature Fluids

P. S. Kubiak*, University of Central Florida, USA; N. Mohajeri, Florida Solar Energy Center, USA; O. S. Ahmed, Y. Sohn, University of Central Florida, USA

Molten nitrate salts as high temperature fluids (HTFs) are one of the most popular methods for the transfer of thermal energy in concentrated solar arrays. However, molten nitrate salts are only capable of operating at temperatures below 600 °C due to chemical degradation of the nitrate group into nitrite. The investigation of nitrate salts as HTFs has focused mainly on the improvement of operating temperature range by the search for better eutectic mixtures, while comparatively little work has been done on understanding and improving their thermal and chemical stability. This study aims to address this by providing a detailed analysis of the degradation mechanisms of these fluids as a function of temperature and impurity concentration. The products of such degradation and the effects they will have on the fluid and its container are of particular interest. Known eutectic mixtures of nitrate salts exhibiting favourable properties will be synthesised using a variety of component purities, and detailed thermal analysis will be carried out using TG/MS, DSC and TPD under a variety of atmospheres. From this study a better understanding of the effects of different components and impurities may be reached, informing the search for improved salt mixtures with higher thermal stabilities. This in turn will allow for greater efficiency of high temperature thermal transfer systems.

5:00 PM

(MCARE-064-2014) Thin film III-V photovoltaics on low-cost, flexible metal substrates using single-crystalline-like Germanium films

V. Selvamanickam*, P. Dutta, Y. Gao, Y. Yao, R. Wang, M. Rathi, E. Galtsyan, University of Houston, USA; P. Ahrenkiel, South Dakota School of Mines and Technology, USA; A. Mehrotra, A. Freundlich, University of Houston, USA

Efficiencies over 40% have been demonstrated with III-V photovoltaics (PV). However, the use of costly substrates has rendered them very expensive for broad terrestrial use. Thin film PV is being pursued by several researchers as a lower-cost alternative to crystalline PV, but their efficiencies are significantly lower. Hence, achievement of single-crystalline-like thin film PV on low-cost substrates can be game changing by combining high efficiency with low cost. We are developing such an architecture that yields single-crystalline-like thin films even on polycrystalline or amorphous substrates using templates made by Ion Beam-Assisted Deposition. Such templates have been used for epitaxial growth of germanium films by reel-to-reel magnetron sputtering. Strongly (400) textured Ge films with an in-plane texture spread of 1° FWHM have been achieved. Optical properties of the Ge films are found to be comparable to that of single crystal Ge and hole mobility values over 900 cm^2/V-s have been achieved. Hetero-epitaxial growth of GaAs thin films by MOCVD has been accomplished on the Ge thin films on metal substrates. The GaAs thin films exhibit strong photoluminiscence and high mobility values. Progress in the development of single-crystalline-like Ge thin films on low-cost substrates for high-efficiency III-V photovoltaics will be presented.

Batteries and Energy Storage

Li-ion Batteries II

Room: Salon E
Session Chairs: Robin von Hagen; Neeraj Sharma, The University of New South Wales (UNSW)

2:20 PM

(MCARE-087-2014) Towards lithium ion 3D microbatteries using TiO2 nanotubes (Invited)

P. C. Knauth*, T. Djenizian, Aix Marseille University-CNRS, France

The development of microbatteries is an important objective for powering microelectronic devices for remote or nomadic use, but they currently lack the necessary power. Three-dimensional (3D) design can significantly improve the power density, by increasing the interfacial area between active components of the battery. In my invited talk, I will present the current status on the development of 3D microbatteries, based on TiO2 nanotubes made by electrochemical anodization of titanium metal films deposited on silicon substrates. The length, diameter and wall thickness of the nanotubes can be designed by changing the electrochemical parameters (potential, time, electrolyte). The remaining back side metal allows direct integration on microelectronic circuitry, because Ti is well known to form TiSi2 with silicon, allowing Ohmic contacts to be formed. Li-ion conducting polymer electrolyte (PEO-PMMA) can be electro-deposited inside the nanotubes, forming a continuous lining. Electrodeposition of the positive electrode material (LiMnOx) on the polymer lining is currently explored and could then give a fully electrochemically fabricated 3D microbattery.

3:00 PM

(MCARE-070-2014) Role of Solution Structure in Solid Electrolyte Interface (SEI) Formation on Graphite (Invited)

B. Lucht*, University of Rhode Island, USA

The investigation of surface reactions of electrolytes with the graphitic anode of Lithium Ion Batteries (LIB) for Electric Vehicle (EV) applications will be presented. In this presentation, we will focus on three novel techniques which have been enabled by the use of Binder Free graphite anodes. The first is a novel method which allows straightforward analysis of the anode SEI by Transmission Electron Microscopy with Energy Dispersive X-ray Spectroscopy. The second, utilizes Multi-Nuclear Magnetic Resonance spectroscopy of the D2O extracts of the cycled anodes. Finally, IR spectroscopy is utilized to assist with the characterization of the electrolyte solution structure. This unique combination of techniques has allow us to develop significant new insight into the anode SEI formation mechanisms and structure.

3:40 PM

(MCARE-071-2014) Graphene Oxide/M2+ Redox Reactions – A Pathway towards Graphene-based Electrode Materials

R. Mueller*, R. von Hagen, R. Raccis, S. Mathur, University of Cologne, Germany

Graphene-based nanomaterials occupy the center stage of current research with respect to the investigation of new and advanced anode materials for Lithium-ion batteries. Whether as phase pure material or as nanocomposites along with various metal oxides, graphene has already been proven of bearing the capabilities to play a key role in the development of next generation rechargeable batteries. In this work, we would like to present a facile microwave assisted reaction for the fabrication of functional graphene/metal oxide nanocomposites. The reduction of graphene oxide (GO) with M2+ ions (M = Sn, Fe, Co) in aqueous media is shown to offer distinct advantages such as effective separation of single and few layered graphene by in situ formed metal oxide nanoparticles as well as stabilization of the oxide phase during electrochemical cycling, leading to anode materials exhibiting high capacities and improved cycling performances. Furthermore, a catalytic route for the controllable reduction of aqueous graphene oxide dispersion will be demonstrated.

4:20 PM

(MCARE-072-2014) Electrochemical-structural relationships probed by in-situ neutron and X-ray diffraction (Invited)

N. Sharma*, The University of New South Wales (UNSW), Australia

Batteries are ubiquitous in society, used in everything from children's toys to mobile electronic devices, providing portable power solutions. There is a continuous drive for the improvement of batteries. A large proportion of the function of batteries arises from the electrodes, and these are in turn mediated by the changes in the crystal structure during an electrochemical process (e.g. battery use). Therefore, a method to both understand battery function and improve their performance is to probe the crystal structure evolution in-situ while an electrochemical process is occurring inside a battery. Our work has utilized the benefits of in-situ neutron diffraction (e.g. sensitivity towards lithium) to literally track the time-resolved evolution of lithium in cathode materials used in lithium-ion batteries. With this knowledge we have been able to directly relate electrochemical properties such as capacity and differences in charge/discharge to the content and distribution of lithium in the cathode crystal structure. In addition, the ability to test smaller samples (e.g. in coin cells) with in-situ X-ray diffraction has allowed us to probe other batteries types, such as primary lithium and secondary sodium-ion batteries. This talk will showcase some of our recent results on electrode structural evolution with respect to electrochemistry in fully functioning batteries.

4:40 PM

(MCARE-073-2014) Stress associated with surface phenomenon in electrode materials for Li-ion Batteries (Invited)

A. Mukhopadhyay*, R. Kali, Indian Institute of Technology (IIT) Bombay, India; A. Tokranov, B. Sheldon, Brown University, USA; X. Xiao, General Motors R&D Centre, USA

Stress development in electrodes during lithiation/delithiation negatively affects the performance of Li-ion batteries. Multi-beam Optical Stress Sensor, in conjunction with custom-made electrochemical (half) cell, has been used for measurement of such stress development in-situ during electrochemical cycling. Formation of solid electrolyte interphase (SEI) on electrode surface results in irreversible Li consumption and cell capacity loss, which gets accrued in case of fracture/disintegration of the SEI layer. In-situ stress measurements with graphitic carbon thin film electrodes allowed analyzing the interrelated changes in voltage, surface reactions and stress development that occur as SEI forms or as Li/solvated Li-ion get inserted. The investigation revealed that SEI formation is associated with nearly 1 GPa compressive stress, which is more than the actual Li-intercalation induced stress by factor of ~4. Experiments involving in-situ stress monitoring during constant voltage holds at different potentials during the first lithiation half cycle, along with HRTEM observations and analysis of SEI layer composition using XPS and SIMS (depth profiling), have indicated that part of the irreversible stress gets developed due to disruption of near surface graphitic structure (at ~0.5V), while considerable fraction of the stress is also borne by the ceramic phases that form at lower potentials.

5:00 PM

(MCARE-074-2014) Nanoscale X-ray Imaging of Advanced Battery Electrodes

R. Winarski*, B. Blaiszik, F. Brushett, L. Trahey, V. Rose, C. Johnson, Argonne National Laboratory, USA

Requirements for higher energy densities, more dynamic cycling, and longer operational lifetimes have directed battery research to studies of fundamental battery operational performance at the nanoscale. New systems will need better overall performance, inexpensive composition and construction, and safe operation. By better understanding chemical interactions at the nanoscale, it is hoped that more efficient systems can be designed and engineered. We are using a combination of nanotomography and nanoscale fluorescence imaging of electrode structures to better understand structural and chemical changes during charge/discharge cycling. Electrodeposited Cu/Sn alloys are inexpensive to produce and have the potential to outperform graphite-based electrodes in rechargeable lithium batteries. It is already known that these alloy electrodes fail due to large volumetric changes during lithium intercalation. Full-field X-ray imaging involves detection of the electrode structures through a 1.5mm diameter capillary and approximately 1mm of electrolyte. The intense X-rays at our beamline allow us to view structural distortions and observe elemental redistribution along the electrode surfaces in-operando. This work was performed at the Center for Nanoscale Materials, a U.S. Department of Energy, Office of Science, Office of Basic Energy Sciences User Facility under Contract No. DE-AC02-06CH11357.

5:20 PM

(MCARE-075-2014) Synthesis of α-Fe2O3 Nanoparticles from Fe(OH)3 Sol and the Hybrids with Reduced Graphene Oxide for Lithium Ion Batteries

J. Sun*, M. Du, C. Xu, Shanghai Institute of Ceramics, Chinese Academy of Science, China; L. Gao, School of Materials Science and Engineering, Shanghai Jiao Tong University, China

α-Fe2O3/reduced graphene oxide (α-Fe2O3/RGO) composite has been synthesized by a facile hydrothermal method. Fe(OH)3 sol is creatively employed as precursor with RGO in lithium ion batteries (LIBs) and the process goes without any nucleating agent. Composites with different ratios between α-Fe2O3 and RGO for comparison are investigated as anode LIB materials. Among the composites, α-Fe2O3/RGO containing 73%α-Fe2O3 exhibits the highest reversible specific capacity of ~ 950 mAh g-1 after 70 cycles at a current density of 100 mA g-1. When the current density is of 800 mA g-1, the capacity still remains ~ 700 mAh g-1, showing superior rate capability. The significant electrochemical property improvements of α-Fe2O3/RGO can be attributed to the uniform α-Fe2O3 nanoparticles (20 - 30 nm) and the RGO substrate, which provides high electrical conductivity and stability.

Tuesday, February 18, 2014

Plenary Session III

Room: Salon E

8:25 AM

(MCARE-PL4-2014) Graphene for Electrochemical Energy Storage

B. Z. Jang*, Angstron Materials, Inc. and Nanotek Instruments, Inc., USA

Recent advancements in the use of graphene for supercapacitors (including electric double layer and redox-based), lithium secondary batteries, and high-power battery cells will be reviewed. Supercapacitors are now at the center stage for designers in the power electronics and electric vehicle (EV) industries. As compared to current lithium-ion batteries, supercapacitors exhibit a much higher power density (can be charged or discharged at a much higher rate), significantly longer cycle life (250,000 vs. 2,000 cycles, for instance), and are much safer. However, conventional activated carbon-based symmetric supercapacitors are capable of storing an energy density of typically < 8 Wh/kg (cell), in contrast to the typically 150 Wh/kg of lithium-ion cells. Significant improvements to the energy density are being made when graphene is used as the electrode active material of a supercapacitor. Graphene is also being implemented as a conductive additive for both the cathode and anode active materials in a lithium-ion battery. In particular, the geometric flexibility, high conductivity, and chemical nature of graphene-based materials have enabled the development of various nano-structured anodes and cathodes. The potential of using graphene as an electrode active material per se in a lithium secondary battery will also be critically reviewed. Our research group has also invented the surface-mediated cells (SMCs), a new type of high-power and high-energy energy storage device. The SMCs are found to exhibit the highest power density of all electrochemical cells ever reported. The principles and limitations of this new high-power device will be discussed.

Hydrogen

Advances in Metal and Complex Hydrides

Room: Salons B - C

Session Chairs: Joseph Teprovich, Savannah River National Laboratory; Ralph Scheicher, Uppsala University

9:20 AM

(MCARE-172-2014) The formation reaction and the hydrogen storage properties of Mg2FeH6 (Invited)

A. Asselli, H. Jacques*, UQTR, Canada

In this study we investigated the formation reaction and the hydrogen storage properties of the complex hydride Mg2FeH6. Samples were prepared by ball milling under Ar and H2 atmosphere mixtures of Mg and Fe or MgH2 and Fe. Kinetics and pressure-composition isotherms of hydrogen absorption/desorption were measured in a Sievert-type apparatus. To investigate the formation reaction of Mg2FeH6, samples were characterized by X-ray diffraction, and scanning and transmission electron microcopy at different stages, e.g., after ball milling and during the hydrogen absorption measurements. Results showed that the milling atmosphere plays a more important role on the Mg2FeH6 synthesis than the starting composition. MgH2 was identified as the Mg2FeH6 precursor. Microscopy analysis showed that Mg2FeH6 is formed from MgH2 by nucleation in the MgH2-Fe interface and it grows with a columnar morphology. Nevertheless, Mg2FeH6 can also be directly formed from Mg and Fe. This direct reaction from the metallic elements occurs at specific conditions of temperature and H2 pressure. Short cycles of hydrogen absorption/desorption revealed a decrease in the hydrogen capacity. It was attributed to the morphology of growth of Mg2FeH6 phase. Efforts have to be made to improve the cyclability and the kinetics of Mg2FeH6.

10:00 AM

(MCARE-173-2014) Hydrogen storage in borohydride and Mg-based materials (Invited)

D. Book*, X. Yi, S. Guo, A. Walton, D. Reed, University of Birmingham, United Kingdom

A number of borohydride compounds have very high intrinsic H2 storage capacity, but require elevated temperatures (200 – 300°C) for H2 desorption and suffer poor reversibility. We have been investigating the storage properties of a range of borohydride-based materials, including LiBH4, Ca(BH4)2, and Mg(BH4)2. We have developed an in situ Raman cell to allow samples to be measured from 30 to 600 °C in 1 to 100 bar H2, and thereby study their dehydrogenation and rehydrogenation behaviour. Different reaction pathways have been identified as a function of H2pressure, during the decomposition of these materials, including the formation of various borane compounds. With a theoretical reversible hydrogen uptake value of 7.6 wt%, Mg is of interest as a potential H2 storage medium. However, the absorption and desorption temperatures need to be reduced (from around 300 to 100 °C), and the sorption kinetics accelerated. The kinetics can be enhanced by introducing a nanoscale microstructure to provide a pathway for H2 diffusion. Mg and Mg-Ni-based alloys have been prepared by rapid solidification using a melt-spinning system. The H2 storage properties were measured using TGA & Sieverts-PCT, and DSC. For a Mg-Ni sample, hydrogen was absorbed under 10 bar H2 at room temperature. The microstructure of the melt-spun and thin film samples have been studied by SEM, TEM and in situ XRD.

10:40 AM

(MCARE-174-2014) Novel multi-purpose metal borohydrides (Invited)

T. 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. We have recently explored mechano-chemical and solvent based methods for synthesis and have discovered new series of metal borohydrides M-M’-BH4, and report an overview of our recent results. This class of materials has extreme structural flexibility, which has led to varieties of new types of materials. In some cases, they hold extreme amounts of hydrogen that may be utilized for hydrogen storage. In other cases, they show very high lithium ion conductivities and may in principle be utilized for preparation of new types of batteries. Novel series of rare earth bi-metallic borohydrides are also discovered, which may have both magnetic and/or luminescence properties. The first nano-porous metal borohydrides were also discovered, with pores in the range of ca. 9 Å, which absorb other smaller molecules, and significant amounts of hydrogen and may contain as much as 20 wt% H2. We conclude, that the chemistry of hydrogen is divers and a lot of new compounds may still be discovered.

11:20 AM

(MCARE-175-2014) Evolution of the physico-chemical properties of nanostructured MgH2 composites upon hydrogen cycles (Invited)

P. De Rango*, S. Nachev, D. Fruchart, CNRS, France; N. Skryabina, Perm State University, Russian Federation; P. Marty, Université Joseph Fourrier, France

Highly reactive nanostructured powders are produced on a large scale by co-milling of MgH2 with transition metals. However, the MgH2 nano-crystallites tend to recrystallize and to induce a progressive swelling of the compacted disks upon cycling. The purpose of this study is to quantify and understand this irreversible phenomenon, through correlations with microstructural evolutions. In-situ dilatometry measurements were performed on samples prepared with different additives. The irreversible phenomenon increases progressively up to about 50 cycles where a stabilisation is achieved. The maximum of deformation strongly depends of the additive. A relaxation of the maximum strain is observed after 50 cycles for Vanadium whereas it remains constant for Ti-V-Cr. SEM and granulometry measurements show that the irreversible dilatation is linked to the coalescence of the MgH2 grains, which tends to create large agglomerates. At nanoscale, it has been correlated to the ability of the fine additive particles to prevent the motion of the grain boundaries, then to limit the recrystallization of MgH2 particles.

Solar Fuels

Solar Fuels: Nanostructuring and Interfacial Aspects in Photoelectrochemical Water Splitting

Room: Salon D
Session Chairs: Hicham Idriss, SABIC; Ru-Shi Liu, National Taiwan University

9:20 AM

(MCARE-027-2014) To what extent the nanostructuring of metal oxide photo-electrodes affects their water splitting efficiency? (Invited)

J. Augustynski*, R. Solarska, P. Barczuk, K. Bienkowski, University of Warsaw, Poland

Several examples from the recent literature show that nanostructuring offers a means to overcome some intrinsic limitations of semiconductor photo-electrodes such as short hole diffusion length or low electron mobility. Although this allows for more effective transport of the charge carriers from the interior of the nanoparticles, that form the photoactive film, to the reactive interface with the electrolyte, it cannot impede the surface recombination. This situation will be illustrated by a comparison of the photo-electrochemical behaviour of a series of thin film metal oxide photo-anodes, either compact or formed from nanoparticles and wholly permeated by the electrolyte, including TiO_2 (both doped and undoped), WO_3 and Fe_2O_3. The essential role of surface reaction intermediates upon the photocurrent efficiency will be delineated.

10:00 AM

(MCARE-028-2014) Advances in quantum confinement effects and interfacial electronic structure for solar water splitting (Invited)

L. Vayssieres*, Xian Jiaotong University, China

The ability to develop novel oxide semiconductor heteronanostructures consisting of highly pure quantum dots/rods entirely made from aqueous chemistry without surfactant at low temperature with controlled surface chemistry and having intermediate bands for high visible light energy conversion and highly quantized band structure for band engineering is demonstrated. Such unique characteristics, combined with the in-depth investigation of their electronic structure at synchrotron radiation facilities as well as optical, structural and transport properties provide comprehensive fundamental understanding of the energetics and structure-property relationships as well as key trends for efficiency optimization. For instance, doped and/or quantum dot sensitized bundled iron oxide oriented quantum rods showing full visible light absorption profile while still being stable against photo-corrosion for efficient and low cost solar hydrogen generation by direct water splitting at neutral pH and very low bias is presented. In addition, the latest development in quantum size effects on electronic structure, surface chemistry and electrical properties of large bandgap semiconductor will be exposed and discussed to improve solar hydrogen generation.

10:40 AM

(MCARE-029-2014) In-situ soft x-ray spectroscopy study of mesoscale interfacial phenomena in solar fuel generation (Invited)

J. Guo, Lawrence Berkeley Natl Lab, USA ; C. Dong*, National Synchrotron Radiation Research Center, Taiwan

Advanced technology arises from the understanding in basic science, and both rest in large on in-situ/operando characterization tools for observing related physical and chemical processes directly at the places where and while reactions occur. In many important energy systems such as solar energy conversion, advanced materials and fundamental interfacial phenomena play crucial roles in device performance and functionality due to the complexity of material architecture, chemistry and interactions among constituents within. To understand and ultimately control the interfaces in solar fuel generation calls for in-situ/operando characterization tools in which soft x-ray spectroscopy offers many unique features. This presentation reports the development of in-situ reaction cells for soft x-ray spectroscopic towards the studies of photosynthesis and catalytic reactions in recent years. The challenge has been that soft x-rays cannot easily peek into a high-pressure catalytic cell or a liquid photoelectrochemical cell. The unique design of the in-situ cell has overcome the burden. Some of the instrumentation design and fabrication principle are to be presented, and a number of experimental studies of nanocatalysts are given as the examples, e.g. the experiment for studying the hole generation and dynamics of photoelectrochemical catalysts under operando conditions.

11:20 AM

(MCARE-030-2014) Self-Powered Flexible Electronic Systems (Invited)

K. Lee*, Korea Advanced Institute of Science and Technology, Republic of Korea

This seminar introduces three recent progresses that can extend the application of self-powered flexible inorganic electronics. The first part will introduce self-powered flexible piezoelectric energy harvesting technology. Energy harvesting technologies converting external sources (such as vibration and bio-mechanical energy) into electrical energy is recently a highly demanding issue. The high performance flexible thin film nanogenerator was fabricated by transferring the BaTiO3 thin film from bulk substrates. Second, we report the nanocomposite generator (NCG) for achieving a simple, low-cost, and large area fabrication based on BaTiO3 (or PZT) nanoparticles and graphitic carbons (CNT or RGO). The second part will introduce flexible electronics including memory and large scale integration (LSI). Flexible memory is an essential part of electronics for data processing, storage, and radio frequency (RF) communication. To fabricate a fully functional flexible memory, we integrated flexible single crystal silicon transistors with an amorphous titanium oxide (a-TiO2) based memristor to control the logic state of memory. Finally, the third part will discuss the flexible GaN LED for implantable biomedical applications. Inorganic III-V light emitting diodes (LEDs) have superior characteristics, such as long-term stability, high efficiency, and strong brightness.

Batteries and Energy Storage

Li-air and Flow Batteries

Room: Salon E
Session Chairs: Madhavi Srinivasan, Nanyang Technical University; Yuxi WANG, TUM CREATE

9:20 AM

(MCARE-076-2014) Insights into Discharge and Charge Chemistries in Li-O2 Batteries from Theory and Experiment (Invited)

L. Curtiss*, K. Amine, Argonne National Laboratory, USA

Nonaqueous Li-O2 batteries have a much superior theoretical gravimetric energy density compared to conventional Li-ion batteries and thus have the potential for making long-range electric vehicles a reality. Two major problems that have limited the successful development of Li-air batteries to date have been related to severe difficulties in attaining reversibility and low charge overpotentials. Recent results from experiment and theory providing insight into the discharge and charge chemistries will be presented. This will include results based on a new cathode architecture that results in a dramatic reduction in charge overpotential. The cathode utilizes atomic layer deposition of small Pd nanoparticles on a carbon surface with an Al2O3 coating for passivation of carbon defect sites. Theoretical calculations show that the low charge potential is enabled by a nanocrystalline form of lithium peroxide with grain boundaries . Density functional studies of the growth and nucleation of lithium peroxide nanoparticles will also be reported and the role they may play in reversibility and charge potenials in Li-O2 batteries. Finally, we will also report results of the role of metal catalysts in Li-O2 batteries.

10:00 AM

(MCARE-077-2014) Recent Development of Lithium Air Battery using Ionic Liquid Based Electrolyte (Invited)

K. Takechi*, Toyota Central R&D Labs., Inc., Japan

One of the key issues in the field of Li-air battery is suppressing decomposition of its electrolyte due to the reaction with oxygen radical species such as superoxide anion radical and/or lithium oxide radical during the discharge process. While many research groups have proposed stable solvents for the electrolyte, we have focused on specific kind of ionic liquids, *N*-methyl-*N*-propylpiperidinium bis-tri(fluoromethansulfonyl)amide (PP13-TFSA) and *N*,*N*-diethyl-*N*-methyl-*N*-(2-methoxyethyl) ammonium TFSA (DEME-TFSA), to meet the required stability as well as non-volatility under the ambient air condition. Li_2O_2 production/decomposition during discharge/charge have confirmed in the battery system, and the mechanism has also been investigated in detail for the both ionic liquids. We also proved that DEME-TFSA provided improved rate capability due to its lower viscosity. To understand and prove the advantages of the ionic liquids, we also developed unique analytical techniques such as the solvent stability test by KO_2 and the quantification method of Li_2O_2 by organic radicals. Those techniques are based on the concept of smart control of the oxygen radical species, and the concept also opens the way to develop new catalysts for the efficient discharge/charge properties. The very recent activity and strategy for the development of lithium air battery in Toyota-team will be presented.

