

CONFERENCE PROGRAM

MATERIALS CHALLENGES IN ALTERNATIVE AND RENEWABLE ENERGY

April 17 - 21, 2016

Hilton Clearwater Beach
Clearwater, FL, USA

ceramics.org/mcare2016

Organized by:



KICHE
The Korean Institute of Chemical Engineers

WELCOME

Dear Colleagues and Friends,

Welcome to the Materials Challenges in Alternative & Renewable Energy Conference (MCARE 2016), organized by The American Ceramic Society (ACerS). MCARE 2016 is a premier forum to address opportunities of emerging material technologies that support sustainability of a global society. MCARE 2016 brings together leading global experts from universities, industry, research and development laboratories, and government agencies to interact collaboratively and communicate materials technologies that address development of affordable, sustainable, environmentally friendly, and renewable energy conversion technologies.

We are happy to announce a partnership recently formed between The Korean Institute of Chemical Engineers (KIChE) and ACerS to co-organize MCARE annually through 2020. MCARE will be hosted in Korea in 2017 and 2019, and in the United States in 2018 and 2020. As a part of this new partnership, one of the plenary sessions at MCARE 2016 will feature the 1st Annual ACerS-KIChE Distinguished Lecture. There will be additional plenary sessions to begin each day. See page vi for details about these special plenary lectures. In addition, the conference includes technical sessions that address challenges and solutions in the areas of hydrogen (production, materials, and the economy); spectral conversion materials; ferroelectrics and multiferroics; nuclear energy; fuel cells; photovoltaics; self-powered generators; batteries and energy storage; direct thermal-to-electrical energy conversion; and critical materials for energy.

We are happy that you are here, appreciate your participation, and hope you enjoy the meeting.

The 2016 Organizing Committee:



Sanjay Mathur
University of Cologne,
Germany



Yoon-Bong Hahn
Chonbuk National
University,
South Korea



H.T. Lin
Guandong University
of Technology, China



Steven Tidrow
Alfred University, USA

Future of MCARE

Yoon-Bong Hahn (left) of Chonbuk National University in Korea; ACerS president Mrityunjay Singh (center) and Do-Heyoung Kim (right) of Chonnam National University in South Korea signed a Memorandum of Understanding that establishes a rotation of the Materials Challenges in Alternative and Renewable Energy conference between the two countries. Kim represented the Korean Institute of Chemical Engineers at the signing.



SAVE THE DATE

FEBRUARY 20 – 24, 2017

MATERIALS CHALLENGES IN ALTERNATIVE & RENEWABLE ENERGY (MCARE 2017) | Jeju, Korea

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Schedule at a Glance

Materials Challenges in Alternative & Renewable Energy 2016

April 17 – 21, 2016

Hilton Clearwater Beach, Clearwater, FL, USA

Sunday, April 17, 2016

Registration	4:00 p.m. – 7:00 p.m.	Salon Foyer
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Monday, April 18, 2016

Registration	7:00 a.m. – 5:30 p.m.	Salon Foyer
Plenary Session	8:30 a.m. – 9:40 a.m.	Salon E
Concurrent Sessions	10:00 a.m. – 5:20 p.m.	Salons A-C, D, E, F, G
Networking Lunch	12:00 p.m. – 1:30 p.m.	Flamingo/Sandpiper Decks
Welcome Reception	6:00 p.m. – 7:30 p.m.	Flamingo/Sandpiper Decks

Tuesday, April 19, 2016

Registration	8:00 a.m. – 5:30 p.m.	Salon Foyer
Plenary Session	8:30 a.m. – 9:30 a.m.	Salon E
Concurrent Sessions	9:50 a.m. – 5:30 p.m.	Salons A-C, D, E, F, G
Networking Lunch	12:10 p.m. – 1:40 p.m.	Flamingo/Sandpiper Decks
Poster Session	6:00 p.m. – 8:00 p.m.	Water's Edge Ballroom

Wednesday, April 20, 2016

Registration	8:00 a.m. – 5:30 p.m.	Salon Foyer
Plenary Session	8:30 a.m. – 9:30 a.m.	Salon E
Concurrent Sessions	10:00 a.m. – 5:30 p.m.	Salons A-C, D, E, F, G
Lunch on own	12:10 p.m. – 1:40 p.m.	