10:40 AM

(MCARE-078-2014) A Novel Refuelable Lithium Battery based on Anodic Lithium Solvated Electrons Solution (Invited)

Y. WANG*, TUM CREATE, Singapore; R. Yazami, K. Tan, Nanyang Technological University, Singapore

Liquid anode has the merits of fast ion transport and stable anode/electrolyte interface. In this work, a novel type of liquid anode based on lithium solvated electrons solution (Li-SES) is developed, which typically comprises a polyaromatic hydrocarbon in terms of naphthalene or biphenyl. We reveal the conductivity of Li-SES as a function of Li content. With a liquid cathode and a ceramic ion conductor electrolyte, a prototype full cell exhibits an OCV close to 3 V at the ambient temperature. To improve the lifespan of the ceramic ion conductor electrolyte used in this Li-SES based battery, a protective thin layer of lithium phosphorous oxynitride (LiPON) is applied. A surface analysis is carried out to further understand the protecting effect. Moreover, we present a prototype cell in form of (-)Li-SES/Ceramic ion conductor/O2(+), showing the practical application of this new anode material in lithium-air battery.

11:00 AM

(MCARE-079-2014) Anion-conducting ionomer membranes for redox flow batteries

M. Di Vona*, Univ. Rome Tor Vergata, Italy; P. C. Knauth, Aix Marseille University-CNRS, France

Redox flow batteries have important potential for large scale energy storage and applications in intelligent grids. All-vanadium redox-flow batteries are one of the most investigated examples; they work in acidic solutions and perfluorinated sulfonated acidic polymers are mostly used as ionic conducting separation membrane. However, this type of membrane presents problems related to cation permeation and insufficient long time stability. In this presentation, we will show our current work on the development of anion-conducting membranes that can significantly reduce the cation permeation and improve the redox-flow battery operation. We have explored various synthesis pathways to obtain anion-conducting membranes. One involves the chlorosulfonation of fully aromatic polymers, such as Poly-ether-ether-ketone (PEEK), followed by amination with various secondary amines. In a third step, the sulfonamide group reacts with an acid solution to obtain an ammonium group fixed on the macromolecular chain and a mobile counter-anion. Another synthesis route is based on chloromethylated aromatic polymers that react with a tertiary amine. The synthesis routes and relevant ionomer properties, including thermal stability, mechanical properties and ionic conductivity, will be discussed.

11:20 AM

(MCARE-080-2014) Nano-structured carbon-based electrodes materials for high-performance vanadium redox battery

C. Flox*, C. Fabrega, M. Skoumal, T. Andreu, J. R. Morante, Catalonian Institute for Energy Research, Spain

Vanadium redox flow battery (VRB) using a newly developed flexible nano-structure materials as electrode is analyzed and its potential performances discussed. The use of nano-electrochemistry features leads to a highly performances that become mandatory to innovative designs and components in VRB system. These nano-structured electrode materials have been synthesized by electro spinning techniques and offers several advantages in comparison with commercial micro-structured felts, i.e. higher surface area, higher electrical conductivity, binder free materials, excellent mechanical, chemical stability, cost-effective, etc. showing an excellent electron transfer properties. The electrochemical characterization using electrochemical impedance spectroscopy and cyclic voltammetric techniques and charge and discharge test have been applied in order to evaluate the electrocatalytic activity. The electrocatalytic activities of the nano-structured electrode have been improved and the reversibility of the VO2+ /VO2+ and V3+/V2+ redox couples increased greatly using several electrolytes. The VRB tested systems exhibit higher coulombic efficiency (>98%) and energy efficiency (>90%) than that with the commercial felts. Consequence on the lifetime, cycling number and improved cost figures will be discussed and its suitability for renewal energy storage or its adaptation for smart grid considered.

11:40 AM

(MCARE-081-2014) Organic-inorganic hybrid anion conducting materials for alkaline fuel cell

P. Zhang*, K. Miyajima, Noritake Co., Limited, Japan; T. Yamaguchi, Tokyo Institute of Technology, Japan; A. Gopinathan M., Noritake Co., Limited, Japan

Alkaline type fuel cell (AFC) is the first commercial device, among various types of FCs, but not become popular due to the lack of good electrolyte membranes. This research aims to develop an hybrid ionic conducting material for AFC, based on layered double hydroxides (LDHs), also known as an anionic clay. Mg-Al LDHs were synthesized from Mg and Al nitrates by a co-precipitation or homogeneous precipitation method, followed by the characterizations using XRD, TG-DTA, and FT-IR techniques. The results suggested that ionic conductivity of LDHs could be increased by decreasing the particle size or crystallinity. Furthermore, the layered structure of LDHs was modified by interlayer intercalation, and zwitterionic surfactant (glycine betaine) intercalation could significantly increase the conductivity of LDHs from 0.056 mS/cm to 0.390 mS/cm under low humidity condition (80C, R.H. 20%). Moreover, delamination was found extremely effective to increase the ionic conductivity of LDHs. These hybrid LDHs are expected to find potential application in the development of composite hybrid electrolyte membranes for alkaline fuel cells.

Nanocomposites and Nanowires Materials for Photovoltaic and Photonic Technologies

Nanocomposites and Nanowires Materials for Photovoltaic and Photonic Devices I

Room: Salon G

Session Chairs: S. Ravi Silva, University of Surrey; Can Xue, Nanyang Technological University

9:20 AM

(MCARE-108-2014) Nanotube and nanowire photonics for photovoltaic devices

G. A. Amaratunga*, H. Butt, T. Butler, R. Rajashekaran, H. Zhou, P. Hiralal, Q. Dai, T. D. Wilkinson, University of Cambridge, United Kingdom

Vertically aligned carbon nanotubes(VA-CNT), ZnO and Si nanowires(NW) can now be realised with defined lengths and spacings in array structures, enabling the exploration of engineered structures in which additional electromagnetic interactions are induced. First the photonic crystal properties of CNTs and Si NW are examined through simulation and confirmed experimentally. The ability to guide light in the visible range using engineered 'defect' structures within he photonic band gap of the arrays are revealed. It is shown that the photonic crystal properties of CNTs can be used to realise meta-materials in the optical frequencies. Second, the quasi-crystalline (QC) photonic properties of vertically aligned CNTs are examined. A pseudo band-gap together with many sub-band gaps are observed. The experimentally measured diffraction patterns of the QC structures show a remarkably rich structure which agrees with that predicted from Fourier optics. The near ideal light absorbing properties of VA-CNTs forests is used to realise another novel application, micro-Fresnel lenses on Si. The exploitation of these structures in PV applications is discussed. Replacing CNTS with transparent NWs such as ZnO allows similar effects using phase contrast instead. Lastly, the use of ZnO NWs to engineer both favourable UV absorption properties as well as providing wide band anti-reflective properties of organic solar cells is presented.

10:00 AM

(MCARE-109-2014) Plasmonic Metal-Semiconductor Nanostructures for Solar Energy Conversion (Invited)

N. Wu*, West Virginia University, USA

Plasmonic nanostructures have great potential in photocatalysts, photoelectrochemical cells and photovoltaic devices. Herein we present the metal-semiconductor composites for improvement in the solar energy conversion efficiency of semiconductors. Both the core-shell nanoparticle and the nanohole array-nanorod structures of metal-semiconductor composites have been proved to be effective in enhancing the solar energy harvesting. This talk also presents the underlying mechanism of the surface-plasmon resonance induced charge separation in the semiconductor. Recent studies show that plasmon can induce the charge separation via three pathways: (i) light trapping, (ii) direct electron transfer, and (iii) plasmon-induced resonance energy transfer from metal to semiconductor.

10:40 AM

(MCARE-110-2014) Metal-TiO2 Composite Nanofibers for Plasmon-Enhanced Solar-to-Hydrogen Conversion (Invited)

C. Xue*, Z. Zhang, Nanyang Technological University, Singapore

We present the preparation of electronspun TiO2 nanofibers co-decorated with Au and Pt nanoparticles. By using these composite nanofibers, we demonstrate the direct evidence of plasmon-enhanced hydrogen generation through through dual-beam irradiation. The Au/Pt/TiO2 nanofibers exhibit certain activity for hydrogen generation under a single irradiation at 420 nm that excites the defect/impurity states of TiO2. Significantly, when a secondary irradiation at 550 nm is introduced to simultaneously excite Au SPR, we observed 2.5 times higher activity for hydrogen generation. Further investigations by finely controlling the irradiation wavelengths reveal that the enhancement factor on hydrogen generation is directly correlated with the plasmon absorption band of the Au nanoparticles in the Au/Pt/TiO2 nanofibers. The enhancement is attributed to the promoted charge separation and photothermal effect upon SPR excitation. Our observation and the enhancement principle would have impact to future plasmonic nanocomposite design for efficient solar energy conversion.

11:20 AM

(MCARE-111-2014) Designing Plasmonic Nanostructures and Quantum Dots for Solar Cell Applications (Invited)

D. Ma*, INRS, Uni Quebec, Canada

Organic photovoltaics (PVs) provide an attractive feature of easy and low-cost fabrication even for large area devices. However their energy conversion efficiency cannot compete with that of inorganic PVs partially because they are only able to strongly absorb “visible” photons, while leaving about 50% of the solar energy in the near infrared (NIR) untapped. In this talk, I will present some of our most recent development in the NIR quantum dots (QDs), such as PbS QDs and PbS@CdS QDs, and their application in PVs. One example is about the controlled hybridization of NIR PbS QDs with carbon nanotubes (CNTs) and their further integration into poly(3-hexylthiophene), which is a hole-transporting polymer. The nanohybrid cells show considerably enhanced power conversion efficiency, which is attributed to the significantly extended absorption in NIR by PbS QDs and the effectively enhanced charge transportation due to CNTs. On the other hand, plasmonic nanostructures have been recently explored for enhancing the efficiency of solar cells. Our recent work on some interesting plasmonic nanostructures (such as Ag nanorices and nanocarrots) that have strong resonances in the NIR regime, and their application in solar cells will also be briefly highlighted. Finally solution processed heterojunction inorganic solar cells based on TiO2 nanorods and QDs will be briefly introduced.

Plenary Session IV

Room: Salon E

1:35 PM

(MCARE-PL5-2014) Recycling and materialization of rare earths with energy sustainability

H. Chae, H. Choi, S. Kim, B. Kim, T. Kim*, Korea Institute of Industrial Technology, Republic of Korea

Rare metal becomes a critical issue due to its drastic increase in industrial demand as well as its rarity. In order to assure it, the recycling among various approaches is vividly conducted in both the scientific and industrial regimes due to a limitation of natural resources with the mass energy consumption. So that convergence in the processes is proposed by these authors, so called RECYMAT (recycling & materialization), as summarized in Fig.1. It means that the materials in-put for recycling move to industry without disposal. In this investigation, an example of RECTMAT is briefly introduced using the recycling of rare earth (Nd-Fe-B) magnets. Those are widely used in various industries such as voice coil motors in hard disk drive, magnetic generators for magnetic resonance imaging and electrical motors equipped in future vehicles. Looking at the process, Nd among Nd-Fe-B magnet scrap was selectively diffused into Mg in the liquid temperature range. On the other hand, Fe-B remains without any reaction with Mg, being a candidate element for high strength Fe-Nd base metallic glass. We will discuss the result obtained by the reaction parameters such as time, temperature, vacuum, etc.

Hydrogen

Fundamentals Studies and Hydrogen Interactions with Nano-Materials

Room: Salons B - C

Session Chairs: Bart van Hassel, United Technologies Research Center; Rana Mohtadi, Toyota Research Institute of North America

2:10 PM

(MCARE-168-2014) Nano Materials for Hydrogen Storage (Invited)

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 field 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.

2:50 PM

(MCARE-169-2014) Elucidation of Hydride Interaction with Carbon Nanostructures and the Formation of Novel Nanocomposites for Energy and Storage Devices (Invited)

J. A. Teprovich*, H. Colon-Mercado, B. Peters, R. Zidan, 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 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. It was determined that a nanocomposite prepared using a 6:1 mole ratio of LiH and C_{60} produced a material that can reversibly store 5 wt % H2 via a chemisorption mechanism and that it spectroscopically resembles a hydrogenated fullerene. Further study of these materials has demonstrated that they could potentially serve as components of new energy storage and covnersion devices.

3:10 PM

(MCARE-170-2014) Nanoconfined hydrides for hydrogen storage and electrochemical conversion (Invited)

C. Zlotea*, Y. Oumellal, S. Bastide, C. Cachet-Vivier, CNRS ICMPE UPEC, France; C. Matei Ghimbeu, C. Vix-Guterl, CNRS IS2M, France; M. Latroche, CNRS ICMPE UPEC, France

Nanosizing and nanoconfinement of metal hydrides are currently emerging as promising routes for the design of new hydrogen storage media and negative electrode materials for lithium ion batteries. Hydrogen storage involves solid-gas interactions in materials whereas electrochemical application relies on Li driven reactions where the metal hydride reacts with lithium ions to form metal/alloy and lithium hydride. The present work reports on the synthesis and properties of hybrid materials obtained by nanoconfinement of Mg-based hydrides within the mesopores of different carbon hosts. The hybrids are synthesized by decomposition and/or reduction of metal precursors directly within the pores of carbon host. Nanoscale effects on physicochemical and thermodynamic properties will be discussed as well as hydrogen sorption and electrochemical behaviors. Experimental results revealed that the hydrogen sorption properties are significantly enhanced by nanoconfinement. The effect of different confining carbon hosts on the fundamental and hydrogen sorption properties will be also addressed. Moreover, the nanoconfined hydrides show promising electrochemical properties. This synthetic strategy holds promise for enhanced hydrogen storage and electrochemical properties and opens the route to better understanding of the underlying nanochemistry.

3:50 PM

(MCARE-171-2014) Measure hydrogen distribution in nano-sized metals: hydrogen microscopy techniques (Invited)

A. Pundt*, University of Goettingen, Germany

Nano-sized metals offer many sites for hydrogen absorption that differ from the conventional interstitial lattice sites, for example sites at grain boundaries or sites at surfaces and interfaces. Thus, the hydrogen distribution strongly depends on the distribution of these defects. Also, the local stress state influences the distribution of hydrogen and further on, the hydride formation. Methods are required that allow measuring the local hydrogen concentration, ranging from the nanometer scale to the micrometer scale. Three different methods will be discussed in this presentation: 1) the tomographical atom probe that allows to measure the hydrogen (deuterium) distribution with atomic resolution [1], 2) the Protron-Proton microscopy [2] with its ultra-high sensitivity and the hydrogenographical microscopy [3] with the largest field of view. These methods allow a detailed view on local hydrogen concentrations such as those at metal/metal, metal/oxide interfaces or at defects. It will be further shown, that hydride formation preferentially happens locally in regions of strong stress-release. The combination of these three methods allows a more detailed view into the hydrogen solution and hydride formation properties of nano-materials. [1] Gemma et al.,Ultramicroscopy 109 (2009) 631. [2] P. Reichart et al., Science 306 (2004) 1537 [3] J. Kürschner, S. Wagner, A. Pundt, JALCOM submitted.

4:30 PM

(MCARE-172-2014) Effect of uniaxial strain on the site occupancy of hydrogen in vanadium: density-functional calculations (Invited)

R. Johansson, R. Ahuja, O. Eriksson, B. Hjörvarsson, R. H. Scheicher*, Uppsala University, Sweden

The preferred site occupancy of hydrogen atoms in uniaxially strained body-centered cubic vanadium has been investigated by density functional based methods. Hydrogen will occupy either tetrahedral or octahedral interstitial sites where the preferred site occupancy is linked to the strength of the uniaxial strain field. The strain field is in itself determined by the concentration and location of hydrogen in the lattice, causing local strains that combine to give rise to a change in volume. Once a critical hydrogen concentration in vanadium is reached, this hydrogen-induced volume change will lead to a change in preferred site occupancy causing a sudden self-amplified shift between tetrahedral and octahedral occupancy. The obtained results point to a hysteresis behavior of tetrahedral and octahedral occupancy in the range of hydrogen concentrations [H/V] of 0.21-0.43. This phenomenon has been experimentally observed and the theoretical calculations presented here provide an atomistic insight to this observation.

Science and Technology of Hydrogen Adsorption

Room: Salons B - C
Session Chairs: Patricia De Rango, CNRS; Theodore Motyka, SRNL

4:50 PM

(MCARE-167-2014) Tutorial on Sorption Storage (Invited)

R. Chahine*, P. Bénard, D. Cossement, R. Zacharia, J. Xiao, Hydrogen Research Institute, Canada

R&D efforts are being directed toward improving the efficiency and economics of hydrogen storage systems to make hydrogen fuel cells competitive, and enable larger than 500 km driving ranges for a wider variety of transportation applications. The majority of today's fuel cell vehicles rely on high-pressure tanks rated at 350 or 700 bar for onboard storage of hydrogen gas. One of the pursued alternatives is cryosorption on nanoporous materials (such as activated carbon, polymers, and metal organic frameworks) due to its inherent reversibility, cyclability, and fast kinetics. While advanced sorption material development is generally directed toward increasing the activity of surface area and hence the excess gravimetric energy density and/or the temperature of operation; hydrogen storage systems need to simultaneously satisfy a set of technical requirements including but not limited to: usable gravimetric and volumetric energy densities, min/max pressure and temperature operability, well to power plant efficiency; acceptable thermal loads and dormancy, charging/discharging rates and fuel purity. We present a set of cascading computing tools that enables a preliminary performance assessment of the storage system based on the knowledge of the basic crystal structure of the constituent adsorbent material. It bridges the gap between materials development and system analysis. Moreover, when it is applied backward it helps orienting materials optimization.

5:30 PM

(MCARE-165-2014) Dense Carbon Monoliths for High Pressure Gas Adsorption

M. Kunowsky*, J. Marco-Lozar, F. Suárez-García, Universidad de Alicante, Spain; J. Carruthers, ATMI, Adsorbent & Gas Technology, USA; ÁNGEL. Linares-Solano, Universidad de Alicante, Spain

Carbon monoliths (CM) with high densities are studied as adsorbents for the storage of H_2, CH_4, and CO_2 at ambient temperature and high pressures. The starting CM (produced by ATMI Co.) was activated under a CO_2 flow at 1073 K, applying different activation times up to 48 hours. Micropore volumes, pore size distributions, and apparent surface areas were deduced from N_2 and CO_2 adsorption isotherms at 77 K and 273 K, respectively. H_2 isotherms were measured up to 20 MPa, CH_4 and CO_2 isotherms up to 3 MPa. The BET surface area of the starting CM (940 m^2g^{-1}) could be significantly increased up to 1580 m^2g^{-1}, and the developed porosity is almost exclusively comprised of micropores < 1 nm. Remarkably high volumetric adsorption amounts are reached for H_2 (10 g l^{-1}), CH_4 (110 g l^{-1}), and CO_2 (440 g l^{-1}). These are higher than for other, high surface area adsorbents, and can be contributed to the high densities of the CMs, which decreased only slightly from 1.0 g cm^{-3} to 0.8 g cm^{-3} upon CO_2 activation. A scale-up study was performed with two tank cylinders, each with a volume of 2.5 liters. One of the cylinders was filled with the starting CM, while the other one remained empty. Measurements were performed for the three studied gases, using maximum pressures of 2 MPa. The findings confirm the results obtained on laboratory scale and reveal the suitability of high density activated carbon monoliths for gas storage application.

5:50 PM

(MCARE-166-2014) Hydrogen densities greater than liquid hydrogen at 77 K in engineered carbon nanospaces

P. Pfeifer*, University of Missouri, USA; A. Gillespie, University of Missouri, USA; E. Dohnke, University of Missouri, USA; Y. Soo, University of Missouri, USA

In response to the DOE's quest for sorption-based hydrogen storage materials that meet the 2017 volumetric storage capacity target of 40 g H2/L system for light-duty fuel cell vehicles, stored densities—total mass of hydrogen stored per volume of pore space—were measured in high-surface-area carbons with variable nanopore structure. Stored density includes the adsorbed film and non-adsorbed gas, and consequently lies between the density of bulk H2 and the density of the adsorbed film at the respective pressure and temperature. Stored densities up to 85 g/L were observed at 77 K and 200 bar, well in excess of 71 g/L, the density of liquid H2 at 20 K and 1 bar, and well above the liquid-gas critical point of H2, 33 K ("supercritical condensation"). Samples have exceptionally low void fractions (0.49-0.70), maxima of gravimetric excess adsorption at exceptionally low pressures (~25 bar), and exceptionally high binding energies (8-10 kJ/mol) consistent with deep potential wells in narrow, 0.7-nm pores. Depending on pore structure, the stored densities do/do not saturate around 200 bar. The resulting saturated film densities outperform previous saturated H2 film densities, 51-69 g/L, in metal-organic frameworks at 50-55 K, by as much as 20% at a 40-50% higher temperature.

Solar Fuels

Solar Fuels: Photonic and Plasmonic Engineering of Water Splitting Photo Catalysts

Room: Salon D
Session Chairs: Leonhard Mayrhofer, Fraunhofer IWM; Jan Augustynski, University of Warsaw

2:10 PM

(MCARE-031-2014) Plasmon-enhanced Upconversion Nanoparticles in Photoelectrochemical Water Splitting (Invited)

R. Liu*, C. Chen, C. Chen, National Taiwan University, Taiwan; S. Hu, National Taiwan Normal University, Taiwan

We report a near-infrared-driven photoelectrochemical water splitting using ZnO nanorod-array decorated with CdTe quantum dots and plasmon-enhanced upconversion nanoparticles. The plasmon enhanced the intensity of the upconversion emission, which improved the photocurrent and the gas evolution rate of the photoelectrochemical reaction greatly. We will demonstrate a process of utilizing NIR to drive the photoelectrochemical water splitting reaction. The Au-UCNs can significantly enhance the upconversion emission intensity by plasmonic effect. Thus, the enhancement of photocurrent and gas evolution was achieved. The results offer a convincing demonstration that energy can be converted from NIR to chemical fuel. We believe that our strategy is fundamental to the design of solar energy devices and should become an accepted technique for solar energy utilization at the NIR and IR regions.

2:50 PM

(MCARE-032-2014) Local structural and chemical property changes of Pt and Pd nanoparticles during catalysis (Invited)

S. Han*, E. Jeong, C. Park, I. Hwang, Z. Jin, J. Park, Chonbuk National University, Republic of Korea

Pt nanoparticles are well-known catalysts and also can be used to generate hydrogen. We investigated the local structural and chemical properties of Pt nanoparticles on various substrates including SiO2, TiO2/SiO2, and ZrO2/SiO2 during catalytic reactions by using in-situ X-ray absorption fine structure (XAFS) measurements. In order to understand the redox of Pt nanoparticles, XAFS data were taken in the temperature range of T = 300 – 720 K in O2 and H2 environments. XAFS analysis at Pt L3 edge showed that the oxidation and the reduction of Pt are quietly sensitive to not only temperature but also supporting materials. The catalytic efficiency of a catalyst is directly related to its size. XAFS results revealed that Pt nanoparticles aggregated to a Pt cluster on SiO2 supports. However, no Pt aggregation was observed when SiO2 supported was covered with TiO2 or ZrO2. XAFS analyses at Ti and Zr K edges suggested that there were strong bonds of Pt-Ti and Pt-Zr pairs. We also studied the local structural and chemical properties of Pd nanoparticles on grapheme. We will discuss the role of supports as well as the local structural and chemical properties of catalytic nanoparticles during catalysis.

3:30 PM

(MCARE-033-2014) Hydrogen production from water; the effect of photonic and plasmonic properties (Invited)

V. Jovic, University of Auckland, New Zealand; K. Wahab, O. Maher, SABIC-CRI, Saudi Arabia; G. Waterhouse, University of Auckland, New Zealand; J. Llorca, UPC, Spain; H. Idriss*, SABIC-CRI, Saudi Arabia

Hydrogen production from water is one of the most promising methods to secure renewable sources for energy in general and chemical industry in particular. There are many methods for producing hydrogen from water and these include reducible oxide materials (solar thermal material), artificial photosynthesis and photocatalysis. At present about ½ of the total amount of H2 produced in the world is used in the ammonia synthesis process. In this work we are addressing the effect of photonic band gap materials and plasmonic responses of Au on the photocatalytic hydrogen production from water over Au/TiO2 and Au-Pd/TiO2 catalysts. By tuning the photonic band gap (PBG) to the electronic band gap (EBG) of Au/TiO2 catalysts enhancement of the photocatalytic water splitting to hydrogen under direct sunlight is achieved. The high photocatalytic activity is attributed to suppression of a fraction of electron-hole recombination rate due to the co-incidence of the PBG with the EBG.

Solar Fuels: Doping of TiO2 for Efficient Water Splitting

Room: Salon D
Session Chairs: Lionel Vayssieres, Xian Jiaotong University; Sang-Wook Han, Chonbuk National University

4:20 PM

(MCARE-034-2014) Tuning the Fermi Level and the Kinetics of Surface States of TiO2 Nanorods by Means of Ammonia Treatments

C. Fabrega*, D. Monllor-Satoca, S. Ampudia, A. Parra, T. Andreu, J. Morante, IREC, Spain

In this work, we present the effects of ammonia treatment on TiO2 rutile nanorods with the aim of improving its photoelectrochemical activity by both tuning the energy Fermi level position and introducing more active surface states that increase holes average lifetime. By tuning the Fermi level position the charge separation was optimized by adjusting the depletion region width to maximize the potential drop inside TiO2 and also filling surface states that lead to a decreased electron-hole recombination mediated by them. Also, by increasing the density of surface hole-traps, which were identified as surface hydroxyl groups, we extended holes lifetime, which is ultimately the limiting factor on the water photooxidation mechanism. Furthermore, nitrogen doping lead to the introduction of a new absorption band that resulted in actual photoactivity within the 420 to 480 nm range. IPCE up to 60% where obtained by this method compared to barely 10% of the non treated samples. A model, based on fundamental physical parameters (e.g. donor density, Fermi level position, depletion width and surface states) is proposed to disclose the relevance of each interfacial property on the observed photoefficiency modification. This model provides a logic that can be used for designing a more rational and tailored material modification that can be also extended to other oxides.

4:40 PM

(MCARE-035-2014) Engineering the electronic properties of titania by doping. An ab-initio approach

L. Mayrhofer*, M. Moseler, Fraunhofer IWM, Germany

Efficient separation of the photoexcited electron-hole pairs is one of the major requirements for high solar energy to hydrogen conversion efficiency in photoelectrochemical cells based on semiconductor materials. Hence the controlled engineering of the electric potential profile across the photoactive semiconductor electrode promises considerable progress towards economic hydrogen production. Here we present our results from ab-initio calculations on the possibility of shifting the electronic bandstructure of titania by incorporation of various metal and nonmetal dopants. Special attention will be paid to the effect of localized defect states and the generation of defect state bands at high dopant concentrations.

5:00 PM

(MCARE-036-2014) Co-doping as a tool to increase photo-electrochemical activity of TiO2 photo-anodes

P. Barczuk*, K. Bienkowski, J. Augustynski, University of Warsaw, Poland

The major drawback of titanium dioxide that is the most widely used photo-catalytic material is its low photo-electrochemical activity under solar light illumination due to the large band-gap energy of 3.2 to 3.0 eV. In order to shift the optical absorption spectrum of TiO2 towards visible light, the doping with a large number of foreign elements both cationic (transition metal elements) and anionic has been attempted. Although such doping generally results in some visible light photo-activity, its counterpart is frequently a drastic decrease of the overall photo-catalytic activity due to the increased charge recombination. In order to avoid formation of the oxygen defects or other recombination centers, co-doping with transition metal cations of varying oxidation state is explored. Such approach allows maintaining charge balance in the TiO2 layer and preventing the formation of the recombination centers. In order to facilitate co-doping of the TiO2 with different elements the sol-gel method was used to obtain both anatase and rutile thin films.

5:20 PM

(MCARE-037-2014) Effects of nano- structuring on TiO2 based photocatalytic materials

Y. Goenuellue*, S. Mathur, University of Cologne, Germany; B. Saruhan-Brings, German Aerospace Center, Germany

In recent years, the well-studied and understood properties of a bulk material are put together with the new properties acquired from its nanostructured counterpart, which in the most cases enables making improvements in applications and device performance. Furthermore the enhanced chemical interactions of the material for photocatalytic applications, high specific surfaces are responsible for the observed improved efficiency of nano materials. Titanium dioxide (TiO2) has attracted considerable attention due to its high potential for application in solar cells, electronics and photo-catalysis based on its excellent chemical stability, semi-conductive properties, non-toxicity and low cost. During last decades, TiO2-based nano-structures have been made more efficient by changing the morphological features and chemical compositions for instance photo-catalysis to gas sensors. In this work, self-ordered and vertically oriented the TiO2 NTs were obtained via electrochemical process by anodization of titanium or its alloy. The TiO2 NTs were modified with different doping techniques to investigate the effects of nano-structuring on photocatalytic application. The TiO2 NTs and also hydrogenated TiO2 NTs were investigated for photocatalytic applications in terms of photoelectrochemical (PEC) measurements.

Batteries and Energy Storage

Sodium-ion Batteries

Room: Salon E
Session Chairs: Sridhar Komarneni, Pennsylvania State University; Dany Carlier, ICMCB-CNRS

2:20 PM

(MCARE-082-2014) Titanate Anodes for Sodium Ion Batteries (Invited)

M. Doeff*, M. Shirpour, Lawrence Berkeley National Laboratory, USA

Identification of a suitable anode material is essential for successful development of sodium ion batteries, because graphite, the most commonly used anode for lithium ion batteries, does not undergo sodium insertion reactions to any appreciable degree. Titanates are one class of materials that are of interest for these devices, based on considerations of earth abundance, low toxicity, reasonable cost, and the probability that redox reactions will take place at low voltages vs. Na+/Na. In the Na-Ti(IV)-O system, several stepped layered and tunnel compounds that can act as hosts for sodium ions are easily synthesized and are redox-active. Tunnel compounds, although structurally robust, have low capacities for sodium due to site limitations, but may be useful in devices targeted to grid storage or other applications not requiring high energy density. Layered compounds exhibit either two-phase or solid solution behavior in electrochemical cells, depending on the exact details of the structure. Some of these are electroactive at extremely low potentials (~0.3V vs. Na+/Na), a feature that may enable high-energy Na-ion cells to be developed. For this presentation, we will discuss the relationship between structure and the physical and electrochemical properties of selected titanate compounds of interest for use in sodium ion batteries.

3:00 PM

(MCARE-083-2014) Advanced materials for low cost Na- ion batteries (Invited)

T. Rojo*, University of the Basque Country, Spain

The development of sodium ion batteries is moving at a much faster rate and its use in the market is expected to be in near future. The choice of electrode materials is a crucial aspect to get an optimized battery. A great range of compounds is being studied as possible cathode materials for Na-ion batteries, from oxides Nax[Fe1/2Mn1/2]O2 to phosphates NaFePO4, fluorophosphates Na3V2O2x(PO4)2F3-2x (where 0≤x≤1) or pyrophosphates Na2FeP2O7 . With respect to the anode materials, unlike the lithium ion batteries, the inability of sodium to insert into graphite, and the up to know uncertain formation of a stable SEI layer is hindering the advance towards preparing full sodium ion batteries. The most used materials utilized as anode are hard carbons, titanates (Na2Ti3O7), Na alloys and phosphorus composites. New Polymer nanohybrids materials, exhibiting conductivities of around 10-5 S cm-1 at 25C and with good conductivity and mechanical properties, have been recently published which can be used as polymer electrolytes for Na-ion batteries. In this talk we will present the most interesting materials for Na-ion batteries and the relationship between the structure and the electrochemical properties of these compounds.

3:40 PM

(MCARE-084-2014) Na2S-P2S5 based solid electrolytes for sodium-ion batteries at room temperature as a renewable source

P. K. Jha*, Thapar University, Patiala, India

The glass samples have been synthesized with composition xNa2S + (100−x)P2S5 for (35 ≤ x ≤ 55) by melt quenching method. The melt quenched samples were characterized by XRD, DTA/TG, FT-IR, Dilatometer, Raman spectroscopy and Impedance spectroscopy. The XRD patterns of all samples showed a broad halo indicated its amorphous nature. Crystallization kinetic is the very important and essential parameters for all glasses have also been calculated. The glass transition and crystallization temperatures of synthesized glasses are found to be different for different compositions. Present glasses have the glass transition temperature lower than silicate, and borate based glasses. Based on DTA/TG results, all the samples are heated above their crystallization temperature to understand the nucleation kinetics of different crystalline phases. FT-IR and Raman study shows that for x = 45 and x = 55 glasses, minor structural changes observed. At ambient temperature, present glasses showed a conductivity in the order of 10-5S/cm-1, which is comparable to that of Li ion based solid electrolyte and can be a substitute for lithium-ion batteries at room temperature.

4:20 PM

(MCARE-085-2014) Designing and investigating novel electrode materials for rechargeable Na-ion batteries with high energy and low cost (Invited)

S. Meng*, J. Xu, C. Ma, University of California San Diego, USA

With the pressing needs for economically feasible and environmentally benign energy storage technologies, Na-ion batteries have re-captured the attentions of the scientific communities due to its natural abundance and broad distribution. In this talk, we report our recent work on layered Na transition metal (TM) oxides, Nax[LiyNizMn1-y-z]O2 (0<x, y, z<1), working as cathode materials in Na-ion batteries. In these compounds, the intercalation in the TM slabs and 2-D transportation of Na-ions occur concomitant with TM redox change during cycling. By identifying the interplay among structural evolution, electronic transition, and electrochemical reactions, the optimized composition is designed and significant improvement in battery performance is achieved. In addition to the cathode study, we have performed a systematic investigation on Na2Ti3O7 as anode in Na-ion batteries, since it is able to provide 177 mAh/g specific capacity at an ultra low voltage, 0.3 V. New phase is identified upon cycling. With carbon coating, the cycling retention and rate performance are enhanced dramatically. The Na-ion full cell fabricated by our group with the two electrode materials above successfully demonstrates high voltage and reversibility, indicating a bright future for Na-ion batteries.

5:00 PM

(MCARE-086-2014) Sodium Layered oxides as positive electrode material for Na-batteries (Invited)

D. Carlier*, M. Guignard, B. Mortemard de Boisse, R. Berthelot, ICMCB-CNRS, France; J. Cheng, C. Pan, NTUST, Taiwan; M. Yoncheva, R. Stoyanova, Bulgarian Academy of Sciences, Bulgaria; A. Wattiaux, ICMCB-CNRS, France; B. Hwang, NTUST, Taiwan; C. Delmas, ICMCB-CNRS, France

Layered oxides AxMO2 (A=Li, Na and M=transition metal) were intensively studied during the 1980's for their electrochemical properties of reversible (de)intercalation of lithium/sodium. Then, for the 20 next years, all researches were focused on lithium batteries that exhibit the high energy density required for portable applications. Since the 2000's, the NaxMO2 phases are studied for potential replacement of the Li-ion technology for stationary applications, where the prevailing parameters are the life time, the low price and the material availability. We recently study several layered materials as positive electrode materials as: NaxCoO2, NaxNiO2, NaxCo2/3Mn1/3O2 and Nax(Fe,Mn)O2. The Mn and/or Fe based systems are especially interesting since Mn and Fe are abundant and non-toxic elements. Depending on the Na/M (and Fe/Mn) ratio and the synthesis conditions several NaxMO2 polytypes could be obtained (O3, P2 or P'3). A detailed study of the initial phases will be presented together with their electrochemical properties in sodium cells. A special focus will be done on the sodium intercalation/deintercalation mechanisms: structural modifications (sheet glidings and/or sodium/vacancy orderings) and redox processes. For these studies, ex-situ and in situ XRD, XAS and Mössbauer spectroscopy have been used as well as ex-situ 23Na MAS NMR and ESR spectroscopies.

Nanocomposites and Nanowires Materials for Photovoltaic and Photonic Technologies

Nanocomposites and Nanowires Materials for Photovoltaic and Photonic Devices II

Room: Salon G

Session Chairs: James Cahoon, University of North Carolina at Chapel Hill; Jordi Arbiol, ICREA and Institut de Ciencia de Materials de Barcelona

2:20 PM

(MCARE-112-2014) Semiconductor nanowires for energy harvesting and conversion (Invited)

S. Gradecak*, MIT, USA

Emerging PV devices based on solution-processable conjugated polymers offer opportunities for the production of low-cost solar cells. To obtain high efficiencies of exciton dissociation and high photocurrent, it is desirable to have an interpenetrating network of electron-donor and electron-acceptor components within the device, referred to as a bulk heterojunction (BHJ). However, current limitations of the all-organic PV devices are inefficient hopping charge transport through the discontinuous percolation pathways in the BHJ films. We have developed an alternative type of nanowire-based solar cells based on organic/inorganic hybrid device structures and demonstrated two distinct hybrid BHJ architectures with enhanced power conversion efficiencies. Furthermore, we have developed a simple method to grow high-quality ZnO nanowires on graphene via the hydrothermal method that preserves the structural and electrical properties of both the nanowires and the graphene. Based on the graphene/ZnO nanowire structure, we have demonstrated graphene cathode-based hybrid solar cells by using two different solution-processed photoactive materials – PbS quantum dots (QDs) and poly(3-hexylthiophene) (P3HT) conjugated polymers – and ZnO nanowires as hole and electron transport layers, respectively. Several critical parameters to further boost the device efficiency and enable scalable and cost-efficient production will be discussed.

3:00 PM

(MCARE-113-2014) Self-Assembled 0D, 1D and 2D Quantum Structures in-a-Nanowire: energy, light and sensing applications (Invited)

J. Arbiol*, ICREA and Institut de Ciencia de Materials de Barcelona, Spain

Inherent to the nanowire morphology is the exciting possibility of fabricating materials organized at the nanoscale in three dimensions. Composition and structure can be varied along and across the nanowire, as well as within coaxial shells. This opens up a manifold of possibilities in nanoscale materials science and engineering which is only possible with a nanowire as a starting structure. As the variation in composition and structure is accompanied by a change in the band structure, it is possible to confine carriers within the nanowire. Interestingly, this results in the formation of local two, one and zero-dimensional structures from the electronic point of view and this, within the nanowire. This novel palette of nano-structures paves the way towards novel applications in many engineering domains such as lasers, high-mobility transistors, quantum information and energy harvesting. Here we summarize and give an overview on recent achievements in the design and growth of advanced quantum structures in nanowire templates. The quantum structures presented have been grown by molecular beam epitaxy and correspond to different confinement approaches: quantum wells (2D), quantum wires (1D) and quantum dots (0D).

3:40 PM

(MCARE-114-2014) Nanofabrication of the superconductive YBa2Cu3O7–x (YBCO) macro-ceramics and electric round wire

A. Rokhvarger*, Retired, USA; L. Chigirinsky, New York University, USA

We developed thermochemical nanotechnology, which results in the full dense sintered YBCO nanocomposite ceramic material, which is electro-conductive at room temperature and superconductive at liquid nitrogen (LN) temperature transmitting with insignificant heat losses dc-current of the extremely high density as can do individual YBCO grains. Metal substrate filament continuously moves through the silicone/toluene-based suspension of YBCO ceramic and silver dope powders. Then, the ceramic nano-crystals of the adhesive coating layer are magnetically oriented and green material is polymerized and fired in a tube furnace where six steps firing mode. There was nanofabricated a self-assembled two-component 3D nano-architecture of the composite ceramics comprising of uniformly oriented and aligned YBCO grains embedded in equal cells located in grain boundary areas. Nano-thick film walls of cells provide uniform 3D network of the vortex pinning centers. The self-controlled thickness of the ceramic coating layer of HTS round wire is ~10 microns, which makes this wire flexible. Developed HTS-YBCO wire is reliable in air and LN and its broad application would save 10% of the generated power and 5 - 10x decrease diameters of cables and sizes and weights of other electricity using equipment and systems incl. photovoltaic systems.

4:20 PM

(MCARE-115-2014) Nanowire-based structure integration for artificial photosynthesis (Invited)

C. Liu*, N. P. Dasgupta, J. Tang, P. Yang, UC Berkeley, USA

From both a scientific and social viewpoint, the conversion of solar energy into fuels has become one of the important topics that people are trying to address. By taking the advantage of large surface area and effective charge collection, nanowire could be applied as efficient building blocks for a fully integrated system of solar-to-fuel conversion. Here it is shown that precise control of the construction and optimization for nanowire-based structures could be achieved from sub-monolayer up to microns, which leads to attractive energy-conversion properties for both efficiency and material cost. The idea of nanowire-based structrue also demonstrates an advance to biomimick the natural photosynthesis by spatially control the whole photosynthetic process at microscopic level.

5:00 PM

(MCARE-116-2014) An 11.1% efficiency nanowire solar cell (Invited)

J. Haverkort*, Y. Cui, J. Wang, S. Plissard, A. Cavalli, L. Gao, A. Standing, Eindhoven University of Technology, Netherlands; M. Verheijen, Philips innovation Services, Netherlands; E. Bakkers, Delft University of Technology, Netherlands

We demonstrate a 11.1% efficiency InP nanowire (NW) axial p-n junction solar cell. The nanowire arrays were grown with in-situ HCl etching on an InP substrate patterned by nanoimprint lithography and the NWs surfaces were cleaned after growth by piranha etching. We find that the post growth piranha etching is critical for obtaining a good solar cell performance. With this procedure, a high diode rectification factor of 10**7 is obtained at ±1V. The resulting NW solar cell exhibits an open circuit voltage (Voc) of 0.73V, a short circuit current density (Jsc) of 21mA/cm**2 and a fill factor (FF) of 72.5% at 1 sun. This yields a power conversion efficiency of up to 11.1% at 1 sun, 10.3% efficiency at 12 suns, and a constant efficiency at very low power, as required for in-house applications. We will also report photo-electrochemical hydrogen evolution on InP and wurtzite GaP nanowires by using Molybdenum Sulfide electrocatalysts. We will report a phtocathode conversion efficiency of 4.1% for InP NWs and a short circuit current of 7.1 mA/cm**2 for GaP NWs.

5:40 PM

(MCARE-117-2014) Characterization of Piezoelectric Nanogenerators Based on ZnO Nanostructures for Self-powering Nanodevices

C. Periasamy, MNNIT-Allahabad, India; P. Sreenath, Indian Institute of Technology (BHU), Varanasi, India, India, Indian Institute of Technology (BHU), Varanasi, India, IndiaSociety Integrated Technology Applied Research), Bangalore, India; P. Chakrabarti*, Indian Institute of Technology (BHU), Varanasi, India, India

The miniaturization of a system involving nanoscale devices is highly constrained by the size of traditional batteries and their recharging/replacement. Therefore, self-powering sources are urgently needed for independent, sustainable, maintenance-free, and continuous operation of such small electronics.For mobile, implantable and personal electronics, solar energy may not be the best choice in many situations. Mechanical energy, including vibration, airflow, and human physical motion, on the other hand may be tapped as an alternative source of energy. We developed a nanogenerator based on platinum rectifying contact on ZnO nanoneedle arrays (NNA) that exploits the piezoelectric property of ZnO for conversion of mechanical energy into electrical energy. The output voltage electrical pulses of nanogenerator are negative and have an average amplitude of around 8-15mV. A finite element simulation was performed in order to understand thepower generation mechanism of the ZnO nanoneedles under applied external stress theoretically by using multi-physics COMSOL software.The simulated results are in good agreement with our experimentally measured data. The simulation tool can be used for optimization of the device. This kind of self-power generating device can be used to develop a battery-less smart systems (MEMS/NEMS) for future applications.

Poster Session

Room: Waters Edge Ballroom

(MCARE-P001-2014) Improving properties of 0.4Li2MnO3-0.6LiNi1/3Co1/3Mn1/3O2 Cathode Materials with Coating LiNi0.5Mn1.5O4

Y. Chen*, K. Xie, Y. Pan, Z. Chen, National University of Defense Technology, China

Lithium- and Manganese-rich cathode materials are currently receiving significant interest for improving the capacity. Both two components of the xLi2MnO3-yLiNi1/3Co1/3Mn1/3O2 have the same framework offer good structure compatibility, but exist large irreversible capacity loss[1] and structure transformation[2] when initially charged to 4.5V or higher. Hence there are many researchers focus their interest to investigate the possibility of integrating core-shell structure on reducing the irreversible capacity loss and improving cycle stability[3]. In this respect, this paper is mainly on the improvement of electrochemical properties of 0.4Li2MnO3-0.6LiNi1/3Co1/3Mn1/3O2, As the core prepared by co-precipitation method, Shell material of LiNi0.5Mn1.5O2 has been integrated onto the surface of the core with assistance of PVP, since PVP has an effect of constraining particle size. For discussion, both the coated and pristine sample were post-treated at the same thermal condition. In a compare of first charge-discharge process of the coated and pristine sample, a remarkable change in the activate process, as coating bring up first cycle efficiency from 73.3% to 83.7% operated at a voltage of 2.0~4.8V vs Li0 at an current rate of c/20(1c=250mAh/g). An an enhancement of cycling properties can also be achieved after coated.

(MCARE-P002-2014) Electrochemical Cycle Life Improvement in RuO2 Nanoplate Architectures

L. Meda*, A. Navulla, Xavier University of LA, USA

Ruthenium oxide (RuO2) nanoplate architectures were grown directly on stainless steel current collector by chemical vapor deposition at low temperatures, 400 °C using ruthenocene, Ru(C5H5)2 as the starting precursor without applying any catalyst. Columnar RuO2 nanoplate of desired thicknesses 800, 450, 400, 320 and 230 nm were obtained by varying the experimental conditions. As-prepared materials were characterized by powder X-ray diffraction and field-emission scanning electron microscope techniques. Galvanostatic charge-discharge experiments were carried out on all the samples versus Li-metal. We obtained extremely high capacity (>1000 mAh/g) beyond the conversion reaction (4Li + RuO2 <——> Ru + 2Li2O, 806 mAh/g). Improved cyclic performance was observed in all the samples when compared to RuO2 nanoparticles and polycrystalline bulk materials. A sample (320 nm thickness) coated with 50 nm of lithium phosphorus oxynitride shows a greater improvement in cycle life.

(MCARE-P003-2014) Metal Organic Chemical Vapor Deposition of α-Fe2O3 nanoparticles and their Electrochemical Properties

A. Dangerfield*, A. Navulla, L. Meda, Xavier University of Louisiana, USA

Transition metal oxides have been studied widely as an anode material for lithium ion batteries due to their high reversible capacities, chemical stability, and low cost. Fe is one of the more abundant metals among the various transition metals and its oxide form, α-Fe2O3 possesses a fairly high capacity of 960 mAh g-1. Direct growth of nanomaterials on current collectors leads to efficient charge transport, and no need of polymer binder and conductive carbon. Because of the preceding facts, α-Fe2O3 nanoparticles have been deposited directly on stainless steel by metal organic chemical vapor deposition (MOCVD) using a volatile precursor material, Fe(acac)3 (acac=acetylacetonate). As prepared materials were characterized by powder x-ray diffraction (PXRD), field emission scanning electron microscope (FESEM) and Cyclic Voltammetry techniques. Galvanostatic charge-discharge experiments were carried out versus Li metal and the details will be presented.

(MCARE-P004-2014) Direct Growth of High-Capacity Manganese Oxide via Chemical Vapor Deposition

M. Jones*, Xavier University of Louisiana, USA

Transition metal oxides have a capacity of 1000 mA*h/g, much higher than that of graphite (372 mA*h/g). They store charge through conversion reactions with lithium metal, where electrochemical reduction leads to the transfer of two or more lithium ions. Low cost, abundant metals, such as Mn, have the potential to provide scalable alternatives for electrode materials. MnO nanomaterials have been deposited directly on stainless steel via chemical vapor deposition (CVD) methods using Mn(acac)2 (acac: acetylacetonate), a volatile precursor. The as-deposited MnO was characterized using scanning electron microscope and x-ray diffraction techniques and found to have a controllable film thickness of less than 100 nm and a cubic structure. Electrochemical charge-discharge experiments versus Li metal yield a high experimental capacity of 975 mA*h/g during the first cycle and high cyclability (>150 cycles). Direct growth of these materials on current collectors is beneficial because it can provide electrical contacts to the current collector, efficient charge transport, and empty space sufficient to accommodate changes in volume. It also eliminates the need for polymer binder and/or conductive carbon, which are currently required for transition metal oxides in battery application.

(MCARE-P005-2014) β-Fe2O3 Nanomaterials by Chemical Vapor Deposition for Innovative Li-Battery Anodes

C. Maccato*, G. Carraro, Padova University, Italy; D. Barreca, CNR-IENI and INSTM, Padova University, Italy; M. Cruz-Yusta, Universidad de Córdoba, Spain; A. Gasparotto, Padova University, Italy; J. Morales, Universidad de Córdoba, Spain; C. Sada, Padova University, Italy; L. Sanchez, Universidad de Córdoba, Spain

The development of suitable materials for rechargeable Li-ion batteries (LIBs), in view of their possible applications in electrical vehicles, portable electronic tools, and implantable medical devices, represents an important and critical challenge. Among the possible candidates, iron oxide is a promising option due to its non-toxicity, low-cost and abundance. Unfortunately, hematite (α-Fe2O3), the most stable and common iron oxide polymorph, presents significant capacity losses upon cycling. This drawback has encouraged the fabrication of more electrochemically efficient materials. A valuable option in this context is offered by a less investigate iron oxide polymorph: β-Fe2O3. Basing on these considerations, in this work innovative β-Fe2O3 nanomaterials have been deposited by CVD and tested as LIB anodes, yielding capacity values up to ca.1300 mAxhxg-1 at low cycling rates thanks their controlled nano-organization, thickness and mass density.

(MCARE-P006-2014) CuxO-TiO2 (x = 1, 2) Nanomaterials by CVD: Promising Anodes for Thin Film Lithium Batteries

D. Barreca*, IENI-CNR and INSTM - Padova University, Italy; G. Carraro, A. Gasparotto, C. Maccato, Padova University and INSTM, Italy; M. Cruz-Yusta, J. Gomez-Camer, Universidad de Córdoba, Spain; C. Sada, Padova University, Italy; J. Morales, Padova University and INSTM, Italy; L. Sanchez, Universidad de Córdoba, Spain

In the last decade, metal oxides have been studied as efficient anode materials for innovative lithium batteries, thanks to their ability to reversibly store a high Li amount. On the other hand, the application of such oxides is still challenging due to their low electronic conductivity and large volume changes upon cycling. An appealing option is the preparation of supported nanocomposite oxides with tailored structure and composition, avoiding the use of any ancillary additive. In the present work, a novel CVD preparation route to

CuxO-TiO2 (x = 1, 2) has been developed trough the following steps: i) growth of CuxO nanomaterials on polycrystalline Ti slides; ii) over-dispersion of TiO2 particles on CuxO. Thanks to its versatility in tailoring the system composition and morphology, the adopted strategy allowed to achieve attractive electrochemical performances due to the intimate contact between CuxO and TiO2 and the synergistic exploitation of their properties.