Thursday, April 21, 2016

Registration	8:00 a.m. – 12:10 p.m.	Salon Foyer
Plenary Session	8:30 a.m. – 9:30 a.m.	Salon E
Concurrent Sessions	9:50 a.m. – 12:10 p.m.	Salons A-C, D, E, F, G

MATERIALS CHALLENGES IN ALTERNATIVE AND RENEWABLE ENERGY

PLENARY SPEAKERS

Monday, April 18



**ACerS-KIChE Distinguished Lecturer:
Sang-Woo Kim**

Sungkyunkwan University (SKKU), Korea

Presentation Title: *Energy harvesting with nano-generators for realizing self-powered small electronics*

Tuesday, April 19



**Plenary Speaker:
Mohammad K. Nazeeruddin**

Swiss Federal Institute of Technology Lausanne (EPFL),
Switzerland

**Presentation Title: *Perovskite solar cells:
A new paradigm in energy sector***

Wednesday, April 20



**Plenary Speaker:
Arumugam Manthiram**

Cockrell Family Regents Chair in Engineering #7; Director,
Texas Materials Institute; Director, Materials Science and
Engineering Program, The University of Texas at Austin

**Presentation Title: *Next-generation battery chemistries:
Materials challenges and prospects***

Thursday, April 21



**Plenary Speaker:
Chris Paradies**

President, Paradies Law

**Presentation Title: *Patenting materials for alternative
and renewable energy: Challenges and opportunities***

Organized by:



MATERIALS CHALLENGES IN ALTERNATIVE

Symposia schedule and organizers

SYMPOSIUM SESSIONS

	MONDAY	
	A.M.	P.M.
S1: Functional Materials for Photoelectrochemical and Electrocatalytic Hydrogen Production		
S2: Spectral Conversion Materials for Energy Applications		
S3: Ferroelectrics and Multiferroics for Energy Applications		
S4: Material Challenges in Nuclear Energy		
S5: Materials Challenges in Fuel Cells		
S6: Critical Materials for Energy		
S7: Emerging Materials for Next Generation Photovoltaics		
S8: Self-Power Generators		
S9: Direct Thermal-to-Electrical Energy Conversion Materials and Applications		
S10: Batteries and Energy Storage		
S11: Hydrogen Materials and Economy		

ORGANIZERS

S1 FUNCTIONAL MATERIALS FOR PHOTO-ELECTROCHEMICAL AND ELECTROCATALYTIC HYDROGEN PRODUCTION

Organizers: Sanjay Mathur, University of Cologne, Germany; Yoon-Bong Hahn, Chonbuk National University, Korea; Steven Tidrow, Alfred University, USA; Silke Christiansen, Helmholtz Energy Zentrum, Berlin; Jan Augustynski, University of Warsaw, Poland; Heli Wang, NREL, Colorado, USA; Juan-Ramon Morante, IREC, Barcelona, Spain; Nianqiang (Nick) Wu, West Virginia University, USA; Gunnar Westin, Uppsala University, Sweden; Gurpreet Singh, Kansas State University, USA

S2 SPECTRAL CONVERSION MATERIALS FOR ENERGY APPLICATIONS

Organizers: Dr. Eva Hemmer, INRS, Quebec, Canada; Dr. Marta Quintanilla, INRS-EMT, Quebec, Canada; Dr. Jose Marques-Hueso Heriot Watt University, Edinburgh, UK

S3 FERROELECTRICS AND MULTIFERROICS FOR ENERGY APPLICATIONS

Organizers: Menka Jain, University of Connecticut, USA; Paula Maria Vilarinho, University of Aveiro, Portugal; Miguel Alguero, CSIC, Spain

S4 MATERIAL CHALLENGES IN NUCLEAR ENERGY

Organizers: Hua-Tay Lin, Guangdong University of Technology YutaiKatoh, Oak Ridge National Laboratory); Ji-Jung Kai, City University of Hong Kong JiYeon Park, Korea Atomic Energy Research Institute, Korea; Tatsuya Hinoki, Kyoto University, Japan; RuobingXie, Shanghai Institute of Applied Physics, China

S5 MATERIALS CHALLENGES IN FUEL CELLS

Organizers: Jonghee Han, KIST, Korea; Sung Jong Yoo, KIST, Korea; Stephen McPhail, ENEA, Italy; Kazumi Tanimoto, AIST, Japan; Olivier Guillon, ForschungszentrumJülich, Germany