(MCARE-P007-2014) Facile synthesis of nitrogen-doped graphene-ultrathin MnO2 sheets composites and their electrochemical performances

X. Song*, P. Zhang, L. Gao, School of Materials Science and Engineering, Shanghai Jiao Tong University, China

Nitrogen-doped graphene-ultrathin MnO2 sheets composites (NGMCs) were prepared through a one step hydrothermal method at low temperature (120 °C). Ultrathin MnO2 sheets were well-dispersed and tightly anchored on graphene sheets, which were doped with nitrogen simultaneously. NGMCs electrode exhibited enhanced capacitive performances relative to those of undoped graphene-ultrathin MnO2 sheets composites (GMCs). As the current density increased from 0.2 to 2 A/g, the capacitance of NGMCs still retained 74.9%, which was considerablely higher than that of GMCs (27%). Moreover, over 94.2% of the original capacitance was maintained after 2000 cycles, indicating a good cycle stability of NGMCs electrode materials.

(MCARE-P008-2014) Carbon coated layered LiNi0.44Mn0.31Co0.25O2 cathode materials with enhanced electrochemical performance

M. Barman*, S. Mitra, Indian Institute of Technology Bombay, India

Due to the high cost, safety issues and toxicity of cobalt, efforts are underway to replace the presently used layered material (LiCoO2) by another layered material like LiNi0.44Mn0.31Co0.25O2, as active cathode material for Li-ion battery. The relatively less expensive LiNi0.44Mn0.31Co0.25O2 -based cathode material shows greater usable capacity as compared to LiCoO2, but suffers from capacity fade during cycling with high rates. To address these issues, we have explored the possibility of coating the cathode active LiNi0.44Mn0.31Co0.25O2 materials, synthesized via by self-combustion method and solid-state process, with carbon via ball milling process. The presence of fairly uniform carbon coating is confirmed by SEM and TEM study. Galvanostatic charge-discharge cycling against Li-metal reveals that the carbon coated LiNi0.44Mn0.31Co0.25O2 samples possess improved cyclic stability and enhanced capacity retention at the higher current rate.

(MCARE-P009-2014) Electrochemical properties of CNT-SnO2-Li4ti5O12 anode for lithium ion battery with hihg capacity

L. Ji Yea*, J. SeungHyn, L. SeokHee, L. KangSoo, W. SungPil, L. YouNa, Y. Young Soo, Gachon university, Republic of Korea

SnO2 has been investigated as an anode material for lithium ion batteries. Because SnO2 have a high theoretical electrical conductivity, and good mechanical properties. However, large volume expansion and agglomeration of tin based nanocrystals during the alloying and dealloying processes affect the decreasing capacity retention. SnO2/ multi-Walled carbon nanotubes (MWCNTs) composite was synthesized by a solution method. Then Li4Ti5O12 has been synthesized on SnO2/ MWCNTs, to improve reversible capacity of electrode, rate capability, strength and safety. The SnO2/ MWCNTs showed a reversible capacity 50 mAh/g after 70cycle (0.1 C). But . additional Li4Ti5O12 / SnO2/ MWCNTs showed a reversible capacity 140 mAh/g after 70cycle (0.1 C) and shows remarkable capability by maintaining 79% of the capacity at SnO2/ MWCNTs (vs SnO2/ MWCNTs /Li4Ti5O12). Consequently, that excellent cycling stability with a capacity retention of 90%.

(MCARE-P010-2014) The revisit of potential of optical fiber modification as solar concentrator/transportation

J. Wang*, NSYSU, Taiwan

Solar energy could be an almost paid-free energy in certain areas if specific technologies can be developed. One of key technology is solar concentrator. First, we would like to revisit the potential of optical fiber as solar concentrator. The dopant, fiber design, wavelength dependence, and thermal effect on the concentrator, transmission, generation properties of solar will be addressed. Furthermore, to exploit efficiently solar energy for any applications, improving the transmission of incident sun light at all wavelengths and all directions is one of common solution but critical. In this study, the transmission at visible, NIR and IR regions from various incident angles of sun light as function of various characteristics of specialty fibers is also discussed.

(MCARE-P011-2014) Synthesis and characterization of preceramic copolymers from ferrocenylsilane by living anionic polymerization to prepare SiC ceramics

Y. Gou*, H. Wang, T. Mao, X. Tong, National University of Defense Technology, China

Linear polyferrocenylsilane(PFS) has been intensively investigated due to its novel magnetic, optical and catalytic properties. There are ferrocene and organic silicon units presented alternatively in its molecular chains. As PFS homopolymers or block copolymers can be pyrolyzed to prepare magnetic porous SiC ceramics, in this work they were used as the precursor system which were synthesized by living anionic polymerization. Firstly, the monomer 1,1'-ferrocenylsilane was prepared and characterized by IR, NMR, etc. The results of gel permeation chromatography showed that the homopolymers and block compolymers obtained by anionic polymerization of the monomers had narrow molecular weight distribution. By changing the ratios of the monomer, co-monomer and initiator (n-butyllithium), the molecular weight, polymeric structure, composition and ceramic yield were well controlled. We can precisely synthesize the target precursors with specific elemental composition and molecular weight. By adjusting the macromolecular state through the self-assembly of the PFS polymer system, the regulation of final ceramic microstructure can be achieved.

(MCARE-P012-2014) Surfactant Free Nanocomposites as Highly Active Catalysts for the Hydrolytic Dehydrogenation Hydrogen from Ammonia Borane

C. Shao*, H. Wang, J. Wang, National University of Defense Technology, China

Recently, ammonia borane complex (AB, H_3NBH_3) is considered to be a distinguished candidate for "on-board" hydrogen applications among all other practical hydrogen storage materials and suitable catalysts is essential for AB to generate hydrogen upon room temperature by hydrolysis reaction. In this study, monodipsperse palladium(Pd) nanoparticles on reduced graphene oxide (RGO) surfaces were successfully prepared by "wet" and "clean" method in aqueous solution. Without any surface treatment, Pd nanoparticles are firmly attached to the RGO sheets. These RGO/Pd nanocomposites exhibited catalyst active in hydrogen generation from the hydrolysis of ammonia borane (AB). Their hydrolysis completion time and activation energy were 12.5 min and 51±1 $kJ \bullet mol^{-1}$, respectively, which were comparable to the best Pd-based catalyst reported. The TOF values (mol of $H_2 \bullet$(mol of catalyst • min)$^{-1}$) of RGO/Pd is 6.25, which appears to be one of the best catalyst among previously reported. We had also incorporated ^{11}B NMR spectrum to investigate the mechanism of this catalytic hydrolysis process. This simple and straightforward method is of significance for the facile preparation metal nanocatalysts with high catalytic activity on proper supporting materials.

(MCARE-P013-2014) Improving Hydrogen Properties of Magnesium Borohydride with M(NH2)(2)(M=Na,Li,Mg)

A. Bateni*, M. Somer, Koc University, Turkey

Mg(BH4)2 with 14.9% has a high potential of becoming one of the most important hydrogen storage materials. However,it has some drawbacks such as,several decomposition pathways and limitations in thermodynamics. For improving thermodynamic properties,one approach is to destabilize Mg(BH4)2 by combination with amides. In this study, three systems, Mg(BH4)2-NaNH2,Mg(BH4)2-LiNH2,Mg(BH4)2-Mg(NH2)2, with 1:1 molar ratio are hand milled for 20 minutes in a N2 filled glove box. Mixtures are analyzed using XRD,TG/MS and IR. The XRD diagram of first blend shows formation of NaBH4 due to metathesis reaction.The XRD pattern in second mixture reveals the presence of MgH2 and LiNH2 and XRD pattern of third system consist of Mg(NH2)2. The existence of amorphous Mg(BH4)2 is proved by IR spectroscopy in all mixtures. According to TG/MS results, H2 onset temperatures for three systems are 543,443 and 473K,respectively. Moreover, NH3 release in last two systems is highly suppressed and also the release of B2H6 in the latter blend is the lowest among the other systems. Interestingly, the dehydrogenation in Mg(BH4)2-Mg(NH2)2 mixtures occurs in two steps, unlike the other blends and pure Mg(BH4)2 which release their hydrogen in three and four steps,respectively. The reduction of the decomposition pathway in the magnesium borohydride/amide blend could be a valuable hint for how to improve the recyclability of Mg(BH4)2.

(MCARE-P014-2014) Influence of support on catalytic (from Ni and Fe functionalized reduce graphene oxide catalysts) in the steam reforming of ethanol for hydrogen production

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Hydrogen is, at present, mainly used as raw material for the chemical and refining industries. The main process for hydrogen production includes steam reforming of natural gas, which is based on a fossil resource and is always associated with the emissions of local pollutants. Therefore, due to the expected increasing demand for energy together with environmental concerns related to reducing atmospheric pollution. An alternative and promising way to produce hydrogen is to use ethanol as the feedstock for the steam reforming process. This alcohol has several advantages compared to fossil fuels but the most important is probably its renewable origin. It can be easily obtained from several biomass sources, including through the fermentation of sugarcane. As a material, graphene oxide (GO) has demonstrated promising physical and chemical properties across a wide range of applications, including the development of novel catalysts and active surfaces. In this study, a comparison between Ni and Fe-supported reduce graphene oxide catalysts in the ethanol steam reforming to produce hydrogen is reported. The promising results shown here support future investigations of our catalys nanocomposite.

(MCARE-P015-2014) Growth of TiO2 nanosheets on SiC nanofibers for promising nanocomposite photoelectrodes

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This work shows a novel nanocomposite mat synthesized by directly growth of TiO2 nanosheets (TiO2 NSs) arrays on the SiC nanofibers (SiC NFs) mat via simple hydrothermal method as promising material for photoelectrodes. In this nanocomposite, TiO2 NSs are designed as high performance material for UV sensitive photocatalytic matrix and SiC NFs act as catalysis supports and also as a charge-transfer material. The synergetic effect between TiO2 and SiC and the unique charge transport property of the nanofibrous mat may endow the new nanocomposite with excellent performance by greatly retarding the recombination of photoinduced electrons and holes and electron trapping. SiC NFs mat were synthesized by carbonthermal reduction reaction between Si powders and electrospun carbon nanofibers at 1300 °C. Subsequently hydrothermal reaction was carried out in a tetrabutyl titanate (0.15 mol/L) solution to grow TiO2 NSs on SiC NFs. The SEM image of TiO2 NSs/SiC nanocomposite displays that TiO2 with the morphology of nanosheets uniformly distributes on the surface of SiC NFs. TiO2 NSs is about 98nm in width and several nanometers in thickness. The XRD pattern of resultant nanocomposite reveals that anatase phase TiO2 NSs were obtained and cubic crystal structure SiC NFs were fabricated. This TiO2 NSs/SiC nanocomposite mat may also be of interest in catalysis, sensors and separation technology.

(MCARE-P016-2014) GaNP Nanowires – a Novel Material System for Solar Cell Applications

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Dilute nitrides is a novel material system that has been recently suggested for applications in intermediated band (IB) solar cells. The purpose of this work is to investigate effects of N incorporation on band structure of dilute nitrides-based GaP/GaNP core/shell nanowires (NWs) using optical spectroscopies. The studied NWs were grown on Si substrates by gas-source molecular beam epitaxy. They had an axial length of ~2.5 μm, a shell thickness of ~50 nm, and a typical diameter of the GaP core of ~110 nm. N incorporation was found to cause the following changes in optical properties of NWs. Firstly, a dramatic increase of photoluminescence (PL) intensity was observed and was accompanied by a shortening of the PL decay time. This indicates that the formed GaNP alloy has a direct band gap, advantageous for increasing light absorption. Secondly, splitting of conduction band (CB) states was observed, as judged from a red shift of the fundament absorption edge and a matching blue shift of the Γ CB state. The lower state can then be utilized as IB. And finally, an efficient two-step absorption process via defect states was observed for photon energies below the GaNP bandgap. This effect can be utilized to extend the spectral range of light absorption. The revealed changes in the band structure are potentially beneficial for the applications of GaNP/GaP NWs in novel IB solar cell structures with a high efficiency.

(MCARE-P017-2014) Efficient counter electrode based on pyrenecarboxylic acid-grafted reduced graphene oxide in dye-sensitized solar cells

W. Rho*, T. Mahmoudi, H. Yang, Y. Hahn, Chonbuk National University, Republic of Korea

In dye-sensitized solar cells (DSSCs), platinum (Pt) is the most commonly used catalyst for iodide/triiodide electrolytes to counter electrode because of its high activity and stability. However, Pt is an expensive metal to use in DSSCs. Several functional materials such as CoS, conductive polymer, carbon, and inorganic oxide are one of the alternatives for iodide/triiodide electrolytes due to high conductivity, chemical stability, and low cost. Carbon black, carbon nanotube, graphite, and graphene are also one of the efficient carbon materials for counter electrode. Graphene is a 2-dimensional crystal of sp2 grafted carbon atoms and used for electronics and optoelectronics because of its high electrical conductivity, chemical and mechanical robustness, optical transparency, and specific surface area. Here, we are demonstrated pyrenecarboxylic acid-grafted reduced graphene oxide (PCA-rGO) for iodide/triiodide elelctrolytes in DSSCs. PCA-rGO is simply prepared at low-temperature reduction method and has high solubility and conductivity of ~ 1.52x105 S/m. By incorporating the PCA-rGO as catalyst for iodide/triiodide based redox electrolytes to counter electrode, the energy conversion efficiency is improved due to its high conductivity and stability. Our method will contribute to the lower cost counter electrode in DSSCs and the large-scale applications.

(MCARE-P018-2014) Bulk heterojunction (BHJ) hybrid solar cells with nanoimprinted ZnO layer

H. Yang*, W. Rho, V. Muhammad, Y. Hahn, Chonbuk National University, Republic of Korea

Bulk heterojunction (BHJ) hybrid solar cells have attracted considerable interest due to their fundamental research and application. Organic p-type donor polymers and inorganic n-type acceptor metal oxides are the most widely used in BHJ hybrid solar cells. The most important advantage of ZnO is higher electron mobility, high transparency, and excellent electrical properties than other metal oxide. However, the charge separation between the organic polymers and the inorganic metal oxides does not show more efficiency because the excited electrons far from interface may recombine with holes during the transporting to ZnO layer. Nanostructured metal oxide has spatially distributed interfaces for charge separation and direct pathways for collecting electrons and holes. Here, we have demonstrated the well-ordered nanostructured ZnO by nanoimprint and its application for hybrid solar cells. The energy conversion efficiency of the hybrid solar cells with well-ordered nanostructures of ZnO is improved due to decreasing recombination and increasing light trapping.

(MCARE-P019-2014) Study & Characterization of Semiconductor Nanowires as Sensing Interfaces for Electrochemical Biosensor Applications

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The ability to optically, electrically and magnetically detect the state of biological systems and species is continually being researched, through innumerable advances in electrical detection techniques. Even though optical & magnetic procedures continue to grow and evolve, electrical detection methods, by-far, continue to remain the most desirable. Nanowires (NW) are emerging as powerful platforms for creating robust & sensitive electrical sensors for biological detection. Their 1D morphology offers significant improvements in sensitivity & specificity. The synthesis and study of semiconductor NW in biosensors have increasingly being taken up as research options worldwide, for a wide spectrum of materials. This paper will specifically deal with the study of common & technologically relevant semiconductor materials, such as Si & ZnO, which have currently become the face of interdisciplinary bio-electrochemical research. Electrical transport properties of semiconductor NW for electro-biosensing operations will be studied. The applications of these NW as potential interfaces for Field Effect Transistor (FET) biosensing will be dealt with. Further, the paper will also address the pros & cons of fabricating such NW based devices & will conclude by reviewing the limitations and predicting the route towards which future research in this arena might be directed.

(MCARE-P020-2014) The Influence of Dopants on the Defect Structure and Sinterability of Actinide and Rare-earth Oxides

J. Henderson*, Netzsch Instruments, USA

Actinide and rare-earth oxides are used in applications ranging from nuclear fuels and burnable poisons to fuel cells, catalyst components and so on. Many of these materials are sintered in off-stoichiometric conditions, which impacts the quality of the oxide and hence its ultimate performance. Despite the impressive amount of work done on this subject many open questions remain. Clearly, the diffusion (→sintering) is controlled by temperature and the defect structure and concentration. These defect properties are, in turn, controlled in part by stoichiometry, i.e. oxygen-to-metal ratio (O/M). The purpose of this work was to quantify the interrelationship between O/M, defects and diffusion and their impact on sinterability. The materials investigated were UO_2, CeO_2 and CeO_2-$GdO_{1.5}$ blends. The measured thermal expansion and O/M data on the single-component systems clearly demonstrate the impact of stoichiometry on sinterability. In the case of the more complex powder blends, the data show that stoichiometry plays an even more important role, because not only is the sintering of the solutionized system O/M dependent, but the diffusion of the gadolinia dopant into the fluorite structure as well. The simultaneous dopant diffusion and sintering create, in some cases, a blocking mechanism which compromises final density and can only be explained with the aid of O/M data.

(MCARE-P021-2014) Evolution and Controlling of Defects during the Preparation of Continuous High-temperature Resistant SiC(Al) Fibers

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Continuous high-temperature resistant SiC(Al) fibers were prepared by polymer-derived method using polyaluminocarbosilane (PACS) as the precursor. The formation and evolution of defects formed in the preparation of continuous high-temperature resistant SiC(Al) fibers were investigated through the analysis of continuous PACS green fibers, cured products, pyrolysis process and continuous SiC(Al) fibers. The results showed that there were two major types of defects in the continuous PACS green fibers: pits and inclusion. These defects were difficult to be eliminated during the next processes. Other new defects can be formed during the preparation process under improper conditions, especially during the pyrolysis and sintering processes. The properties of the fibers are greatly affected by the defects. It could reduce the formation of defects and prepare high performance SiC(Al) fibers if effective measures are taken according to the formation mechanism of defects.

(MCARE-P022-2014) Structure of zirconium alloy consolidated by high voltage electric discharge consolidation

E. Grigoryev, L. Lebedeva*, E. Olevsky, NRNU "MEPhI", Russian Federation; E. Olevsky, San Diego State University, USA

High-density samples of the alloy Zr +1% Nb were obtained by high voltage electric discharge consolidation (HVEDC). Optimal parameters of the HVDEC strongly depend on the initial properties of consolidated powders, in particular, on the conductivity of metal powders and alloys at different applied mechanical pressures. The conductivity of metal powders is strongly dependent on the size distribution of powder particles. Thereby it is necessary to know the influence of particle size and particle shape of a powder on the processes of high voltage electric discharge consolidation. The impact of mechanical pressure on the value of the conductivity of the powders was studied. Apart from the above mentioned, the influence of current pulse amplitude on the final density of the consolidated zirconium powder alloy samples was investigated for different applied pressures. We established the maximum amplitude of the current density above which the consolidation process becomes unstable. This research was supported by the Ministry of Science and Education of Russian Federation (grant Contract 11.G34.31.0051).

(MCARE-P023-2014) Novel biogas purification design utilizing Botryococcus braunii as a method of carbon capture

Y. Shin*, J. Albanese, M. Chen, J. Chiao, L. Cho, H. Huang, P. Puppala, B. Lin, M. Meyerson, A. Sekaran, D. Wang, C. Zhou, M. Yu, University of Maryland, College Park, USA

Biogas is an alternative energy source produced from the anaerobic digestion of organic matter by bacteria. It is composed primarily of methane and carbon dioxide (CO2), with trace amounts of other toxic compounds such as hydrogen sulfide (H2S). The presence of CO2 lowers the energy yield from biogas combustion. Past studies have used expensive and environmentally harmful chemicals to purify biogas. This study involved the design and construction of a biogas purification system that utilizes the microalgal species, Botryococcus braunii, as a form of carbon capture. Using biogas produced by anaerobic digestion, H2S was removed from the biogas using a steel wool scrubber. CO2 was then removed from the gas with a water scrubber, and the CO2 laden water was then fed to the microalgae. This method has the distinct advantage of being renewable due to the self-propagation of the microalgae. The microalgae also produces hydrocarbon products that can be utilized as a biofuel. We expect our biological system to purify biogas to a degree similar to that of most commonly used chemical methods while increasing cost-efficiency, thereby creating a viable energy source.

(MCARE-P024-2014) Catalytically enhanced combustion in porous media utilizing thermoelectric devices for power conversion

B. T. Beaman*, M. D. Robayo, A. Terracciano, B. Hughes, N. Orlovskaya, R. Chen, University of Central Florida, USA

Highly porous silicon carbide ceramic is used to support combustion inside a steel casing chamber. A premixed methane fuel and air are used to ignite a flame, and eight thermocouples are utilized to track the temperature changes along the porous media. Perovskite catalysts, catalysts with a crystal structure of ABO3, are used to coat the silicon carbide foam to enhance combustion, allowing for a lower equivalence ratio and a more efficient combustion. Power is produced using thermoelectric generators, which convert thermal energy into usable electric power. The efficiency of the device and the minimum equivalence ratio possible within the combustion chamber are observed and reported for both perovskite enhanced and inert combustion.

(MCARE-P025-2014) Syngas Combustion in Porous Media: Creation of an Experimental Porous Combustor

B. Hughes*, A. C. Terracciano, B. Beaman, M. D. Robayo, N. Orlovskaya, S. S. Vasu, University of Central Florida, USA

The syngas created from combustible gasses found in products of solid waste disposal sites and in sewage treatment facilities can be recycled effectively. However, the variability of produced syngas mixture composition presents or causes instability in conventional combustion systems. When designing a suitable system for combustion of such mixtures, the varying composition of syngas produces a wide range of heating values, creating an issue of flame quenching or thermal damage to the combustor. Combustion in porous media has been shown to be a type of robust combustion process as the insertion of a refractory ceramic material, such as silicon carbide, into the flame provides additional pathways for heat transfer. Heat transfer through the solid structure, not exhibited in conventional combustion, allows for longer preheating lengths of ignition of extremely low heat value air mixtures while also allowing a wider range of feasible burn velocities. In order to supplement a concurrent numerical modeling study, a design for an experimental porous combustor is presented; which will be used to later validate the produced model. Design will include a poly-enclosure combustion chamber allowing for the use of laser diagnostics. Care will also be taken to ensure adequate boundary conditions of the heat flux out of the system, reducing the complexities of a numerical modeling analysis.

(MCARE-P026-2014) Charge transfer dynamics in perylene diimide-C60/poly(3-hexylthiophene) blend films studied by transient absorption

K. Kaunisto*, P. Vivo, M. Niemi, R. Dubey, T. Ruoko, N. Tkachenko, H. Lemmetyinen, Tampere University of Technology, Finland

Perylene diimide (PDI) derivatives are interesting materials for optoelectronic applications since wide possibilities for altering their optical and photoelectrical properties,1,2 and for their ability to be covalently linked to another molecule to form a molecular dyad with a desired function. Such a photo functional molecule with capability for intramolecular charge separation can be used as a building block in photovoltaic applications. In this research, NIR absorbing pyrrolidine substituted PDI derivative covalently attached to C60 (PyPDI-C60 electron transfer dyad) was blended with the well-known light active polymer poly(3-hexylthiophene) to establish a molecular assembly for efficient photoinduced charge generation. Transient absorption spectroscopy in ultra-fast to millisecond time domain was used to model the charge generation phenomena in the complex molecular blend. First, photoinduced electron transfer from the PDI core to the C60 moiety of the dyad was demonstrated in solution and in a film by using the femtosecond transient absorption spectroscopy. Finally, complex charge transfer scheme in the blend film was revealed by using the femtosecond and millisecond transient spectroscopy.

(MCARE-P027-2014) Reduction of CO2 by nanocrystals of metal-organic framework photocatalyst

Y. Lee*, J. Kang, Korea Advanced Institute of Science and Engineering, Republic of Korea

Over the decade, Metal-organic frameworks (MOFs) have been suggested for various application fields such as gas storage or separation, sensing, drug delivery and catalysts due to their diverse characteristics by design of molecular structure. MOFs can have specific properties because they can be designed through combination of metal elements and organic ligands. Here, we will present about MOF photocatalysts for a CO2 reduction as the development of technologies on converting light energy into chemical energy has been needed. In order to synthesize MOF photocatalysts, light harvesting organic ligands which can generate electron-hole pairs by absorption light and catalytic metal elements which can potentially catalyze CO2 into reactive compounds were used. There are several criteria for MOF photocatalysts. They have to be stable to water because CO2 reduction is occurred under water atmosphere and their energy band structure of MOF photocatalysts should be appropriate for CO2 reduction potential. Therefore, we synthesized MOF photocatalysts based on water stable metal ion. It successfully regenerated CO2 into useful chemical compounds with water under light irradiation. The charge generation and transfer during photocatalysis was also investigated by various photo-physical measurements.