S6 CRITICAL MATERIALS FOR ENERGY

Organizers: Taek-SookKim, Korea Institute of Industrial Technology, and Univ. of Science & Technology, Korea; Ryan Ott, The Ames Laboratory, USA; Tadachika Nakayama, Nagaoka University, Japan; Annett Gebert, IFW, Germany; Bum Sung Kim, Korea Institute for Rare Metals, Korea; Wei-Sheng Chen, National Cheng Kung University, Taiwan; Dudley J. Kingsnorth, Curtin University, Australia; Nobuhito Imanaka, Osaka University, Japan; Lorenzo Martínez Gómez, Instituto de Ciencias Físicas, UNAM, Mexico

TUESDAY		WEDNESDAY		THURSDAY	
A.M.	P.M.	A.M.	P.M.	A.M.	

S7 EMERGING MATERIALS FOR NEXT GENERATION PHOTOVOLTAICS

Organizers: Hyun Suk Jung, Sungkyunkwan University, Korea; Hua Zhang, Nanyang Technological University, Singapore; Hanwei Gao, Florida State University, USA; Dan Wang, Chinese Academy of Sciences, China; Iván Mora Seró, Jaumel University, Spain; Bin Liu, Nanyang Technological University, Singapore; Sang Hyuklm, Kyung Hee University, Korea

S8 SELF-POWER GENERATORS

Organizers: Sang-Woo Kim, Sungkyunkwan University, Korea; Christian Falconi, Univ. of Rome Tor Vergata, Italy; Husam N. Alshareef, King Abdullah University of Science & Technology, Kingdom of Saudi Arabia; Caofeng Pan, Beijing Institute of Nanoenergy and Nanosystems, China ; Jeong Min Baik, Ulsan National Institute of Science and Technology, Korea; Yu-LunCheuh, National Tsing-Hua University, Taiwan

S9 DIRECT THERMAL-TO-ELECTRICAL ENERGY CONVERSION MATERIALS AND APPLICATIONS

Organizers: Terry M. Tritt, Clemson University, USA; Lidong Chen, Shanghai Institute of Ceramics, Chinese Academy of Sciences, China

S10 BATTERIES AND ENERGY STORAGE

Organizers: Palani Balaya, National University of Singapore, Singapore; Dany Carlier-Larregaray, ICMCB-CNRS, Bordeaux, France; MickaelDolle, Université de Montréal, Canada; Robert Dominko, National Institute of Chemistry, Slovenia; Kisuk Kang, Seoul National University, Seoul, Korea; Partha P. Mukherjee, Texas A&M University, USA; Neeraj Sharma, University of New South Wales, Australia

S11 HYDROGEN MATERIALS AND ECONOMY

Organizers: Steven Tidrow, Alfred University, USA

MATERIALS CHALLENGES IN ALTERNATIVE AND RENEWABLE ENERGY

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Cell phones silent



No photography/recording

Technical Meeting and Exhibition

MS&T16

MATERIALS SCIENCE & TECHNOLOGY

OCTOBER 24-26, 2016 | SALT PALACE CONVENTION CENTER | SALT LAKE CITY, UTAH, USA

TECHNICAL PROGRAM

- Additive Manufacturing
- Biomaterials
- Ceramic and Glass Materials
- Electronic and Magnetic Materials
- Energy
- Fundamentals, Characterization, and Computational Modeling
- Iron and Steel (Ferrous Alloys)
- Materials-Environment Interactions
- Nanomaterials
- Processing and Manufacturing
- Special Topics

VISIT MATSCITECH.ORG TO VIEW THE **84 SYMPOSIA TOPICS**, FOR MORE DETAILED INFORMATION, AND SUBMISSION INSTRUCTIONS.

Organizers:

The American Ceramic Society
www.ceramics.org

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ASM
INTERNATIONAL

TMS
The Minerals, Metals & Materials Society

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Oral Presenters

Name	Date	Time	Room	Page Number	Name	Date	Time	Room	Page Number
A					J				
Adams, S.	20-Apr	9:50AM	Salon E	11	Islam, M.R.	20-Apr	10:30AM	Salon F	10
Ahmad, I.	20-Apr	3:50PM	Salons A-C	11	J				
Almeida, R.M.	18-Apr	2:10PM	Salon D	4	Jain, M.	19-Apr	11:30AM	Salon F	6
Alshareef, H.N.	19-Apr	1:40PM	Salon G	8	Jalem, R.	19-Apr	3:20PM	Salon E	8
Amin, M.R.	18-Apr	2:10PM	Salon E	5	Jiang, Q.	20-Apr	10:10AM	Salon D	10
Ang, C.	20-Apr	2:40PM	Salons A-C	11	Jones, J.L.	18-Apr	2:10PM	Salon F	4
Anoufa, M.	19-Apr	2:50PM	Salon F	7	Joya, K.S.	19-Apr	3:30PM	Salons A-C	6
Augustynski, J.	19-Apr	10:30AM	Salon D	5	Jung, E.	20-Apr	11:10AM	Salon D	10
Ayan, I.	20-Apr	1:40PM	Salon D	12	Jung, Y.	20-Apr	4:10PM	Salons A-C	11
B					K				
Baik, J.	19-Apr	4:10PM	Salon G	8	Kang, C.	18-Apr	2:10PM	Salon G	5
Balachandran, B.	21-Apr	11:10AM	Salon D	13	Kato, Y.	19-Apr	9:50AM	Salon E	6
Balachandran, P.	18-Apr	3:20PM	Salon F	4	Katoh, Y.	20-Apr	2:10PM	Salons A-C	11
Balasubramanian, S.	18-Apr	4:30PM	Salon F	4	Khabibullin, A.R.	20-Apr	4:00PM	Salon G	12
Banerjee, S.	19-Apr	11:50AM	Salon F	6	Kim, B.	21-Apr	11:10AM	Salon F	13
Bär, M.	20-Apr	10:50AM	Salon D	10	Kim, H.	18-Apr	11:00AM	Salon G	3
Bhattacharyya, A.J.	20-Apr	10:30AM	Salon E	11	Kim, M.	18-Apr	4:40PM	Salon G	5
Bibienne, T.	19-Apr	11:30AM	Salon E	6	Kim, S.	18-Apr	8:40AM	Salon E	3
Boona, S.	20-Apr	9:50AM	Salon G	11	Kim, T.	20-Apr	2:40PM	Salon F	11
Bordia, R.K.	21-Apr	9:50AM	Salon D	13	Kim, Y.	20-Apr	5:00PM	Salon F	12
Bowen, C.R.	18-Apr	10:00AM	Salon F	3	Kolodziejak, K.	19-Apr	6:10PM	Salons A-C	7
C					L				
Chen, A.	19-Apr	11:00AM	Salon F	6	Koyanagi, T.	20-Apr	10:20AM	Salons A-C	10
Chen, W.	20-Apr	1:40PM	Salon F	11	Kumar, A.	18-Apr	3:50PM	Salon D	4
Chen, Z.	19-Apr	4:40PM	Salon E	8	Kumar, A.	18-Apr	4:50PM	Salon F	4
Chiu, K.	18-Apr	5:30PM	Salon E	5	Kwon, G.	19-Apr	2:50PM	Salons A-C	6
Choi, D.	19-Apr	4:50PM	Salon G	8	L				