(MCARE-P028-2014) Local structural, optical, and electrical properties of ion-implanted ZnO nanorods

S. Han*, Z. Jin, C. Park, E. Jeong, I. Hwang, Chonbuk National University, Republic of Korea

We investigated the structural, optical, and electrical properties of ZnO nanorods implanted with various ions, including N+, H+, Co+, and Fe+ at different energies and fluxes. The structural, optical, and electrical properties of ion-implanted ZnO nanorods were studied by using XRD, XAFS, SEM, TEM, EDS, IR, PL, and I-V measurements. We observed that the electrical properties of ZnO nanorods were substantially enhanced by ion implantation. Although there was structural degradation in ZnO nanorods, the shape of ZnO nanorods was not destroyed due to the ion implantations. We will demonstrate the details of the structural changes of the ion-implanted ZnO nanorods.

(MCARE-P029-2014) FTO/CuO/Graphite as counter electrode in DSSC

C. O. Avellaneda*, E. Portugal, T. Sampaio, E. Santos, Universidade Federal de Pelotas, Brazil; A. Gundel, W. H. Flores, Universidade Federal do Pampa, Brazil; N. Carreño, Universidade Federal de Pelotas, Brazil

During the past two decades, dye-sensitized solar cells (DSSC) have emerged as one of the most promising candidates for useful photovoltaic applications in good quality of their low manufacturing cost and relatively high efficiency to convert solar energy into electricity. The function of the counter electrode is to transfer electrons arriving from the external circuit back to the redox electrolyte and to catalyze the reduction of the triiodide ion. Usually, Pt is used as the catalytic material, but it is extremely expensive and has the problem of reserves for large scale application. In this work we studied the use of graphite as a counter electrode in DSSC in order to develop inexpensive materials for CEs which also exhibit high electrical conductivity, good chemical stability and good catalytic activity to the reduction of electrolyte. The sol of CuO was prepared by the sol-gel method and the film was deposited by dip-coating technique at 12cm/min and heat treatment of 450 oC during 30 min. After that the graphite layer was produced by spraying graphite 33 (Kontakt Chemie) on the CuO/FTO. The graphite counter electrode was then put in the oven at 150°C for 24 hours. The addition of the CuO film improved the adhesion of the graphite film Key Words: DSSC, graphite, counter electrode

(MCARE-P030-2014) Narrowband infrared emitter for Energy Harvesting Applications

S. Sharma*, E. Stefanakos, D. Y. Goswami, J. Zhou, University of South Florida, USA

A photonic crystal structure is designed to control thermal emission spectrum tailored to suit applications in biosensors, detectors and thermophotovoltaic devices. The hybrid photonic crystal structure uses the effect of surface morphology on the optical properties to introduce the selectivity in frequencies for the emission. The thermal emission in a certain set of frequencies can be suppressed while allowing the crystal to emit radiation limited in a narrow band of frequencies. The emission spectrum tunability has been confirmed by using experimental setup as well as theoretical calculations. A metal-dielectric composite with the top metal surface etched into sub wavelength nanostructures is made the base case for the emitter design. From thereon, various periodic arrays of rectangular or circular holes as well as gratings were introduced in the base case. While simulating the emission spectrum different metals including Silver, Gold, Tungsten, Nickel and Platinum were considered. Also, changing the dielectrics with varying indexes was also seen to impact the shape of the emission spectrum. Effect of etch depth in such periodic structures was also taken into account. Variations in period of the array and the dimensions of each hole were also noted to affect the narrowness of spectrum.

Wednesday, February 19, 2014

Plenary Session V

Room: Salon E

8:25 AM

(MCARE-PL6-2014) Theoretical Study of Growth and Electronic Structure of Graphene and Graphene-based Nanostructures

S. Hong*, Sejong University, Republic of Korea

Recently, interesting subjects in the graphene research is graphene growth mechanism on various substrates and band gap engineering of pristine gapless graphene. First, we have performed density functional theory (DFT) calculations to understand the initial stage of graphene growth on the oxide substrates such as sapphire and magnesium oxide. The single carbon atom is found to bind favorably to an oxygen atom on the substrates. By increasing the number of adsorbed carbon atoms, we find that at least one carbon atom of the carbon structure binds to an oxygen atom of the surfaces due to strong bond between carbon and oxygen atoms. Combined with the experimental results, these theoretical findings may imply that carbon atoms on the oxide substrates form the nanocrystalline graphite structure within a limited area. Next, a periodically modulated graphene (PMG) generated by nano-patterned surfaces is reported to profoundly modify the intrinsic electronic properties of graphene. DFT calculations performed on a model of PMG reveals a possible tuning of a band gap by considering both strain caused by periodic bending of graphene and doping through chemical interactions with underlying substrate oxygen atoms. *This research was supported by NanoMaterial Technology Development Program (2012M3A7B4049888) through MSIP/NRF and Basic Science Research Program (2010-0020207) through MOE/NRF.

Solar Fuels

Solar Fuels: Frontiers in Materials Development for Water Splitting Photocatalysts I

Room: Salon D

Session Chairs: Thomas Hamann, Michigan State University; Davide Barreca, IENI-CNR and INSTM - Padova University

9:20 AM

(MCARE-038-2014) Materials aspects of solar water splitting (Invited)

D. Wang*, Boston College, USA

Photosynthesis harvests solar energy and converts it into chemical forms, allowing for easy storage and redistribution of the most abundant energy we are blessed with on the surface of earth. It is a fundamentally important process in nature. From a thermodynamic perspective, the process may be carried out at a significantly higher efficiency using artificial systems, such as semiconductor-based photoelectrochemical ones. In order to do so, we need stable photoanodes that can effectively oxidize water to produce oxygen, extracting electron from water. The electron can then be excited again at the photocathode to either directly reduce water to produce hydrogen as a clean energy carrier or reduce carbon dioxide for fuel production. Presently, the main challenge in the field is the lack of suitable materials that are both inexpensive and efficient. This talk will examine materials-related issues in photoelectrochemical water splitting. We will use hematite as a model system to discuss problems encountered in photoanode design and present our strategies to combat these issues. Si nanowires are discussed within the context of photocathode design, with a focus on carbon dioxide reduction. This work paves the way toward economically competitive production of solar fuels by inexpensive materials.

10:00 AM

(MCARE-039-2014) Development of Precursor Chemistry for Metal Oxide Thin Films and Nanostructures (Invited)

S. Mathur*, T. Fischer, L. Brueckmann, J. Schläfer, G. Fornalczyk, J. Leduc, L. Appel, University of Cologne, Germany

Chemistry in the past few decades has played a major role in the convergence of life, physical and engineering sciences enabling controllable manipulation of matter at molecular length scale. The successful synthesis, modification and assembly of nanobuilding units such as nanocrystals, -wires and –tubes of different materials have demonstrated the importance of chemical influence in materials synthesis, and have generated great expectations for the future. Precursor-based synthesis of nanostructured materials is a viable and versatile method to overcome thermodynamic limitations, which are based on equilibrium states, necessary for the controlled growth of doped-systems and metastable compounds. The chemical configuration of precursor is highly sensitive to the decomposition processes involved in the transformation of molecules into material. By variation of the steric profile of the organic ligands and cation combination, the chemical configuration of different molecules have been optimised to obtain precursors with labile metal-ligand bonds that enable chemically controlled decomposition and growth of nanostructures. Following this strategy, various nanocrystalline oxides and composites have been obtained. This talk will present how chemically grown and designed nanoparticles, nanowires and nanocomposites of different metal oxides open up new vistas of material properties, which can be tuned by the chemical input and transformed into advanced material technologies.

*Denotes Presenter

10:20 AM

(MCARE-040-2014) Design of photoelectrodes for efficient solar water spliitting (Invited)

J. Lee*, Ulsan National Institute of Sci & Tech (UNIST), Republic of Korea

Sunlight is a clean, renewable and abundant energy source on the earth. Its conversion to hydrogen has been considered an ideal solution to counter the depletion and environmental problems of fossil fuels. Photoelectrochemical water splitting is an ideal technology for the purpose, since H2 could be produced directly from abundant and renewable water and solar light from the process. The key to the technology is photoelectrodes of high efficiency, high stability, and low cost. In addition of the discovery of new materials, the structure and morphology of the known materials could be controlled to enhance the performance of the photoelectrodes. In this presentation, the concepts of materials design and their examples are proposed for efficient photoelectrodes of photoelectrochemical cells for visible light water splitting. We discuss the material designs including: i) p-n heterojunction photoanodes for effective electron-hole separation, ii) electron highway to facilitate interparticle electron transfer, iii) metal doping to improve conductivity of the semiconductor, and iv) one-dimensional nanomaterials for vectoral electron transfer. High efficiency has been demonstrated for all these examples due to efficient electron-hole separation. Modern material processing techniques have been explored to materialize these concepts.

11:00 AM

(MCARE-041-2014) Enhancement of sensitivity and charge carrier collection in mixed metal oxides photo-anodes employed for photo-electrochemical water splitting

R. Solarska*, K. Bienkowski, M. Sarnowska, J. Augustynski, University of Warsaw, Poland

An effective solar light-driven water splitting in photo-electrochemical devices requires use of materials which combine both high photo-conversion efficiency and long term stability goals. For the latter reason the choice of the suitable systems is restricted to the semiconducting oxides that, in most cases, do not undergo photo-corrosion in aqueous solutions but which are also able to absorb efficiently the visible light. The low optical absorption coefficients near the fundamental band edge, which determine the extent of solar light absorption by many photo-anode materials, are the critical factors for a number of semiconductors characterized by an indirect optical transition. This is also the case of n-type semiconducting WO_3 or Fe_2O_3 responding to the blue, respectively, green part of the solar spectrum for which the optical absorption depths exceed the minority charge carriers collection distances. The results regarding the improved charge collection in doped and/or mixed semiconducting oxide photo-anodes including mixed WO_3-Fe_2O_3 oxide will be presented.

11:20 AM

(MCARE-042-2014) The synthesis of Ti alloying DLC coating for the application on bipolar plates in fuel cell (Invited)

D. Jung, N. Lee, K. Moon, KITECH, Republic of Korea; G. Yakup*, S. Mathur, University of Cologne, Germany

DLC coatings is widely used in machinery and medical industries due to high hardness, low friction, high wear resistance and chemical stability. However, the problems of DLC coatings such as thermal unstable, poor adhesion on ferrous material is limited on its wide uses. So, there have been developed the modified DLC coatings by doping or alloying of different elements to improve the properties in respect to pure DLC coatings. In this study, the effect of Ti addition has been studied on the properties of DLC coatings. Especially, the improvement of the electrical conductivity of DLC coatings without losing the chemical properties have been examined to find out the usefulness of DLC coatings for the application in fuel cell. In this study, DLC coatings were deposited by PECVD equipped with sputter gun and Ti was added to DLC coatings with increasing RF power. On sputter gun as a result, Ti content in DLC coatings could be controlled by varying RF power and process pressure for Ti target. Also Ti-DLC coatings were deposited by PECVD of C_2H_2, Ar, H_2 and precursor of tetrakis(dimethylamino)titanium (TDMAT, Ti[$(CH_3)^2N]^4$). The crystal structure of DLC coatings were measured by Raman, XPS. The mechanical properties of DLC coatings was investigated by scratch test, nano-indenter, wear test with the type of ball on disc. The chemical and electrical properties of the DLC coatings was measured with dynamic tests and four point probe methods.

11:40 AM

(MCARE-043-2014) Nano-hybrid Structured Regioregular Polyhexylthiophenes Blend Films for Photoelectrochemical Applications

M. K. Ram*, P. Basnayaka, P. Villalba, E. Stefanakos, A. Kumar, University of South Florida, USA

Recently, we have shown 8 to 20 times enhanced photoelectrochemical in the nanodiamond (ND)-ragioregular polyhexylthiophene (RRPHTh) nanostructured blend film than most of the nanoparticle inserted, hybrid or composite structures. Later, the extensive research has been carried out to investigate the photovoltaic effect of ND- poly (3-dodecylthiophene), another derivative of PTH. The particle size dependent to photovoltaic effect of ND-poly (3-acylthiophene) polymer blends have also been investigated. We made attempt to characterize the polythiophenes-ND structures using AFM, SEM, FTIR, UV-visible spectroscopy and the Raman spectroscopy. Later, zeta potential has been used to understand the ND hydrodynamic particle size in the hybrid structures. The photoelectrochemical study on RRPHTh for multiwalled carbon nanotube (MWCNT), molybdenum disulfide (MoS2), ZnO and TiO2 nanoparticles have been studied and their photoelectrochemical properties are compared. Various electrolytes (0.2M TBATFB, 0.2 M LiClO4, 1 M H2SO4 and 0.2 M LiBF6) were used to estimate the photocurrent for MWCNT-polythiophene films films. The optimized ND-polythiophenes structures have been used for the fabrication of solid photovoltaic cell.

Batteries and Energy Storage

All Solid State Batteries

Room: Salon E

Session Chairs: Mickael Dolle, University of Montreal; Derek Johnson, Prieto Battery, Inc

9:20 AM

(MCARE-069-2014) Porous and Nanostructured Electrodes for Energy Storage Devices (Invited)

A. Stein*, A. Vu, N. Petkovich, B. Wilson, Y. Fang, Y. Qian, University of Minnesota, USA

Electrode materials containing well-defined pores offer interesting features for electrical energy storage applications. Pores provide good access of electrolyte to the electrode surface; large surface areas facilitate charge transfer across the electrode/electrolyte interface; nanometer-sized walls reduce path lengths for ion diffusion and increase utilization of active material. Structured porous carbon materials can act as conductive hosts to disperse and stabilize other electrochemically active materials. This talk will focus on methods of synthesizing porous and nanostructured electrode materials for lithium-ion batteries and supercapacitors, using hard and soft templating methods to control the electrode architecture and distribution of phases in multi-component electrode systems. These methods produce bicontinuous structures with continuous transport paths through the active phase (walls) and the electrolyte phase (pores), yielding improved rate capabilities for lithiation and delithiation. Furthermore, they allow the preparation of composites of a conductive scaffold with poorly conducting but otherwise desirable electrode materials to overcome limitations in electrical conductivity of those materials, increasing the choice of feasible electrode materials. Templating methods can also provide discrete nanoparticles of active material with uniform size distribution.

10:00 AM

(MCARE-088-2014) Materials Challenges to Develop Reliable "All-Solid-State" Batteries (Invited)

L. Castro, CEMES/CNRS, France; A. Kubanska, MADIREL/CNRS, France; R. Bouchet, LEPMI/CNRS/INPG, France; C. Jordy, SAFT, France; L. Tortet, MADIREL/CNRS, France; V. Viallet, V. Seznec, LRCS/CNRS, France; G. Caillon, SAFT, France; M. Dolle*, University of Montreal, Canada

All solid state batteries have always been considered with a peculiar interest due to the advantages they offer, especially when safety and reliability issues are concerned. Since 1982 and the works of Hitachi Co, Ltd. Japan, thin film micro-batteries have been widely studied. However, their use remains limited to micro-electronic applications. In order to answer today's energy needs, bulk-type "all-solid-state" batteries would be of great interest since they offer higher energy densities than thin films. However, their development has been hindered by the difficulty to assemble laminated ceramics together as it is often very complicated to sinter sufficiently such compacts when compositions of each layer generally require different optimal sintering temperatures. Our approach was then to develop bulk-type all solid state batteries by means of the Spark Plasma Sintering (SPS) technique. Such a method turns out to be perfectly adapted to guarantee high quality contacts between materials in very short times. In this presentation, we will consider the choice of materials to develop such technology. The different steps to reach our goal will be detailed starting with the development of composite ceramic electrodes. Finally the electrochemical performances of half cells and full cells will be presented.

10:40 AM

(MCARE-089-2014) Three-Dimensional Solid-State Lithium-ion Cell Fabrication with Integrated Electrodes (Invited)

D. C. Johnson*, Prieto Battery, Inc, USA; A. L. Prieto, Colorado State University, USA

Traditional lithium-ion (Li-ion) batteries have the inherent tradeoff between energy and power density. When designing a high power density cell, the electrode thickness is typically reduced resulting in a decrease in energy density. Conversely, high energy cells can be achieved through an increase in the electrode thickness. The result, however, is diminished cell power due to an increase in the Li-ion diffusion length. While Li-ion batteries have become the primary energy choice for low power applications, this inversely proportional relationship between energy and power density is limiting their use in high power applications. The use of three-dimensional (3D) electrodes with high surface areas while simultaneously integrating the electrodes has the ability to yield an energy storage device with both high energy and power density. This is due to the combination of both high surface areas between the electrodes as well as nanoscale Li-ion transport distances through the electrolyte. While these architectures were first proposed ten years ago, many synthetic challenges remain in successfully fabricating a 3D cell. To that end, our approach is to utilize electrodeposition as the main synthetic tool for fabricating a 3D solid-state cell. A discussion of the component fabrication as well as the performance, both individually and as a functioning solid-state cell, will be presented.

11:00 AM

(MCARE-090-2014) 3D-New Lithium Battery Technology Platform

J. Prochazka*, HE3DA, Czech Republic

Thin film technology (2D) producing lithium ion accumulators has nearly been optimized. The capacity limits are given and the production cost is high. In addition, ultimate safety of this type of batteries cannot be provided. It has been demonstrated that a significant increase of lithium battery capacity is feasible by removing organic binders and extending the electrode thickness from micrometers (2D) to millimeters (3D). The HE3DA® concept of several millimeters thick electrodes gives the battery incomparable safety and brings a number of new attributes, which are not achievable by the existing thin film technology. 3D electrodes provide a significant volumetric capacity increase. Recently developed internal cooling system, with electrolyte as the cooling media, radically shrinks the battery pack size and extends battery life. during operations, The safe, robust construction with a multifunctional frame, easy degassing and possibility of electrolyte exchange and regeneration provides a new lithium accumulator technology platform ideal for large energy storage modules.

11:20 AM

(MCARE-091-2014) Stability Increase of Cathode Materials by NASICON structured electrolyte for all-solid-state batteries

S. Jee*, S. Lee, K. Lee, S. Woo, Y. Lee, J. Lee, Y. Yoon, Gachon Univeristy, Republic of Korea

In the last few decades, NASICON electrolytes have been investigated for all-solid-state batteries. Especially, Li-Al-Ti-Ge-Si-P-O electrolyte with high electrochemical stability in contact with electrode materials has been developed. Therefore, fully crystalline electrolytes, especially NASICON electrolytes are appealing for solid-state systems for cathode improvement and electrode/electrolyte interfacial quality enhancement. The material search for optimized NASICON lithium ion conductors is still continuing. A LiCoO2 target on was sputtered in order to grow the LCO cathode thin films, which were deposited for 1~10 hours on the Li-Al-Ti-Ge-Si-P-O electrolyte plate. The Li-Al-Ti-Ge-Si-P-O electrolyte had relatively high ionic conductivity. The ionic conductivity of Li-Al-Ti-Ge-Si-P-O electrolyte were 1.3 × 10^–4 S/cm. The Li-Al-Ti-Ge-Si-P-O electrolyte was very stable in the operating potential range between 0 and 5.5V full-cell test. Moreover, the stability of the all-solid-state battery with the Li-Al-Ti-Ge-Si-P-O electrolyte was improved because no chemical reaction between Li-Al-Ti-Ge-Si-P-O electrolyte and LiCoO2 was observed. Consequently, these results indicated that the Li-Al-Ti-Ge-Si-P-O electrolyte can be applied for stability increase between the solid electrolyte and the cathode in the all-solid-state battery.

Nanocomposites and Nanowires Materials for Photovoltaic and Photonic Technologies

Nanocomposites and Nanowires Materials for Photovoltaic and Photonic Devices III

Room: Salon G
Session Chairs: Esther Alarcon-Llado, EPFL; Yoon-Bong Hahn, Chonbuk National University

9:20 AM

(MCARE-118-2014) 4G Hybrid Organic Solar Cells for Energy Harvesting: Inorganics-in–Organics

S. P. Silva*, K. Jayawardena, L. J. Rozanski, C. A. Mills, M. J. Beliatis, G. R. Dabera, University of Surrey, United Kingdom

Clean energy production is one of the most significant challenges faced by humanity. Unlike any other problem there is a source of energy with unlimited potential in the form of the Sun, but harvesting this energy in a sustainable, clean and socially cost effective manner is challenging. Recent developments in solution processable single junction polymer solar cells have led to a significant improvement in power conversion efficiencies from ~5% to beyond 9%. Much of the initial efficiency improvements were driven through judicious design of donor polymers. We believe that by engineering of device architectures through the incorporation of inorganic nanostructures and better processing, this 4G hybrid technology can continue to deliver more efficiency gains. Inorganic nano-components such as carbon nanotubes, graphene and its derivatives, metal nanoparticles and metal oxides have been central in improving device performance and longevity beyond those achieved by conventional 3G polymer solar cells. This talk will summarise the diverse roles played by the nano-scale design to improve the performance of solar cells and discuss key features in state of the art next generation (4G) polymer solar cells. The challenges associated with the engineering of such devices for future deployment are also discussed.

10:00 AM

(MCARE-119-2014) Semiconductor nanowires for next generation photovoltaics (Invited)

E. Alarcon-Llado*, A. Fontcuberta i Morral, EPFL, Switzerland

We are seeing an expanding interest in finding novel concepts for increasing the efficiency-to-cost ratio in solar cells. Among the different possibilities, semiconductor nanowires provide various paths towards this objective. In this presentation, we will discuss different aspects that indicate semiconductor nanowires are ideal candidates for next generation photovoltaics: 1) increased device design freedom for optimizing the carrier extraction and light absorption, 2) a self-concentrating effect in single nanowires, which provides a way to surpass the Shockley-Queisser limit, and 3) three-dimensional-heterostructure fabrication in up-conversion designs.

10:40 AM

(MCARE-120-2014) Designing Sub-Wavelength Silicon Nanowires for Photovoltaics: Synthesis, Measurement, and Modeling (Invited)

C. Pinion, J. Christesen, X. Zhang, J. Cahoon*, University of North Carolina at Chapel Hill, USA

Semiconductor nanowires have been widely pursued as a platform for solar energy devices. Here, we present general principles for the synthesis, measurement, and modeling of photovoltaic devices based on silicon nanowires with sub-wavelength diameters. We address the growth and doping of these materials using the vapor-liquid-solid mechanism and present a method to encode morphological features as small as 10 nm along the wire axis. These features include nanogaps, bow-ties, tapers, sinusoids, and gratings. Morphology is used to impart specific and tunable optical resonances, which can substantially enhance long-wavelength light absorption through photonic effects. In addition, the performance of nanowires with axial or radial p-n junctions is evaluated using a device-physics model. Direct comparisons between experimental and simulated current-voltage measurements highlight the key parameters that limit the performance of each p-n junction geometry. Finally, we show that direct time-resolved measurements of charge carrier dynamics using ultrafast microscopy quantitatively reveal the fundamental recombination processes that dictate the performance of devices fabricated from these materials. The combination of synthesis, measurement, and modeling enables a full evaluation of silicon nanowires as fundamental components for photovoltaic technologies.

11:20 AM

(MCARE-121-2014) The use of TiO_2 nanotubes arrays for photoanodes in dye-sensitized solar cells

L. Suhadolnik, Jozef Stefan Institute, Slovenia; I. Jerman, National Institute of Chemistry, Slovenia; A. Kujan, Cinkarna Celje, d.d. Inc., Slovenia; M. Krivic, K. Zagar, M. Ceh*, Jozef Stefan Institute, Slovenia

TiO_2 nanotubes arrays fabricated by anodization of titanium foil can be used as photoanodes in dye-sensitized solar cells (DSSCs) due to reduced intertube connections, slow electron recombination and enhanced light scattering. A self-ordered, vertically aligned TiO_2 nanotubes were grown on electropolished titanium foil by anodic oxidation in viscous organic electrolyte. In our work we chose two different anodization times to obtain TiO_2 nanotubes of app. 9 μm and 17 μm in length. The anodized nanotubes after thermal treatment were polycrystalline and composed of well-crystallized anatase grains. Some of the TiO_2 nanotubes were post-treated with $TiCl_4$ or hydrothermally with TiO_2 P25. The structure and morphology of processed nanotubes were investigated by X-ray diffraction and various electron microscopy techniques (SEM, TEM). In order to avoid problem of insufficient sensitizing the high aspect ratio TiO_2 nanotubes with a dye we used a new approach of dye infiltration at elevated temperatures in an autoclave. The absorption spectra of the dye and optical losses due to counter electrode and electrolyte were measured with UV/VIS spectroscopy. Chosen photoanodes were assembled into back-side illuminated DSSCs. The measured current voltage characteristics of test solar cells gave an average energy conversion efficiency of 5.7% for untreated TiO_2 nanotubes.

11:40 AM

(MCARE-122-2014) Hollow-flowered ZnO as scattering layer for improving energy conversion efficiency in dye-sensitized solar cells

W. Rho*, M. Vaseem, D. Jung, Y. Hahn, Chonbuk National University, Republic of Korea

Dye-sensitized solar cells (DSSCs) have gained great interest due to high energy conversion efficiency and low cost alternative. However, the energy conversion efficiency of DSSCs needs to be improved to alternate conventional photovoltaic devices. There are several parameters that can be investigated, including dimensionality of TiO2 for electron transport, light harvest, molar absorption coefficiency, energetically suitable HOMO–LUMO levels, available surface area for dyes, transport kinetics of the electrons, regeneration by a redox couple, and losses of recombination and back reactions. To improve the energy conversion efficiency of DSSCs, scattering layers are one of best research areas in the light harvesting. In principle, 3-dimensional structure has good collection and good light absorption due to scattering effects. Additionally, hollow structure has attracted a great deal of attention due to low density, high surface area, good surface permeability. Here, we reported characterization of hollow-flowered ZnO as scattering layer and its application to DSSCs for improving energy conversion efficiency. The hollow-flowered ZnO is synthesized by solution method and characterized by FE-SEM, TEM, and XRD and then DSSCs with hollow-flowered ZnO were fabricated and characterized by I-V and incident photon-to-current efficiency (IPCE).