Chotard, J.	20-Apr	2:20PM	Salon E	12	Lee, J.	19-Apr	10:50AM	Salon D	5
D					M				
De Vittorio, M.	18-Apr	3:20PM	Salon G	5	Mahmoudi, T.	20-Apr	2:20PM	Salon D	12
Dedryvere, R.	20-Apr	11:10AM	Salon E	11	Manthiram, A.	20-Apr	8:30AM	Salon E	10
Dehkordi, A.	20-Apr	10:50AM	Salon G	11	Marcinek, M.	18-Apr	4:10PM	Salon E	5
Deluca, M.	18-Apr	11:10AM	Salon F	3	Marques-Hueso, J.	19-Apr	11:50AM	Salon D	6
Doeff, M.	18-Apr	10:00AM	Salon E	3	Martorell, J.	19-Apr	11:10AM	Salon D	5
Dunn, S.	19-Apr	4:10PM	Salon F	7	McNeary, W.W.	21-Apr	10:30AM	Salon D	13
Dunn, S.	19-Apr	4:30PM	Salon F	8	Meijerink, A.	18-Apr	11:20AM	Salon D	3
Dunn, S.	19-Apr	9:50AM	Salon G	6	Méndez-Ramos, J.	19-Apr	9:50AM	Salon D	5
Dunn, S.	20-Apr	2:00PM	Salon D	12	Mistry, A.	19-Apr	4:20PM	Salon E	8
E					N				
Eapen, J.	20-Apr	3:20PM	Salons A-C	11	Mistry, A.	20-Apr	11:50AM	Salon E	11
Ehsan, M.A.	20-Apr	4:40PM	Salon F	12	Mitlin, D.	19-Apr	10:30AM	Salon G	6
Elissalde, C.	19-Apr	9:50AM	Salon F	6	Morante, J.R.	20-Apr	5:00PM	Salon E	13
F					O				
Fischer, S.	18-Apr	10:40AM	Salon D	3	Mouis, M.	19-Apr	2:20PM	Salon G	8
Funahashi, R.	21-Apr	11:50AM	Salon G	14	Moya, X.	19-Apr	1:40PM	Salon F	7
G					N				
Groen, W.A.	18-Apr	10:40AM	Salon F	3	Mukherjee, P.	21-Apr	11:30AM	Salon E	14
Gu, L.	21-Apr	10:50AM	Salon E	14	Mukhopadhyay, A.	19-Apr	5:00PM	Salon E	8
Guignard, M.	20-Apr	4:20PM	Salon E	12	N				
Guillon, O.	21-Apr	10:50AM	Salon D	13	Nakayama, T.	20-Apr	5:20PM	Salon F	12
H					O				
Hayashi, A.	19-Apr	10:30AM	Salon E	6	Nazeeruddin, M.	19-Apr	8:30AM	Salon E	5
He, J.	20-Apr	1:40PM	Salon G	12	Nersisyan, H.	18-Apr	3:10PM	Salon E	5
He, J.	21-Apr	10:30AM	Salon G	13	Nishimura, C.	18-Apr	10:40AM	Salon G	3
Hinchet, R.	19-Apr	5:30PM	Salon G	8	Nolas, G.S.	20-Apr	10:10AM	Salon G	11
Hoffmann, M.J.	18-Apr	10:40AM	Salon E	3	O				
Holgate, T.C.	20-Apr	3:20PM	Salon G	12	Oez, S.	20-Apr	9:50AM	Salon D	10
Hong, S.	21-Apr	11:50AM	Salon F	13	O				
Huang, Q.	20-Apr	1:40PM	Salons A-C	11	O				
Hummelen, J.	18-Apr	3:10PM	Salon D	4	O				
Hussain, A.	18-Apr	4:10PM	Salon F	4	O				
I					O				
Imanaka, N.	20-Apr	3:20PM	Salon F	11	O				