Other Energy Issues

Other Energy Technologies I

Room: Salons B - C
Session Chairs: Rachael Robertson, Melbourne University; Ali Kaouk, AK Mathur, Institute for Inorganic and Material Sciences

9:20 AM

(MCARE-140-2014) Life in the freezer - leadership, water and energy challenges in Antarctica (Invited)

R. Robertson*, Melbourne University, Australia

Antarctica is at the forefront of climate change research. Its pristine environment is an early warning indicator of ecological change. Every year hundreds of scientists descend on the continent to undertake research that improves our understanding of global warming and human impacts on the planet. At the end of Summer the scientists return home and a small team remain behind, through the long, dark winter, to maintain the facilities and continue baseline data collection. The environment is harsh, with months of darkness and freezing temperatures, but the inter-personal pressure of living together, around-the-clock is tougher. Minimising our ecological footprint is also critical so water and energy use is always monitored, reported, and front of mind. This presentation is an inspiring and entertaining look at a year in the life of a small Antarctic community of 18 people, the highs & lows, the ups and downs. Complete with extraordinary photographs and video, Rachael shares her leadership journey and provides several insights and tools along the way.

10:00 AM

(MCARE-141-2014) Pyrolysis of Rush Grass and Wood investigated by TG-GC-MS

E. Post*, NETZSCH Geraetebau GmbH, Germany; B. Fidler, NETZSCH Instruments NA, LLC, USA

Biomass materials like special weeds, wood parts etc. are precious organic materials for the generation of second-generation bio-fuels. The advantages of these materials are their neutral CO2 balance, the high availability and non-competing with edibles. During “non-complete” combustion or pyrolysis a large number of gaseous organic substances were produced which were extremely difficult to identify by TG-MS or TG-FTIR alone. A pre-separation of the gas mixtures by gas chromatography makes the identification by library search much easier. The pyrolysis of rush grass and wood material were investigated by a thermo balance connected to a gas chromatograph with mass spectrometer (TGA-GC-MS). This instrument combination facilitates measuring the mass change of the substances versus temperature and time. The GC-MS allows the identification of gaseous products in real time (quasi-continuous), meaning direct correlation to actual temperature/time/mass. Alternatively, the gas products condensable at -50°C were collected in a cryo-trap and analyzed after the TGA measurement by high resolution GC-MS analysis. In this contribution, the principle of the TGA-GC-MS will be explained along with the measurement modes employed for these investigations. The TGA-GC-MS results will be shown and explained for rush grass and selected wood samples.

10:20 AM

(MCARE-142-2014) Switchable Antibiofouling Coatings

M. Denton*, M. Kirtk, Sandia National Laboratories, USA; S. Stafslien, North Dakota State University, USA; B. Hernandez-Sanchez, S. Dirk, Sandia National Laboratories, USA

Marine Hydrokinetic (MHK) energy generation systems harness the energy of water as it moves and are vital in providing clean and sustainable energy. Biofouling presents a problem for these technologies 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. Our work has focused on the development of an alternative switchable type of surfactant that incorporates both antibacterial and fouling-release properties. Antibacterial ammonium salts containing long chain an aliphatic moiety disrupt the bacterial cell wall leading to cell death. Siloxane coating materials have a low modus and surface energy which facilitates easy removal of organisms from surfaces by the application of fluid shear stress. We have been exploring the use of switchable polymers that start as sulfonium and ammonium based polymers with antimicrobial properties, and can be transformed from antibiofouling to fouling release materials. When the polymers are switched to the fouling release form, attached fouling will be lifted away from the surface. 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.

10:40 AM

(MCARE-143-2014) Thermoelectric power generation coupled with perovskite catalyst enhanced combustion in porous media

M. D. Robayo*, B. Beaman, B. Delose, N. Orlovskaya, R. Chen, University of Central Florida, USA

Thermal to electrical power conversion device that incorporates perovskite enhanced combustion on porous media and thermoelectric generators. Highly porous silicon carbide ceramics are used as a support structures for a catalytically-enhanced matrix-stabilized combustion of a lean mixture of methane and air. Perovskite catalysts, catalytic active materials with a crystal structure of ABO3, are used to coat the porous ceramic decreasing the minimum possible equivalence ratio that the burner can sustain. The efficiency of the device and the minimum possible equivalence ratio within the combustion chamber are reported for both perovskite enhanced and inert combustion in porous media.

11:00 AM

(MCARE-144-2014) On the Electrodeposition of Antimony and Cobalt in Citrate Solutions

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

Over the past decade, there has been a great interest in research on thermoelectric materials that can be used to harvest energy from waste heat and convert it to electricity. Among these thermoelectric materials, skutterudites such as cobalt triantimonide (CoSb3) showed promising thermoelectric properties at intermediate temperatures (ca. 400–700 oC). Despite intense research and vast literature data on bulk CoSb3 and its derivatives, very few studies have been done on the nanostructured skutterudites. Our recent studies on the Co-Sb system provided a detailed understanding of the co-deposition of Co and Sb from aqueous solutions. Additionally, discrepancy in elemental composition of nanorods and thin films grown under the same experimental conditions were observed. It was found that even though the use of citrate and complex formation can increase the solubility of Sb2O3, the electrodeposition of Sb at large overpotentials is controlled by diffusion of Sb(III) complexes due to their still low concentrations. The deposition of Co, on the other hand, is controlled by reaction at the cathode. When both Co(II) and Sb(III) are combined in citrate solution, the electrochemical behavior is similar to their respective single solutions although the relative content of Co is slightly lower. Our results explain the higher relative content of Co found in Co-Sb nanorods.

11:20 AM

(MCARE-145-2014) Parameter Calibration for Glass Strength Prediction Model Considering the Influence of Environment

C. Ronchetti*, Roma Tre University, Italy

Structural use of glass has been increasingly spreading and represents a big challenge, considering its brittle nature. The use of glass is strictly related to environmental sustainability issues and requires a deep understanding of material mechanical behaviour. Linear elastic fracture mechanics (LEFM) explains that brittle material strength is highly reduced by the presence of surface micro-defects. However, glass strength and lifetime also depend on environmental attack, in particular on temperature and humidity, which are combined with mechanical tensile stress by accelerating crack propagation. This phenomenon is known as stress-corrosion and an explicit correspondence between glass strength and environmental variables is lacking. On the one hand, the present work provides lifetime prediction model for glass considering the influence of temperature and humidity. On the other hand, it proposes a numerical algorithm, which allows chemical-physical parameters to be calibrated, in order to give prediction value to the model. The algorithm is based on numerical interpolation of experimental data, obtained through tests used joint to experimental data from the literature. Parameter calibration is performed according to sensitivity numerical procedure. Finally, lifetime prediction curves are obtained for different environmental conditions, even at high temperature levels.

Plenary Session VI

Room: Salon E

1:35 PM

(MCARE-PL7-2014) Non Palladium-based Alloy membranes for Hydrogen Separation and Production

C. Nishimura*, National Institute for Materials Science, Japan

There is growing interest on hydrogen selective membranes to be applied in hydrogen energy technology. Non-porous membranes for extraction and purification of hydrogen are key components for the establishment of hydrogen energy system. Non-porous membranes, which are essentially 100% hydrogen selective, can serve as a final clean-up mean of hydrogen gas before its use in PEFC, which requires hydrogen gas with ultra high purity. Alloys based on group V elements, vanadium, niobium and tantalum, have attracted the attention of researchers in chemical engineering and materials science, because of their extremely high hydrogen permeability. Japan has been leading the world in the research activities to develop hydrogen separation membranes based on these metals. Some alloy membranes have come to a stage of application test in catalytic membrane reactor systems. Here, I present the current status of development of non palladium-based alloy membranes for hydrogen separation. Mainly, the works on vanadium alloys, in which the authors have long been engaged, will be presented.

Solar Fuels

Solar Fuels: Materials for Water Splitting: Hematite

Room: Salon D

Session Chairs: Gunnar Westin, Uppsala University; Ashok Kumar, University of South Florida

2:10 PM

(MCARE-044-2014) Photocatalytic Water Oxidation with Hematite Films (Invited)

T. Hamann*, O. Zandi, Michigan State University, USA

Hematite has long been a potential candidate for photocatalytic water splitting, however only very poor conversion efficiencies have been achieved. This is generally attributed to a short minority carrier collection length. In principle, the short collection length can be overcome through nanostructuring the electrode. Thin films represent ideal model systems of nanostructured electrodes which allow for detailed mechanistic investigations. We utilize atomic layer deposition (ALD) to make conformal thin film hematite electrodes with controllable thickness for this purpose. Films less than 20 nm thick, however, are plagued by a dead layer near the substrate contact. We found that the dead layer can be alleviated by the incorporation of dopant atoms in the hematite film, which lead to dramatically improved water oxidation efficiencies. A series of electrochemical, photoelectrochemical and impedance spectroscopy measurements were employed to elucidate the cause of the improved photoactivity of the doped hematite thin films. This performance enhancement was determined to be a combination of improved bulk properties (hole collection length) and surface properties (water oxidation efficiency). The non-ideal water oxidation efficiency constrains the overall water splitting efficiency. Recent results of adding catalysts to the hematite surface in order to improve the water oxidation efficiency will also be presented.

2:50 PM

(MCARE-045-2014) Tailored Fabrication of Fluorine-Doped Fe2O3 Nanomaterials via PE-CVD: Synthesis, Characterization and Photo-Activated Performances (Invited)

D. Barreca*, IENI-CNR and INSTM - Padova University, Italy; G. Carraro, Padova University, Italy; A. Gasparotto, IENI-CNR and INSTM - Padova University, Italy; C. Maccato, C. Sada, Padova University, Italy; S. Mathur, A. Mettenborger, Cologne University, Germany; O. Lebedev, Laboratoire CRISMAT, CNRS-ENSICAEN, France; S. Turner, G. Van Tendeloo, EMAT, Antwerp University, Belgium

A single-step plasma enhanced-chemical vapor deposition (PE-CVD) route for the synthesis of F-doped iron(III) oxide nanomaterials is presented. Growth experiments were performed in the temperature range 100-400°C on both Si(100) and Indium Tin Oxide (ITO) substrates, using Fe(hfa)2TMEDA (hfa = 1,1,1,5,5,5-hexafluoro-2,4-pentanedionate; TMEDA = N,N,N',N'-tetramethylethylenediamine) as single-source precursor for both Fe and F. Under the adopted processing conditions, pure and single-phase α- or β-Fe2O3 nanodeposits were obtained. Interestingly, their morphology and fluorine content could be tailored as a function of growth temperature. Such features candidate the present systems as technologically appealing materials for photo-assisted applications, as demonstrated by photo-electrochemical and photo-catalytic tests aimed at H2 generation via water splitting or photo-reforming processes.

3:30 PM

(MCARE-046-2014) Photoelectrochemistry and Surface Science of Composite Hematite Photoelectrodes (Invited)

B. E. Koel*, P. Zhao, C. X. Kronawitter, Princeton University, USA

The physical and photoelectrochemical properties of composite oxide photoelectrodes comprised of α-Fe2O3 (hematite) and other oxides are investigated. We combined thin-film and nano-materials synthesis with surface-science type experiments designed to elucidate new information on the surface phases formed in hematite and about their specific stability and reactivity toward photoelectrochemical water splitting. We prepared α-Fe2O3 model catalysts with different morphology and geometry, and investigated their structure by LEED and STM. Then, TPD, XPS, and AES were used to develop a molecular level understanding of the photocatalyst surface chemistry, exploring reactions in the light and dark and determining the differences in the thermal and photochemical reaction mechanisms. We investigated the properties of mixed-oxide surfaces formed by vapor deposition under controlled conditions, and also wet chemistry methods, of a second metal or oxide component, e.g., Ni or WO3. For a composite oxide photoelectrode comprised of α-Fe2O3 and WO3 crystals, the composite films exhibit a water oxidation photocurrent onset potential as low as 0.43 V vs RHE, a value considerably lower than that of pure α-Fe2O3 photoanodes prepared in comparable synthesis conditions. This result represents one of the lowest onset potentials measured for hematite-based PEC water oxidation systems.

Solar Fuels: Materials for Water Splitting: Hematite & Multiferroics

Room: Salon D

Session Chairs: Bruce Koel, Princeton University; Renata Solarska, University of Warsaw

4:20 PM

(MCARE-047-2014) Nonaqueous sol-gel chemistry: From nanoparticles to particle-based aerogels, films and metal foams (Invited)

M. Niederberger*, ETH Zurich, Switzerland

Nonaqueous sol-gel processes represent a powerful way to prepare metal oxide nanoparticles in a wide variety of sizes, shapes and compositions. They offer advantages such as high crystallinity of the nanoparticles, small crystal sizes in the range of just a few nanometers, and the possibility to dope the nanoparticles with other metals to tailor their properties. But similarly important as the synthesis is their processing into films and their assembly into 3-dimensional architectures. The talk will introduce the basic concepts of nonaqueous synthesis approaches and their underlying chemical mechanisms. It will be shown how the use of microwave irradiation accelerates the organic and inorganic processes, offering an efficient tool to prepare doped and undoped metal oxide nanoparticles within just a few minutes. We will also discuss the use of nanoparticles as building blocks for films and multicomponent aerogels. Such a modular approach over several length scales enables the processing of nanoparticles into a form optimized for applications in e.g. water splitting, gas sensing, photocatalysis or as transparent conducting oxides. Nonaqueous sol-gel chemistry beyond metal oxides will be discussed in the context of copper, which can be prepared as self-supporting foil, as polymer-supported film or as templated metal foam.

5:00 PM

(MCARE-048-2014) Plasma Deposition and Modification of Semiconducting Thin Films for Photoelectrochemical Hydrogen Production

A. Mettenboerger*, S. Mathur, University of Cologne, Germany

The PE-CVD is a unique technique for thin film deposition, since it provides a good control over several parameters and therefore over the properties of the resulting films. In addition PE-CVD processes show a high reproducibility and they are scalable for large area productions. It finds applications in growth and processing of nano-materials, such as semiconductor thin films or carbon structures like graphene, carbon nanotubes (CNT), or DLC. Since the PE-CVD is a low temperature process it is possible to deposit under mild conditions onto sensitive materials like polymers. In this work we present the deposition and modification of semiconducting metal oxides (TiO2, Fe2O3) for photoelectrochemical (PEC) hydrogen production. The deposition parameters for thin film creation were optimized with respect to the PEC performance of the resulting materials. Furthermore the as deposited films were modified using plasma techniques as simple and effective strategy for modifying the existing substrate to improve significantly the band edge positions and photoelectrochemical (PEC) performance. Namely those modifications were the partial reduction of the metal oxides by hydrogen plasma. This technique allowed the selective tuning of the optical and electrical properties of the films and therefore leads to a substantially enhanced PEC performance.

5:20 PM

(MCARE-049-2014) Novel Fe2O3 Nanostructures: From Synthesis to Photo-assisted H2 Production (Invited)

C. Maccato*, Padova University, Italy; D. Barreca, CNR-IENI and INSTM, Padova University, Italy; A. Gasparotto, G. Carraro, Padova University, Italy; P. Fornasiero, V. Gombac, ICCOM-CNR - INSTM, Trieste University, Italy; O. Lebedev, Laboratoire CRISMAT, CNRS-ENSICAEN, France; T. Montini, ICCOM-CNR - INSTM, Trieste University, Italy; S. Turner, G. Van Tendeloo, EMAT, Antwerp University, Belgium

Fe2O3 is an interesting low-cost and versatile material. Thanks to its promising properties, it has recently been the focus of a renewed attention in several applicative fields. Among the various iron oxide polymorphs, hematite (α-Fe2O3) is largely used even in photo-assisted processes for hydrogen production. Unfortunately, α-Fe2O3 performances are still limited by its low absorption coefficient and high recombination losses. Conversely, the metastable β- (bixbyite) and ε-phases, existing only on the nanoscale, present appealing features which allow to overcome hematite drawbacks. However, β- and ε- are significantly less studied as a consequence of their hard-won synthesis. In this work, we report on a flexible synthetic approach which provides a simultaneous structural and morphological control on the obtained iron oxide materials. In particular, the optimization of a chemical vapor deposition (CVD) route starting from a fluorinated iron(II) diketonate-diamine compound as a single-source precursor enabled the selective production not only of α-Fe2O3 phase, but also of the scarcely investigated β- and ε-Fe2O3 polymorphs. For the first time, such nanostructures have been used in photoreforming processes for H2 generation starting from renewable resources and yielding very attractive performances.

Batteries and Energy Storage

Supercapacitors

Room: Salon E

Session Chairs: Karina Cuentas-Gallegos, Universidad Nacional Autónoma de México; Amartya Mukhopadhyay, Indian Institute of Technology (IIT) Bombay

2:20 PM

(MCARE-093-2014) Nanoporous Carbon Based Materials for Energy Storage Application (Invited)

A. Vinu*, The University of Queensland, Australia

The depletion of traditional energy resources and the requirement of power for a number of portable electronic devices have stimulated the research on the development of alternative energy storage devices such as supercapacitors and batteries. Among the energy storage devices, supercapacitors have been receiving much attention as they possess higher energy density than dielectric capacitors and higher power density than batteries. Different types of carbonaceous material ranging from amorphous carbons to carbon nanotubes (CNTs) have been used as electrodes for supercapacitors. Nanoporous materials have been receiving much attention in the recent years owing to their excellent textural features. In this talk, I will present the results about the synthesis, and supercapacitor performance of nanoporous carbons and nitrides with different pore diameters and structures. It is found that the pore diameter of the nanoporous carbon plays a critical role in controlling the supercapacitance performance of the material. In addition, the role of the functional elements and the metal or metal oxide species in the nanochannels of the carbon affecting the supercapacitance of the materials will be demonstrated. Finally, the tuning of the EDLC and pseudocapacitance behaviour of the nanoporous carbon functionalized with different elements with a simple adjustment of the structural features will be demonstrated.

3:00 PM

(MCARE-094-2014) High Performance Supercapacitors Using Graphene Nanoribbons

J. B. Gaillard*, H. Colon-Mercado, Savannah River National Laboratory, USA; R. Czerw, NanoTechLabs, Inc., USA

We have investigated graphene nanoribbons (GNRs) as the electrode material in supercapacitors. Graphene structurally has two regions: the basal plane, consisting of a 2D honeycomb lattice of sp2-hybridized carbon atoms and the edge, comprising a single line of disordered carbon atoms. For electrochemical applications, the edge is known to store significantly more charge than the basal plane. Using previously reported experimental values of the areal capacitance for both the edge (10^5 μF/cm^2) and plane (4 μF/cm^2) [Yuan, et al. 2013], we calculated total contributions to energy density based on total volumetric content of the edge and plane. Our results show that GNRs (modeled as a 30 nm wide, 1 μm long ribbon) provide a theoretical volumetric energy density 10X greater than its graphene counterpart (modeled as a 1 μm diameter disk). We have produced supercapacitors using unzipped multiwalled carbon nanotubes (MWNTs) and hence GNRs as flexible electrode material. The GNRs were produced by chemically unzipping 30 nm diameter MWNTs with concentrated sulfuric acid and 500 wt% KMnO4. Using a 6M KOH aqueous solution as the electrolyte, we measured a high specific capacitance of 260 F/g and 200 F/g at a scan rate of 2 mV/s and 20 mV/s (after 100 cycles), respectively. The specific capacitance of the GNRs is ~5X greater than the original MWNTs. The specific energy reached 36 Wh/kg with a high specific power of 238 kW/kg.

3:20 PM

(MCARE-095-2014) Effect of the number of rings on the capacitance of bamboo-type titania nanotube arrays prepared by alternating voltage anodizing

F. J. Quintero*, P. J. Arias, J. D. Reyes, J. Agreda, H. Zea, National University of Colombia, Colombia

Titania nanotube arrays prepared by anodizing are known to be supercapacitors, though few studies are available. In this study we aim to increase the capacitance of the material by using alternating voltage anodizing to produce bamboo-type titania nanotube arrays. Titanium foils will be anodized in ethylene glycol containing 0.1 % ammonium fluoride and 5 % water, using another titanium foil as cathode and applying different squared-pulse voltage profiles consisting of one step at a low voltage of 20 V followed by one at a high voltage of 80 V. Partial results show that rings are formed on the outside of the nanotube walls during the low voltage step, as a consequence, total anodizing time and steps holding time will be varied in order to study the effect of the number of rings on the properties of the nanomaterial. Anodized titanium foils will be annealed in atmospheric air at 500 °C for two hours to crystallize the titania nanotube arrays prior to cyclic voltammetry measurements. Morphology will be studied by SEM, crystallography by XRD, and surface area by BET sorptometry. We expect to find an increase of the capacitance of the titania nanotube arrays when the number of rings, and thus their specific surface area, increases. The material is expected to be a supercapacitor with capacitance values around or above 100 μF cm^{-2}.

3:40 PM

(MCARE-096-2014) Mesoporous graphene synthesized by sacrificial template approach for electrochemical capacitor applications

J. Cao*, J. Xu, Z. Chen, Changzhou University, China

Electrochemical capacitors (ECs) have attracted broad interest as potential power sources due to their high power density, excellent cycling stability and low impact on the environment. As the commonly used active materials for ECs, porous carbon materials such as ordered mesoporous carbons, carbon nanotubes, carbon nanofibres, carbon aerogels, and graphenes have been intensively studied due to their low cost, high electrical conductivity, and large specific surface area. In particular, effective surface area and pore volume in carbon nanostructure can dramatically improve the performance of ECs by providing active sites available for charge-separation at the electrode/electrolyte interface. Mesoporous graphenes (MGs) was synthesized via one-pot pyrolysis reaction using dicyandiamide as a sacrificial template. The resulting MGs exhibit high surface area, large mesopore size (9.3 nm) and excellent conductivity. Benefiting from large mesopores and interconnected mesoporous nanostructures, MGs manifest outstanding specific capacitance (200 Fg-1) and excellent cycling stability when it is applied in ECs.

4:20 PM

(MCARE-097-2014) Surface Modification of Carbon Materials for Improved Capacitance (Invited)

K. Cuentas-Gallegos*, D. A. Baeza-Rostro, E. Fuentes-Quezada, Universidad Nacional Autónoma de México, Mexico; D. Pacheco-Catalán, J. M. Baas-López, Centro de Investigación Científica de Yucatán A.C., Mexico

Supercapacitors (SC) are energy storage devices with higher power but lower energy density than Li batteries. SC stores energy based on two mechanisms: double layer capacitance (non-Faradaic) and pseudocapacitance (faradaic). Porous carbon materials have been extensively used as electrodes in SC, where their great surface area and pore size distribution have been the main properties for capacitance improvement. Nevertheless, these properties show limitations since they cannot be highly increase without losing electric conductivity, which is detrimental for the power requirements of SC. An alternative approach to increase capacitance has been the modification of the surface of carbon materials by introducing pseudocapacitive contributions. In this work, the effect of grafted functional groups and electroactive nanoparticles has been studied to improve the intrinsic capacitance values of different carbon materials, such as: graphene oxide (GO), carbon aerogels (CA), and activated carbon (AC). Different characterization techniques were used to monitor the surface modifications made on the different carbons, such as: N2 and CO2 isotherms to determine BET surface area and pore size distribution attenuated Total Reflectance (ATR) to identify the formed chemical bonds, and cyclic voltammetry to evaluate the electrochemical performance for their use as electrodes in supercapacitor cells.

4:40 PM

(MCARE-098-2014) Self-assembled porous α-Fe2O3 mesocrystals-graphene hybrid nanostructures for Enhanced electrochemical capacitor

L. Gao*, X. Song, P. Zhang, S. Yang, School of Materials Science and Engineering, Shanghai Jiao Tong University, China

Self-assembled porous α-Fe2O3 mesocrystals-graphene hybrid nanostructures have been successfully synthesized by a simple route, which possesses a unique mesocrystals porous structure and a large specific surface area. Mesocrystals porous structure has recently attracted attention due to their increased levels of energy storage in electrochemical capacitors. However, porous mesocrystals-graphene nanohybrid and their grow mechanism has not been clearly investigated. Here we show the formation of Fe2O3/graphene nanohybrid by self-assembly of α-Fe2O3 mesocrystals on graphene. The Fe2O3/graphene nanohybrid exhibits enhanced capacitance of 306.9 F g-1 at 3 A g-1, and demonstrates superior rate capability and good cycling stability.

5:00 PM

(MCARE-099-2014) Carbon Monoliths for EDLC Electrodes with Outstanding Volumetric Capacitances

M. Kunowsky*, University of Alicante, Spain; A. Garcia-Gomez, V. Barranco, J. Rojo, Instituto de Ciencia de Materiales de Madrid, CSIC, Spain; J. Carruthers, ATMI, Adsorbent & Gas Technology, USA; ÁNGEL. Linares-Solano, University of Alicante, Spain

High density carbon monoliths (CM) are studied as supercapacitor electrodes. The starting CMs, produced by ATMI Co, were treated: 1. Under a N_2 flow at 1073 K to modify the carbon surface chemistry, and 2. Activated with CO_2 at the same temperature, using different activation times, to increase their porosity. Electrochemical measurements were performed in two-electrode cells with 2 M H_2SO_4 solution as electrolyte. The obtained CMs reveal high densities (up to 1.2 g cm^{-3}), high electrical conductivities (9-10 S cm^{-1}), high contents of surface oxygen groups (up to 2411 μmol CO g^{-1}), and large specific surface areas (1000-1600 m^2g^{-1}). The results show that the porosity of the starting CM is increased by physical activation with CO_2. The high density of the starting CM is slightly reduced by the heat treatments; however, they remain higher than values reported for other porous carbon monoliths. The performance of the CMs as supercapacitor electrodes show: i) high specific capacitances values (up to 290 F g^{-1}) due to their appropriate structure and porosity, ii) exceptional high volumetric capacitances (up to 339 F cm^{-3}), due to their high densities and iii) high energy as well as power densities. The volumetric capacitance values are the highest ever reported for porous carbon monoliths and are achieved due to both, their high specific capacitances and high densities.

5:20 PM

(MCARE-100-2014) High Reliability Ceramic Capacitors based on Temperature and Voltage-Stable Relaxor Dielectrics for High Operating Temperature Inverter Applications

G. Brennecka, H. J. Brown-Shaklee*, Sandia National Laboratories, USA; N. Raengthon, Oregon State University, USA; M. A. Blea, Sandia National Laboratories, USA; D. P. Cann, Oregon State University, USA

Advanced inverters based on wide band gap (WBG) semiconductors are attractive for increased efficiency and power handling capabilities over their Si-based counterparts. New dielectric materials are required because existing capacitor technologies of sufficiently high energy densities are not compatible with desired operating temperatures higher than 200°C. This presentation will focus on materials based on BaTiO3–Bi(Zn1/2Ti1/2)O3, a relaxor dielectric with a large relative permittivity that exhibits remarkable stability under large electric fields. This composition can be doped to produce very stable performance across broad temperature ranges >200°C. Low equivalent series resistance and equivalent series inductance multilayer ceramic capacitors based on this composition family and having capacitance values >200nF for operation above 1.5kV have been fabricated. This work was supported in part by the Energy Storage program managed by Dr. Imre Gyuk for the Department of Energy's Office of Electricity Delivery and Energy Reliability. 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.

5:40 PM

(MCARE-101-2014) Novel Approach of Increasing Capacitance by Coating Polyvinylidene Fluoride Langmuir-Schaefer Film on Graphene-Polyaniline Nanocomposite Electrode for Supercapacitor Applications

M. K. Ram*, P. Bolisetty, A. Takhi, Y. Goswami, E. Stefanakos, A. Kumar, University of South Florida, USA

Supercapacitors do not possess high energy density unlike the batteries, so research is mainly focused in improving the energy density by enhancing the material physical and chemical properties, and research is always in search of a new material. A nanocomposite of high energy density and surface area is considered to be an effective electrode material for enhancing performance and energy density of a supercapacitor. The supercapacitor fabricated based on G-PANI nanocomposite have shown to be an excellent electrode material in terms of obtained magnitude of specific capacitance, energy and power density. However, the G with PANI and its derivatives such as graphene-poly (o-anisidine) (G-POA) and graphene-poly (o-toluidine) (G-POT) have shown to exhibit specific capacitances of about 400 F/g, 380 F/g and 425 F/g, respectively. Recently, the increase of capacitance value has been proposed on carbon electrode by coating the barium titanate as high dielectric layer. However, the insulating properties have been found to affect the formation of electrochemical double layers (EDLCs). We tried to understand the enhancement of specific capacitance by coating an electrochemical active dielectric material over G-PANI electrode. Recently, we have fabricated symmetric and asymmetric supercapacitor based on several graphene (G)-conducting polymer (polyaniline (PANI), polypyrrole, poly (ortho-anisidine), polythiophene, and polyethylenedioxythiophene) nanocomposite, and obtained the specific capacitance varying from ~100-500 Farad/gram (F/gm). However, the G- PANI nanocomposite has been found to be promising material for supercapacitor applications with specific capacitance of around ~400 F/g. An attempt has been made to enhance the specific capacitance by depositing electrochemical active polyvinylidene fluoride (PVDF) polymer ultrathin film over G-PANI electrode. The pressure–area isotherm of PVDF Langmuir monolayer was studied, and Langmuir-Schaefer (LS) monolayer/monolayers film was deposited on G-PANI electrodes. The quality of PVDF LS film on G-PANI electrode was controlled by measuring optical (UV-Vis), morphological (scanning electron microscopic (SEM)) and surface (atomic force microscopic (AFM)) properties, respectively. The symmetric and asymmetric supercapacitor configured LB-PVDF on G-PANI based electrodes has been studied. This paper presents for the first time the experimental findings of PVDF LS films applications on G-PANI based electrodes for enhancement of specific capacitance of a supercapacitor.

Nanocomposites and Nanowires Materials for Photovoltaic and Photonic Technologies

Nanocomposites and Nanowires Materials for Photovoltaic and Photonic Devices IV

Room: Salon G

Session Chairs: Dongling Ma, INRS, Uni Quebec; Shi-Woo Rhee, POSTECH

2:20 PM

(MCARE-123-2014) Nanocomposite Hybrids Photoelectrodes for the High Efficiency Flexible Dye-Sensitized Solar Cells

M. Ko*, Korea Institute of Science and Technology (KIST), Republic of Korea

Over the last decade, dye-sensitized solar cell (DSSC) has attracted much attention due to the high solar-to-electricity conversion efficiency up to 12% as well as low cost compared with p-n junction photovoltaic devices. Replacing the heavy glass substrate with plastic materials is crucial to enlarge DSSC applications for the competition with inorganic based thin film photovoltaic devices. One of the biggest problems with plastic substrates is their low-temperature tolerance, which makes sintering of the photoelectrode films impossible. Therefore, the most important step toward the low-temperature DSSC fabrication is how to enhance interparticle connection at the temperature lower than 150 oC. In this talk, the key issues for high efficiency plastic solar cells will be discussed, and several strategies for the improvement of interconnection of nanoparticles and bendability will also be proposed.

3:00 PM

(MCARE-124-2014) Amorphous and Graphitic Carbon Nanoparticles for Energy Conversion: New Kids on the Carbon Block (Invited)

W. Kwon, S. Rhee*, POSTECH, Republic of Korea

Fluorescent carbon nanoparticles (FCNPs) have been the subject of extensive research because of their distinct benefits such as low cost, less toxicity, biocompatibility, and excellent photoresponses. There are now available a number of types of FCNPs, and they may generally fall within two major categories of carbon structures: amorphous and graphitic. Amorphous FCNPs (A-FCNPs), also called 'carbon nanodots' or 'carbon quantum dots', have a structure that some sp2 carbon clusters are embedded in a heterogeneous sp3 carbon matrix. Graphitic FCNPs (G-FCNPs), also widely known as 'graphene quantum dots', are nanometer-sized flakes of one or few-layer graphene, composed of a regular hexagonal lattice of sp2 carbon atoms edged with heteroatomic (in most cases oxygenic) functional groups. In this talk, we discuss similarities and differences between A- and G-FCNPs based on our novel synthetic method employing amine as a passivation agent. By investigating and comparing them, we can examine the origin of their opto-electronic properties, and therefore establish one fundamental principle successfully describing all their similarities and differences. We finally introduce some examples of real applications of FCNPs, especially regarding energy conversion devices such as solar cells, photo-electrochemical cells, and light-emitting diodes.

3:40 PM

(MCARE-127-2014) graphene base solar cell by incorporation new organic aromatic functionalized graphene oxide as charge transfer amplificator

T. Mahmoodi*, W. Rho, Y. Hahn, Chonbuk National University, Republic of Korea

In this study, we have demonstrated charge carrier amplification of the rGO coupled with Pyrenecarboxylic acid (PCA) and Isoguinoline-5-carboxylic acid (IQCA) could enhance the charge mobility property in BHJ solar cells. GO can act as an excellent hole-extraction layer while its PCA and IQCA- doped-derivatives (doped-rGO) are excellent charge carrier materials. The exceptional charge carrier performance is attributed to their tunable work functions through charge delocalization of the rGO via dopant and the amibipolar transporting ability of rGO basal plane. The inverted devices based on GO and doped-rGO:ZnO as hole- and electron-extraction layers and doped-rGO:P3HT active layer all outperform the corresponding standard BHJ solar cells. A 105 % improvement in the performance of inverted solar cells as a result of increased short-circuit current (Jsc) obtained using a composition of doped-rGO as electron carrier/ extraction material. Doped-rGO nanocomposites show higher electron conductivity than intrinsic samples; moreover, they show reduced contact resistance at the interface between the active layer and n-type buffer layer, thereby significantly increased the Jsc value. Thus, substantial increase in efficiency (up to 2.85%) was achieved for inverted solar cells with rGO nanocomposites layer in Glass/ITO/ZnO:doped-rGO/P3HT:doped-rGO/GO/Ag device.

4:20 PM

(MCARE-126-2014) Graphene-based Sensors and Solar Cells (Invited)

H. Zhu*, Tsinghua University, China

In this talk, I will demonstrate a graphene-based woven fabric made by interlacing two sets of graphene micron-ribbons and its uses in high sensitivity strain sensors and heterojunction solar cells. The conductive graphene/polymer hybrid films can act as electromechanical sensors under uniaxial tension. Tensile test accompanied by simultaneous electrical measurement shows a significant increase of resistance during the tensile cycle. The repeatable results of stretching in two different ways reveal that the graphene/polymer resistance is sensitive to the elongation rather than the shear strain. The exponential response on elongation implicates a subtle metal-insulator transition by strain engineering due to the macroscopic motion of graphene sheets in polycrystalline micron-ribbons. Graphene has the potential for creating thin film devices, owing to its two-dimensionality and structural flatness. Graphene serves multiple functions as transparent electrode, active junction layer, hole collector and anti-reflection layer in the graphene-on-semiconductor solar cells. Chemical doping, organic filling of graphene reduce the sheet resistance and facilitate the hole injection and extraction, resulting in high-quality heterojunctions and enhanced solar energy conversion efficiency. Our results show that the use of this carbon-based composite film may lead to a new line of portable and wearable nanodevices.

5:00 PM

(MCARE-128-2014) Comparative Study of the Output of Amorphous Silicon Photovoltaic Solar Cells when Receiving Direct and Diffused Radiations

M. O. Olatinwo, O. Oyeleke*, O. H. David, Federal Polytechnic Offa, Kwara State,Nigeria, Nigeria

Four amorphous silicon photovoltaic cells rated 12v, 20amps, 30watts DC were subjected to solar radiations study with the aim to determine their output at different positions. The amorphous silicon photovoltaics were paired in two. A pair was placed on a sun tracker while the other was placed on a fixed position. An LDR cell was constructed to control the tracking system while a LED was connected to indicate the radiation intensity at a particular time. The output powers for both arrangements were recorded at 10minutes interval for a period of two months. The data obtained were compared and treated to obtain a model of mean output power at a particular temperature for the two pairs separately. It was observed that the mean output power of the set up on tracking mechanism has a higher mean output power.

5:20 PM

(MCARE-129-2014) Application of nitrogen-doped TiO2 Films for Inverted Polymer Solar Cells

D. Kim*, H. Kim, H. Cho, Chonnam National University, Republic of Korea

Direct utilization of sunlight into electrical power is of great interest as a clean and safe energy source. Among various types of solar cells, Si-based solar cells can yield high power conversion efficiency and thus, is in mass production for practical usage. However, the expensive fabrication cost of the Si-based solar cells stimulated a research for alternative types of solar cells. Polymer solar cell (PSC) is considered as one of the promising candidates for the partial replacement of Si-based solar cell due to its advantages of low cost, easy fabrication, and moderate power conversion efficiency compared Si-based solar cells. However, poor stability of a conventional PSC in ambient condition should be resolved for commercialization. To improve the stability, there has been great attention in the alternative architecture, inverted structures where indium tin oxide (ITO) acts as electron collecting layer by lowering its work function with thin layer of inorganic metal oxides. TiO2 is the most commonly used material to improve charge extraction for electrons. Surface modification, morphology control, or direct modification of electrical properties of TiO2 by doping of metal or non-metal were proposed to enhance the performance and improve the stability of PSCs. Particularly, nitrogen doped TiO2 film has been successfully applied in PSCs and strong effects were observed.

Other Energy Issues

Other Energy Technologies II

Room: Salons B - C
Session Chairs: Michele Denton, Sandia National Laboratories; Dylan Cuskelly, University of Newcastle

2:20 PM

(MCARE-146-2014) Positioning to Win Government Research, Development, and Demonstration Funding

P. Winkler*, Government Contracting Specialists, LLC, USA

Learn how to identify government funded R, D, and D programs and how to position your technology to win government funding. Some of the key issues to be aware of will be reviewed. Several success stories will be presented. The advantages of working with the government include leveraging your company's research capabilities, using government funding as part of your open innovation process, enhancing your competitive edge by pursuing higher risk projects, increasing external resources for your project, and decreasing the time it takes to go to market.

2:40 PM

(MCARE-147-2014) Low Temperature Hydrogen Free Large Scale Graphene Growth Using Plasma-Enhanced Chemical Vapor Deposition for Energy Applications

A. H. Kaouk*, T. Singh, S. Mathur, Institute of Inorganic and Material Chemistry, Germany

Due to the very high mobility and the possibility to tune the electronic conduction via the field effect, graphene is very promising material for future electronic applications. In order for graphene fulfil the promises of future nanoelectronic devices, an easy and cheap route for mass production is an essential prerequisite. In this presentation, an easy and simple approach to extend the capabilities of plasma-enhanced chemical vapour deposition (PE-CVD) to the synthesis of few-layer graphene in a large temperature window (700oC < T > 250 oC) is presented, whereby the achieved deposition temperature of 250 °C is the lowest reported value for gas phase synthesis of graphene. Large micrometer grain size consisting of three to six atomic layers of stacked graphene sheets have been synthesized by controlled recombination of carbon radicals in a plasma. A simple and highly reproducible technique is essential, since the resulting sheets can be synthesized without the need for a catalyst on the surface of Cu substrate. A thorough structural analysis of the few layer graphene is performed with electron microscopy, X-ray diffraction, Raman spectroscopy and scanning tunnelling microscopy. Further the conjugations of graphene sheets with MOx films for energy applications will be discussed to fabricate novel graphene-based nanocomposites.

3:00 PM

(MCARE-148-2014) Modeling of thermal treatment of raw briquet in the course of foam glass production

D. Anton*, SPbGASU, Russian Federation

One of the main stages in the technology of foam glass producing is the thermal treatment (TT) during which the final item structure and its operational properties are formed. The TT process consists of 3 steps: preheating, foaming and annealing. We submit a mathematical model of TT in the course of foam glass producing which describes all steps of the process. The foam glass producing from raw briquet (brick of glass powder) without moulds is considered. The basic of TT model is boundary value problem of heat conduction. In order to find temperature dependences of properties of the raw briquet (coefficients in the thermal conductivity equation), the method of calculation is suggested. The feature of the model is statement of moving-boundary problem and taking into account temperature dependence of raw briquet properties. The model allows to find temperature distribution in raw briquet at any time moment, to calculate process and material parameters and to predict end-use foam glass properties. The model can be used to analyze, optimize and control TT process in the course of foam glass producing. The model adequacy was checked experimentally.

3:20 PM

(MCARE-149-2014) Numerical Study of Heterogeneous H-O-C-N-S Syngas Combustion System with a Porous Ceramic Media

A. C. Terracciano*, B. Hughes, N. Orlovskaya, S. S. Vasu, University of Central Florida, USA

Highly reactive gaseous species evolved at solid waste disposal sites and sewage treatment facilities present a serious human health and environmental risk; products evolved from decomposition produce combustible gasses, with a varied composition of primarily: H_2S, $(CH_3)_2S$, NH_3, and CH_4, these chemicals when in bodies of water disturb the delicate pH of already stressed aquatic ecosystems; while the gasses which remain airborne are key attributers to global climate change. Combustion of these gasses, within a porous combustion system, renders these extremely harmful byproducts into forms which exhibit less reactivity while also providing a renewable energy source. Utilizing collected data from literature, a characteristic syngas mixture utilizing H-O-C-N-S compounds has been constructed as a fuel for combustion in porous media, along with the inclusion of sulfur combustion mechanisms into an existing H-O-C-N system. The composite reaction mechanism and fuel mixture is then to be utilized in conjunction with an already experimentally verified physical model. Modeling simulations utilizing CHEMKIN-PRO of a porous combustor have been produced to provide a means of determining the optimal use of combustion in porous media, according to the syngas mixture, including a parameter expressing the maximum effective length of the porous solid.

3:40 PM

(MCARE-150-2014) MAX Phase Synthesis Via Reduction Reactions

D. Cuskelly*, University of Newcastle, Australia

Processes such as nuclear power, concentrated solar thermal power or thermal energy storage involve not only extremely hazardous conditions, demanding new combinations of properties not found in everyday materials. MAX phases (e.g. Ti3SiC2) have the potential to emerge as leading materials due to outstanding individual properties such as resistance to oxidation and chemical attack. These are useful in their own right, but perhaps more importantly in MAX phases they occur in combination with thermal shock resistance, damage tolerance and machinability which are extremely useful in energy applications. A promising method for reducing the synthesis cost, while maintaining the functionality of the MAX phase, is synthesis directly from the ore via an exchange reaction. For example our experiments have shown that TiO2 is reduced by Al in the presence of Si and C forming a Ti3SiC2-Al2O3 composite. Synthesis via both self-propagating synthesis, where the heat of reaction provides all the energy needed, and reactive sintering have produced MAX phase-Al2O3 composites free of contaminate phases such as TiC and titanium silicides. The composites can be put to use in high temperature applications such as concentrated solar thermal electricity generation, can be used as coatings for oxidation resistance, or the MAX phase can be refined via removal of the Al2O3 allowing it to be used for high thermal shock or damage tolerant applications.

4:20 PM

(MCARE-151-2014) Carbon Nanotubes Integrated with Superconducting NbC

G. Zou*, Soochow University, China

The formation of carbon nanotube and superconductor composites makes it possible to produce new and/or improved functionalities that the individual material does not possess. Here we show that coating well-aligned carbon nanotubes with superconducting niobium carbide (NbC) does not destroy the microstructure of the nanotubes in two different ways. NbC also shows much improved superconducting properties such as a higher irreversibility and upper critical field. An upper critical field value of ~5 T at 4.2 K is much greater than the 1.7 T reported in the literature for pure bulk NbC. Furthermore, the aligned carbon nanotubes induce anisotropy in the upper critical field, with a higher upper critical field occurring when the magnetic field is parallel to the carbon nanotube growth direction. These results suggest that highly oriented carbon nanotubes embedded in superconducting NbC matrix can function as defects and effectively enhance the superconducting properties of the NbC.

4:40 PM

(MCARE-152-2014) High Temperature Reactions of Agricultural Wastes as Material Resources for EAF Steelmaking

N. Mohd Yunos*, A. Ismail, M. Idris, University Malaysia Perlis, Malaysia

Agriculture waste is renewable source found in iron and steelmaking production that ability to reduce anthropogenic CO2 emission in the world next tackled the world's most problematic waste stream. Palm shells waste recycled as a carbon source replacing metallurgical coke in EAF steelmaking. The present paper studies the slag/carbon interaction, and Fe reduction of the palm shells char by physical and chemical activation that carbonized with H3PO4 acids. Analytical tools such as XRD, TG-MS and SEM are used to analyse and understand the structural transformations and gas formation during release of volatiles that occur at high temperature. The interactions of coke and palm shells with EAF slag were investigated at 1550 °C using sessile-drop in Ar atmosphere where the slag/carbonaceous residue interactions were conducted in a horizontal tube furnace using the sessile drop approach. Foaming was improved when palm shell char was used as carbon material. The palm shells kinetic advantage might come from its richer hydrogen content, in comparison to metallurgical coke, because the reduction reaction (FeO + H2(g) = Fe + H2O(g)) is much faster than the reduction of FeO with C. These results indicate that partial replacement of coke with palm shells char is efficient due to improved interactions with EAF slag.

Thursday, February 20, 2014

Plenary Session VII

Room: Salon E

8:25 AM

(MCARE-PL8-2014) Materials Development Synergies in Alternative and Renewable Energy Technologies

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

Many commonalities and synergies exist in the materials needs between various alternative and renewable energy technologies. The identification of synergies and leveraging of efforts can accelerate progress and provide benefits across technology areas. This presentation will describe examples and opportunities through the U.S. Department of Energy's, Office of Energy Efficiency and Renewable Energy's (EERE) Fuel Cell Technologies Office, which has maintained a comprehensive program to develop advanced hydrogen production and storage technologies for a number of years. Significant efforts have been devoted towards addressing materials challenges in these fields, specifically the development of materials for photoelectrochemical (PEC) hydrogen production, high energy density metal hydride, highly porous adsorbent materials and advanced carbon fiber composite technology for hydrogen storage. Today, joint efforts across EERE technology offices and the Advanced Research Projects Agency – Energy (ARPA-E) are being carried out on: a) wide bandgap semiconductors as more efficient PEC and photovoltaic materials and improved power control devices; b) metal hydrides as thermal energy storage materials for concentrated solar energy systems and efficient hydrogen compressors; c) highly porous materials for natural gas storage and carbon capture and sequestration; and d) low-cost, advanced carbon fiber composites for high-pressure tanks for H_2 and CNG, lightweight vehicle bodies and lighter weight, stronger wind turbine blades. Through coordinated, synergistic development efforts across technology offices the rate of development can be accelerated and carried out at lower overall costs.

Solar Fuels

Solar Fuels: Frontiers in Materials Development for Water Splitting Photocatalysts II

Room: Salon D

Session Chairs: Markus Niederberger, ETH Zurich; Riad Nechache, INRS-EMT

9:20 AM

(MCARE-050-2014) Photovoltaic proprieties and Photocatalytic activity of Multiferroics-based systems (Invited)

R. Nechache*, S. Li, F. Rosei, INRS-EMT, Canada

Photocatalytic water splitting with semiconductor materials has been investigated as a clean and renewable process for directly converting sunlight into chemical energy. In particular, multiferroics MFs have recently been used for applications in both photocatalysis (PC) and photovoltaics (PV) due to their ferroelectric properties and narrow band gaps, allowing them to harness the majority of solar radiation in the visible range. As typical MFs, BiFeO3 (BFO) and Bi2FeCrO6 (BFCO) have been recognized as potential materials for PV and visible-light PC applications owing to their suitable band gap (1.4-2.8 eV) and good chemical stability. However, the investigations on such materials for photocatalytic water splitting are still limited and efforts have to be undertaken to demonstrate their full potential. An efficient PV system is at the basis on an effective PC process. Thus, the control of PV properties of MFs is a critical issue for achieving highly efficient photocatalytic system. Here we will present, the controlled growth and characterization of BFCO and BFO thin films and nanostructures via pulsed laser and hydrothermal techniques. The PV properties of such systems and their photocatalytic activity will be also discussed.

10:00 AM

(MCARE-051-2014) Solution synthesis routes to advanced materials (Invited)

G. Westin*, Uppsala University, Sweden

Here we describe two approaches to synthesis of complex oxides, metals and nano-composites; (i) Metal alkoxides yielding pure complex composition oxides as nano-particles, thin or ultra-thin films and coatings, core-shells, wires and mixed nano-phase materials. Precursors and synthesis routes to different oxide systems relevant for energy materials will be described. Purely alkoxide based routes provide many beneficial possibilities such as low temperature synthesis of complex composition oxides, extended doping levels beyond the thermodynamic range and ultra-thin oxide coatings on nano-structured electrodes. (ii) Low-cost routes based on metal salt complexes that yield thin- or ultra-thin films and coatings, core-shells, and sponge or foam-like materials. Many structures have been achieved including: nano-structured metals and alloys as films and sponges, down to 1 nm ultra-thin Ni coatings on wires and nano-structured oxide electrodes as well as metal-in-ceramic composite films and thin or ultra-thin coatings on wires and porous oxide electrodes with a wide range of metals and oxide matrixes, having particle sizes down a few nm. The processes were up-scaled to large industrial or pilot 50 m roll-to-roll scale, resulting in superior hardness/toughness WC-Co mining tools and record efficient spectrally selective solar thermal absorbers with Ni-Al2O3 films.

10:40 AM

(MCARE-052-2014) Atomic Layer Deposition Modified Electrospun Nanofibers for Energy Conversion

A. Lepcha*, T. Singh, S. Mathur, University of Cologne, Germany

Application of tailor-made molecular precursors in low pressure or plasma-enhanced chemical vapor deposition techniques offers a viable solution for overcoming thermodynamic impediments involved in thin film growth. The use of atomic layer deposition and cold plasmas enables the realization of various functional coatings whose application spectrum spans from transparent conductive coatings, scratch-proof films to anti-bacterial materials. Over the past decade, we have developed several new precursor systems in order to demonstrate the competitive edge of molecule-based plasma coatings. Our work on a large number of metal oxide systems and their characterization towards microstructure, compositional and functional properties supports the advantages of chemical design in simplifying deposition processes and optimizing functional behavior. This talk will present electrospun one dimensional nanofiber mats coated with nanometric thin films for solar water splitting applications atomic layer deposition (ALD). The chemically amiable method of electrospinning allows the fabrication of photoactive materials in a large quantity with defined morphology and precise control of thin films deposition with ALD ultimately resulting in the elevation in the photocurrent of the photoanodes.