Presenting Author List

Oral Presenters

Name	Date	Time	Room	Page Number	Name	Date	Time	Room	Page Number
Ohtaki, M.	21-Apr	9:50AM	Salon F	13					
Okumura, T.	18-Apr	11:20AM	Salon E	3					
Ott, R.T.	20-Apr	9:50AM	Salon F	10					
		P					V		
Padiyan, D.	19-Apr	4:10PM	Salons A-C	7	van der Kolk, E.	19-Apr	4:00PM	Salon D	7
Paradies, C.	21-Apr	8:30AM	Salon E	13	Van der Ven, A.	19-Apr	1:40PM	Salon E	8
Pavel, C.	20-Apr	11:30AM	Salon F	10	Vattikuti, S.	19-Apr	5:50PM	Salons A-C	7
Pei, Y.	20-Apr	4:20PM	Salon G	12	Vayssieres, L.	19-Apr	2:10PM	Salons A-C	6
Pfeifer, P.	18-Apr	10:00AM	Salon G	3	Vilarinho, P.	18-Apr	3:50PM	Salon F	4
Ponrouch, A.	20-Apr	3:00PM	Salon E	12	Voiculescu, I.R.	18-Apr	4:00PM	Salon G	5
Post, E.	20-Apr	4:40PM	Salon G	12	Vomiero, A.	19-Apr	3:20PM	Salon D	7
Pralong, V.	18-Apr	1:30PM	Salon E	5					
		Q					W		
Qi, Y.	19-Apr	2:20PM	Salon E	8	Wang, Y.	20-Apr	11:30AM	Salon D	10
Quintanilla, M.	19-Apr	4:40PM	Salon D	7	Wang, Y.E.	19-Apr	3:40PM	Salon E	8
		R			Waske, A.	20-Apr	4:00PM	Salon F	11
Reddy, S.N.	21-Apr	11:30AM	Salons A-C	14	Wei, K.	20-Apr	11:30AM	Salon G	11
		S			Westin, G.	19-Apr	2:20PM	Salon D	7
Santato, C.	19-Apr	5:00PM	Salon D	7	Westin, G.	19-Apr	4:50PM	Salons A-C	7
Sauder, C.	20-Apr	11:10AM	Salons A-C	10	Winkler, P.	20-Apr	11:10AM	Salon F	10
Schmid, S.	21-Apr	10:10AM	Salon E	14	Wolfenstine, J.	19-Apr	11:10AM	Salon E	6
Schropp, R.E.	18-Apr	10:00AM	Salon D	3	Wood, D.L.	21-Apr	9:50AM	Salons A-C	14
Schweizer, S.	18-Apr	4:10PM	Salon D	4	Woods, L.M.	20-Apr	2:20PM	Salon G	12
Seifert, H.J.	20-Apr	9:50AM	Salons A-C	10	Wu, W.	18-Apr	1:30PM	Salon G	4
Shahbazian-Yassar, R.	21-Apr	9:50AM	Salon E	14	Wysmulek, K.	19-Apr	5:30PM	Salons A-C	7
Singh, G.	20-Apr	11:30AM	Salons A-C	10					
Singh, R.N.	20-Apr	5:40PM	Salon E	13			X		
Solangi, M.S.	21-Apr	11:30AM	Salon F	13	Xu, G.	19-Apr	3:00PM	Salon E	8
Sopori, B.	20-Apr	2:40PM	Salon D	12					
Spanier, J.E.	19-Apr	3:30PM	Salon F	7			Y		
Srinivasan, S.	18-Apr	11:40AM	Salon G	3	Yabuuchi, N.	20-Apr	1:40PM	Salon E	12
		T			Yang, Y.	19-Apr	1:30PM	Salons A-C	6
Tabuchi, Y.	21-Apr	10:30AM	Salons A-C	14	Yao, K.	21-Apr	11:10AM	Salons A-C	14
Tamburello, D.A.	18-Apr	11:20AM	Salon G	3	Yartys, V.A.	21-Apr	11:50AM	Salon E	14
Terrani, K.	20-Apr	10:40AM	Salons A-C	10	Yin, S.	18-Apr	2:40PM	Salon F	4
Tidrow, S.	18-Apr	1:30PM	Salon F	4	Yoo, B.	20-Apr	2:20PM	Salon F	11
Tidrow, S.	20-Apr	5:00PM	Salon G	12	Yu, Z.	19-Apr	11:10AM	Salon G	6
		U			Yuzyuk, Y.	18-Apr	5:10PM	Salon F	4
Uršič, H.	19-Apr	2:20PM	Salon F	7					
							Z		
					Zeng, X.	18-Apr	2:50PM	Salon E	5
					Zeng, X.	21-Apr	11:10AM	Salon G	13
					Zhao-Karger, Z.	20-Apr	5:20PM	Salon E	13
					Zhao, H.	18-Apr	1:30PM	Salon D	4
					Zhou, C.	20-Apr	6:00PM	Salon E	13
					Zhu, T.	21-Apr	9:50AM	Salon G	13