11:00 AM

(MCARE-053-2014) Production, Applications and Toxicology of nano TiO2 (Invited)

J. Prochazka*, HE3DA, Czech Republic

Nano applications of TiO2 in photocatalysis, catalysis and cosmetics take an increasing share of the TiO2 market. Since 1999, when only 4000 tons of nano TiO2 were sold, the market with nano titanium dioxide has grown more than 20 times. Consequently, there are an increasing number of new nano TiO2 syntheses and manufacturing technologies. While the number of new syntheses is large, there are only few manufacturing processes capable of producing TiO2 nanoparticles under $10,000/ton. The high price limits development of many applications. In this work we want to introduce a technology, where the manufacturing cost is comparable to the TiO2 white pigment process, which will allow mass scale use of nanoparticles in the future. The most dynamically growing applications of nano TiO2 are in photocatalytic coatings, paints and concrete. Good photocatalytic coatings contain high amounts of nano TiO2, and literally, any common surface can be functionalized by them, bringing new values to the daily life. Irregularities in behavior of nanoparticles brought many safety concerns and an increased focus on nano toxicology. A serious, resposible and professional approach to the toxicology of nanoparticles is very important in order to protect human health and the environment, without causing significant damage to the economy by unreasonable, speculative or naive claims about the issue.

11:20 AM

(MCARE-054-2014) In-Situ investigations on CVD grown photo catalysts for photoelectrochemical water splitting

T. Fischer*, S. Mathur, University of Cologne, Germany

The chemical vapor deposition (CVD) is a well established tool for the synthesis of homogeneous thin films and anisotropic nanostructures, but the details during film growth still remains unclear, especially when using tailored single source precursors which allow the deposition of materials with a defined stoichiometry, morphology and phase, due to their preformed molecular structure. Using metal organic precursors with complex decomposition and reaction pathways, a deeper insight into the film formation relies on in-situ diagnostic tools like mass spectrometry and electrical spectroscopy, resolving the chemical composition of the gas phase products as well as the evolution of the electrical properties of the resulting film, respectively. Especially the direct monitoring of the materials' electrical resistance during the CVD process is a suitable tool in tailoring the materials properties needed for the targeted application. This presentation will focus on the growth of TiO2 and Fe2O3 nanostructured thin films and their application in photocatalytic and photoelectrochemical (PEC) water splitting applications.

11:40 AM

(MCARE-055-2014) Electrocatalysts for Water Splitting and Solar Fuel

K. Joya*, Leiden University, Netherlands

Recently, there is a lot of research activity related to artificial photosynthesis in order to develop an artificial solar to fuel conversion device, the "Artificial Leaf". A key component of an artificial leaf is a robust and efficient water oxidation catalyst (WOC). In combination with a suitable CO2 reduction catalytic system, the electrons and protons released from water oxidation can be reduced directly into liquid fuels. We here disclose a very simple electrochemical approach to make electrocatalytic materials on electrode surface in a neutral pH system that can be efficiently employed for water oxidation, H2 generation and CO2 reduction system. The surface morphology, materials features and catalytic abilities of so generated electrocatalytic materials are identical to those generate by other methods, and catalytic performance of these surface-assemblies for water splitting is remarkable over a wide range of pH (pH 6-11). These electro-assembled catalysts are very efficient for H2/O2 evolution systems, and in combination with suitable CO2 reduction module at the cathode, they are able to generate liquid fuel (formic acid, methanol) from water.

Batteries and Energy Storage

Li-S and Li-ion Batteries

Room: Salon E
Session Chairs: Stefan Adams, National University of Singapore; Sebastian Osswald, Naval Postgraduate School

9:20 AM

(MCARE-102-2014) Insight into Li-S batteries using analytical tools in operando mode (Invited)

M. Patel, National Institute of Chemistry, Slovenia; I. Arčon, CO-NOT, Slovenia; G. Aquilanti, Elettra-Sincrotrone Trieste S.C.p.A., Italy; R. Dominko*, National Institute of Chemistry, Slovenia

Lithium sulfur (Li-S) batteries are gaining significant importance due to their high energy density. The remaining challenge before commercialization is to control the polysulfide formation and consequently to stabilize capacity retention. Understanding the mechanism(s) of polysulfide formation along with knowledge about the interactions of sulfur and polysulfides with a host matrix and electrolyte are essential for the development of long cycle life lithium sulfur (Li-S) batteries. To achieve this goal, new analytical tools need to be developed. We recently started to develop and use three different analytical tools in operando mode which enable us quantitative and qualitative determination of polysulfides in the separator and within cathode composite. Using a 4-electrode modified Swagelok cell we can quantitatively detect polysulphides that are migrating from cathode. Complimentary information can be obtained from UV-Vis spectroscopy, which besides quantitative determination of polysulpfides offers qualitative determination. The last analytical tool is based on a sulfur K-edge XAN study of battery components and batteries run in operando mode and it give us information about interactions and concentration of sulfur in the different parts of electrode. The setup for in operando measurements can be viewed as valuable analytical tools that can aid in the understanding of the Li-S batteries behavior.

10:00 AM

(MCARE-103-2014) Lithium Sulfur Batteries: Fundamental Understanding Towards Practical Application (Invited)

J. Xiao*, J. Zheng, D. Lv, T. Lozano, J. Liu, Pacific Northwest National Laboratory, USA

Lithium sulfur (Li-S) batteries have attracted increasing attention because of their high theoretical capacity, natural abundance, low cost and environmental friendliness. However, the low electrical conductivity of sulfur and the "shuttle reaction" caused by the soluble polysulfides are detrimental to Li-S battery performances, leading to low utilization rate of sulfur, poor Coulombic efficiency, fast capacity fading and self-discharge. Although there are many approaches reported in literature to address the challenges in Li-S system, the sulfur content in S/C composite, electrode thickness and testing conditions vary largely in different groups, making the direct comparison or evaluation of various methods a difficulty. This talk will discuss the fundamental research in Li-S batteries from electrochemical point of view by using consistent sulfur cathode baseline cathode and testing conditions. The knowledge gained from these baseline cathodes were then successfully transferred into thick sulfur cathode with practical usable mass loadings. The entangled electrochemical and chemical reactions associated in Li-S batteries were further elaborated by using advanced characterization techniques in an attempt to provide new insights for this battery system.

10:40 AM

(MCARE-104-2014) High energy density batteries using thiophosphate solid electrolytes (Invited)

S. Adams*, National University of Singapore, Singapore

Fast ion conducting (FIC) solids more and more grow beyond the thin film battery niche to crucial elements for a wide range of high energy density battery concepts ranging from bulk all-solid-state e.g. Lithium-sulfur batteries to battery/fuel cell hybrids (such as redox flow and Lithium-air batteries). Key advantages of FICs include their potential to improve safety and stability over conventional batteries. Moreover the scalability of battery/fuel cell hybrids renders them promising for grid support applications. Identifying electrochemically stable lithium or sodium FICs and designing viable processing routes is thus crucial to achieve high energy density batteries with viable power performance. Our studies of thiophosphate-based FICs highlight the role of disorder in the immobile sublattice for maximizing conductivity both for argyrodite-type halide-doped thiophosphates Li6PS5X (X=Cl, Br) as well as for Li10MxP3-xS12, where the local anion disorder limits packing density and leaves free volume for fast ion transport channels and their interconnection to an anisotropic 3D pathway network. To reduce the synthesis costs of these two classes of thiophosphate solid electrolytes, we developed low temperature or no heating routes for the preparation of the various thiophosphate solid electrolytes and demonstrate the performance of Lithium-sulfur batteries employing these solid electrolytes.

11:00 AM

(MCARE-105-2014) Thermodynamics and Kinetics of Semi Solid Flow Cells (Invited)

S. Osswald*, Naval Postgraduate School, USA

The increasing utilization of renewable energy sources is driving the need for low-cost medium-to-large scale energy storage systems. A promising approach is the Semi Solid Flow Cell (SSFC), which operates on the principle of moving suspensions of active materials past inert electrodes to store or utilize electricity. Energy and power density can be scaled independently, which gives these systems distinct advantages over existing technologies. While SSFCs have great potential for future applications, they are subject to complex physical and electrochemical processes. To date, the SSFC approach has only been applied to the lithium ion chemistry and its suitability for other chemistries remains largely unknown. Here we present a thorough analysis of the thermodynamics and kinetics of such battery systems, with the goal to identify crucial design and performance requirements. Using the example of the lead acid chemistry, suspension stability and particle-to-electrode resistance were identified as the performance-limiting parameters. The results of the study were used to develop tools for evaluating the suitability of different battery chemistries for the SSFC approach and to provide a road map for the design of a functional SSFC.

11:20 AM

(MCARE-106-2014) Fabrication of TiO2/graphene in core-shell structure as advanced anode materials

Y. Yao, R. Sisson*, Worcester Polytechnic Institute, USA; Q. Xu, Z. Xia, University of North Texas, USA; Y. Cen, J. Liang, Worcester Polytechnic Institute, USA

In this report, anatase TiO2 nanoparticles (NPs) were synthesized by a facile sol-gel method. In order to improve the lithium insertion and extraction, graphene was introduced by a self-assembly process: first, TiO2 NPs were modified by APTES to introduce positive charges to their surface; second, the TiO2 NPs were wrapped by negatively charged graphene oxide by electrostatic interaction; finally the TiO2/GO composite was reduced by hydrazine, a TiO2/graphene composite in a core-shell structure was obtained. The morphology and crystalline structure were investigated by TEM, SEM and XRD studies. Several important factors, such as size and phase control of TiO2 NPs during the sol-gel process and the mechanism of improved conductivity in the composite were discussed. The thickness of graphene coating on individual TiO2 were identified by TEM and agreed well with calculated thickness based on TGA result. The conformal and uniform graphene coating was identified as the key contributor to the enhanced electrochemical performance. The initial capacity of TiO2/graphene composite was as high as 409mAh/g and a promising specific capacity of 141mAh/g even at 20C current rate was observed. Long term cycling tests at 1C current rate yielded a specific capacity of 343mAh/g, and Coulumbic efficiency of above 98% at 100 cycles.

11:40 AM

(MCARE-107-2014) High capacity Li2MnSiO4/C nanocomposite prepared by a resorcinol-formaldehyde assisted sol-gel method

K. Xie*, Y. Pan, College of Aerospace Science and Engineering, National University of Defense Technology, China

As a new cathode material for lithium batteries, lithium manganese silicate (Li2MnSiO4) is able to achieve two lithium insertion/extraction theoretically, which means it has a high theoretic specific capacity of 330 mAhg-1, nevertheless, it also shows advantages such as abundance and low cost of raw materials, good safety, and environmental friendliness, thus it has attracted increasing interest to researchers in recent years. However, the extremely low electronic conductivity and bad cycling stability of this cathode material have greatly limited its development and application. Aimed at solving the existing problems of the Li2MnSiO4 material, in-situ carbon coating and nano technique were adopted successfully by a resorcinol-formaldehyde assisted sol-gel method, and its electrochemical performance was greatly improved, the obtained Li2MnSiO4/C nanocomposite delivers a high initial discharge capacity of 251.6 mAh g-1 at a current density of 10 mA g-1 under optimal conditions. The improved electrochemical performance can be ascribed to the nanoparticle size and the coated carbon on the Li2MnSiO4 crystalline formed by the decomposition of resorcinol-formaldehyde resin during calcination, which can enhance the electronic conductivity as well as lithium-ion diffusion coefficient.

Nanocomposites and Nanowires Materials for Photovoltaic and Photonic Technologies

Nanocomposites and Nanowires Materials for Photovoltaic and Photonic Devices V

Room: Salon G
Session Chairs: Michael Filler, Georgia Institute of Technology; Zhifeng Ren, University of Houston

9:20 AM

(MCARE-130-2014) Vapor-Liquid-Solid Synthesis as a Route to Manipulate Energy Flow at the Nanoscale (Invited)

N. Shin, M. Filler*, Georgia Institute of Technology, USA

The vapor-liquid-solid synthesis of semiconductor nanowires offers exciting opportunities to control energy conversion and transport. However, the robust tuning of photon absorption/scattering or thermal transport in kinking, defect, and/or diameter-modulated superstructures is likely to remain elusive without significant advances in structural fidelity and user-programmability. Here, we will show that sidewall surface chemistry plays a critical role in determining nanowire structure. Our experimental approach couples the in-situ infrared spectroscopic interrogation of chemical bonding with post-growth structure and property characterization. We connect nanowire crystal structure with the specific chemical bonds present during synthesis and, in doing so, provide a firm foundation from which to control morphology and therefore function. Our recent results show that well-defined Si nanowire kinking superstructures result from interplay between adsorbed hydrogen atoms and a continuous twin boundary that reduces the symmetry of the catalyst droplet. Changes to surface chemistry also favor {111} sidewall facets, which deform the catalyst droplet, drive transverse twin boundary nucleation, and open the door to twinning superlattices in Si. Both of these findings identify the root cause of well-known growth phenomena and highlight the importance of designing novel precursors for engineering nanowires.

10:00 AM

(MCARE-131-2014) Nanostructures for High Efficient Photovoltaic Solar Cells and Flexible Transparent Electrode (Invited)

Z. Ren*, University of Houston, USA

Photovoltaic technology converting solar energy into electricity is playing more and more important role in providing the society with clean energy and reduces the impact of burning fossil fuels on environment. How to increase the photovoltaic conversion efficiency has been studied very intensively during the past couple of decades. In this talk, I will present our effort using nanostructures to improve the conversion efficiency by both designing new structures and inventing new transparent electrode, specifically I will discuss our development on nano coaxial cable solar cells to separate the photon and charge path ways, ultra thin film solar cells for efficient light absorption, and super flexible transparent electrode for efficient collection of charges.

10:40 AM

(MCARE-132-2014) Iron Pyrite Films with Passivated Surface States for Photovoltaic Applications

J. A. Frantz*, C. C. Baker, S. C. Erwin, N. D. Bassim, S. B. Qadri, J. D. Myers, J. A. Freitas, E. R. Glaser, J. S. Sanghera, Naval Research Laboratory, USA

We evaluate the potential for surface passivation in thin films of iron pyrite (FeS_2) – a material that is promising for photovoltaic (PV) applications but has electronic properties that are degraded by surface defects – by use of wide bandgap semiconductor capping layers. Bulk FeS_2 crystallizes in the cubic pyrite structure, and its sulfur atoms are paired in an S-S bond. Its surfaces, however, are typically terminated by S monomers. The resulting surface states exhibit defects within the FeS_2 bandgap, and the surface has properties similar to the iron monosulfide phase with a bandgap of ~0.3 eV. In PV devices, these surface states lead to high dark currents and low open circuit voltages. In order to passivate the surfaces, thin films of sputtered FeS_2 are sandwiched between 15 nm layers of ZnO and ZnS and compared with films deposited without capping layers. The films' interfaces are characterized via X-ray diffractometry, transmission electron microscopy, X-ray photoelectron spectroscopy (XPS), photoluminescence spectroscopy, and electron paramagnetic resonance measurements. ZnS-capped films show a significant decrease in monosulfide character as evidenced by a decrease in the XPS peak associated with the surface states. This result is supported by a density functional theory model that shows nearly perfect surface passivation. ZnS is thus identified as an especially promising passivation layer.

11:00 AM

(MCARE-133-2014) Photonic Metal Oxide Nanomaterials for Energy Related Applications & Solar Fuels

E. Redel*, KIT (Karlsruhe Insitute of Technology), Germany

A straightforward, cost effective and technologically relevant synthetic method will be presented to produce an extensive composition library of different metal oxide as well as hybrid nanomaterials and hierarchical multilayer constructions thereof. Potential applications will be shown e.g. as white light Bragg Reflectors (Tandem & Gradient Architectures), tune able and porous 1D Photonic Crystals, porous and transparent conducting thin films, electrochromophotonic switches as well new single & multilayered photocatalytic architectures. Additionally, new 1D Hybrid Photonic Materials as optical sensing devices will be discussed, including novel metal-organic thin film materials for light harnessing will be presented.

11:20 AM

(MCARE-134-2014) Nitrogen doped TiO2 and Eosin-Y dye for Dye sensitized solar cell (Invited)

K. C. Mohite*, University of pune, India; M. T. Sarode, Mahatma Phule Arts, Science and Commerce College, India; B. B. Kale, Centre for Materials for Electronics Technology (C-MET), India

In this paper, photovoltaic properties of Dye sensitized solar cell based on pure TiO2 and nitrogen (N) doped TiO2 film electrode with eosin-Y dye as a photo sensitizer are reported. The carbon coated indium tin oxide is used as a counter electrode. This TiO2 film electrode was prepared by using (1) sol-gel dip-coating method; and (2) Doctor's blade method. The resultant films were characterized by using XRD, Raman spectroscopy, XPS, SEM, TEM and UV-Visible spectroscopy. The X-ray diffraction patterns shows the pure anatase TiO2 phase at annealed temperature of 400 0C. The morphological studies with SEM indicated nearly uniform distribution of spherical agglomerates with average size 20-25 nm. The TEM studies indicated nanocrystalline state of films (average particle size ~ 15- 20 nm) consistent with XRD results of crystallite size (~15 - 25 nm). A profound effect of variation of film thickness on optical and eosin-Y sensitized photovoltaic characteristics of TiO2 films is observed. The band gap of the pure TiO2 was observed to be 3.22 eV and it shifted to 2.69 eV after doping with nitrogen in the ratio of Ti:N (1:15). The presence of nitrogen was also confirmed by XPS characterization. The results of the investigation showed that the DSSCs made with N-TiO2 film electrode has improved photocurrent efficiency than nanocrystalline TiO2 film.

Author Index

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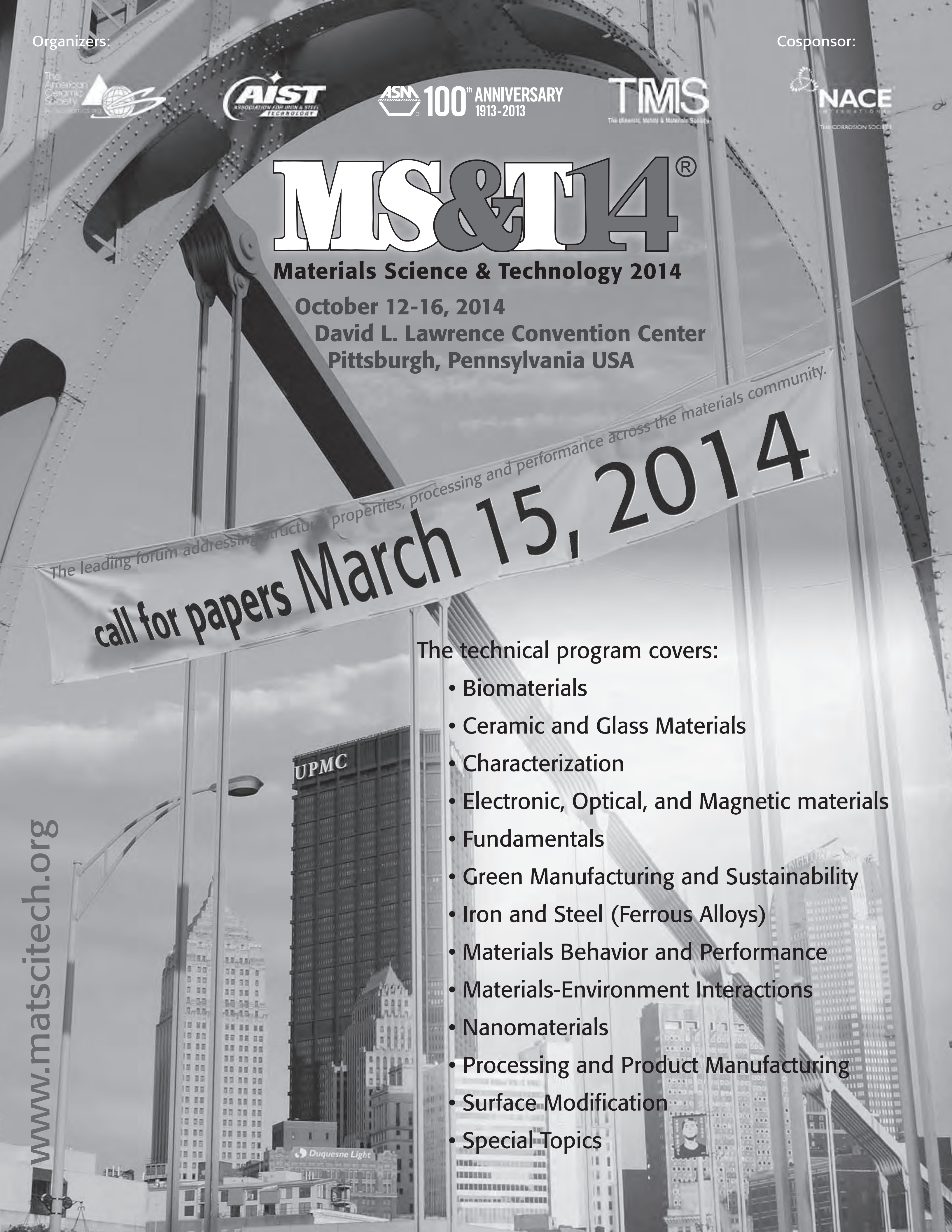
*Denotes Presenter

Author Index



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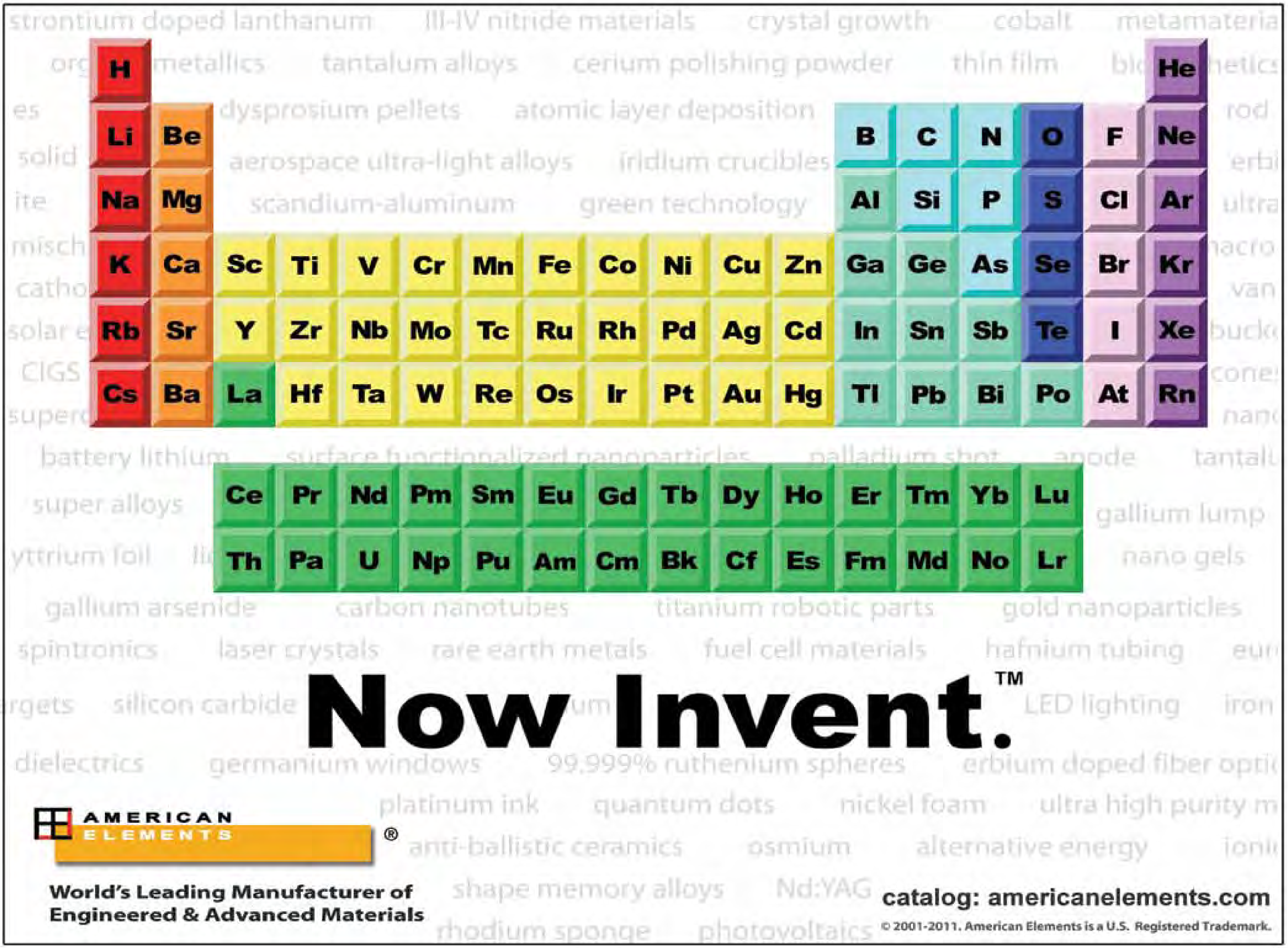
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K Ca Sc Ti V Cr Mn Fe Co Ni Cu Zn Ga Ge As Se Br Kr
Rb Sr Y Zr Nb Mo Tc Ru Rh Pd Ag Cd In Sn Sb Te I Xe
Cs Ba La Hf Ta W Re Os Ir Pt Au Hg Tl Pb Bi Po At Rn
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Th Pa U Np Pu Am Cm Bk Cf Es Fm Md No Lr
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crystal growth
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metallics
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