Poster Presenters

Name	Date	Time	Room	Page Number	Name	Date	Time	Room	Page Number
Algueró, M.	19-Apr	6:00PM	Water's Edge Ballroom	9	Post, E.	19-Apr	6:00PM	Water's Edge Ballroom	9
Babu, V.	19-Apr	6:00PM	Water's Edge Ballroom	9	Razumnaya, A.	19-Apr	6:00PM	Water's Edge Ballroom	9
Carreno, N.L.	19-Apr	6:00PM	Water's Edge Ballroom	9	Redel, E.	19-Apr	6:00PM	Water's Edge Ballroom	9
Cervera, R.M.	19-Apr	6:00PM	Water's Edge Ballroom	9	Rho, W.	19-Apr	6:00PM	Water's Edge Ballroom	9
Choi, J.	19-Apr	6:00PM	Water's Edge Ballroom	9	Rodriguez, J.	19-Apr	6:00PM	Water's Edge Ballroom	9
Djebbi, M.A.	19-Apr	6:00PM	Water's Edge Ballroom	9	Seo, S.	19-Apr	6:00PM	Water's Edge Ballroom	9
Groen, W.A.	19-Apr	6:00PM	Water's Edge Ballroom	9	Seung, W.	19-Apr	6:00PM	Water's Edge Ballroom	9
Han, S.	19-Apr	6:00PM	Water's Edge Ballroom	9	Silva, R.M.	19-Apr	6:00PM	Water's Edge Ballroom	9
Hwang, S.	19-Apr	6:00PM	Water's Edge Ballroom	8	Tung, P.	19-Apr	6:00PM	Water's Edge Ballroom	9
Iso, Y.	19-Apr	6:00PM	Water's Edge Ballroom	9	Vaso, C.	19-Apr	6:00PM	Water's Edge Ballroom	9
Jung, Y.	19-Apr	6:00PM	Water's Edge Ballroom	9	Vilarinho, P.	19-Apr	6:00PM	Water's Edge Ballroom	9
Kim, Y.	19-Apr	6:00PM	Water's Edge Ballroom	9	Wang, Y.	19-Apr	6:00PM	Water's Edge Ballroom	8
Kosaraju, R.	19-Apr	6:00PM	Water's Edge Ballroom	9	Yang, H.	19-Apr	6:00PM	Water's Edge Ballroom	9
Kuznetsova, Y.	19-Apr	6:00PM	Water's Edge Ballroom	9	Ye, B.	19-Apr	6:00PM	Water's Edge Ballroom	9
Kwon, S.	19-Apr	6:00PM	Water's Edge Ballroom	9	Yin, S.	19-Apr	6:00PM	Water's Edge Ballroom	9
Lim, S.	19-Apr	6:00PM	Water's Edge Ballroom	9	Yoon, H.	19-Apr	6:00PM	Water's Edge Ballroom	9
Mahmoudi, T.	19-Apr	6:00PM	Water's Edge Ballroom	9	Zhang, G.	19-Apr	6:00PM	Water's Edge Ballroom	9
Mehmandoust, E.	19-Apr	6:00PM	Water's Edge Ballroom	9					

Monday, April 18, 2016

Plenary Session I - ACerS-KICe Distinguished Lecture

Room: Salon E

8:30 AM

Opening Remarks

8:40 AM

(MCARE-PL-001-2016) Energy harvesting with nanogenerators for realizing self-powered small electronics

S. Kim*; 1. Sungkyunkwan University, Republic of Korea

9:40 AM

Break

S2: Spectral Conversion Materials for Energy Applications

Upconversion, Downconversion /Quantum Cutting and Luminescent Downshifting for Solar Cells I

Room: Salon D

Session Chairs: Eva Hemmer, INRS; Jose Marques-Hueso, Heriot-Watt University

10:00 AM

(MCARE-S2-001-2016) Upconverter Solar Cells: from Materials to Device Applications (Invited)

R. E. Schropp*; J. de Wild; W. G. van Sark; J. Feenstra; J. Schermer; 1. Eindhoven University of Technology (TU/e), Netherlands; 2. Luxembourg University, Luxembourg; 3. Utrecht University, Netherlands; 4. Radboud University, Netherlands

10:40 AM

(MCARE-S2-002-2016) Upconversion of Sub-Bandgap Photons for Solar Energy Harvesting: Recent Progress, Obstacles, and Future Perspective (Invited)

S. Fischer*; 1. Lawrence Berkeley National Laboratory, USA

11:20 AM

(MCARE-S2-003-2016) Modelling Energy Transfer in Lanthanide Doped (Nano)Crystals (Invited)

F. Rabou; D. Yu; A. Meijerink*; 1. Utrecht University, Netherlands; 2. Rutgers University, USA

S3: Ferroelectrics and Multiferroics for Energy Applications

Ferroelectrics for Energy

Room: Salon F

Session Chair: Catherine Elissalde, ICMCB-CNRS

10:00 AM

(MCARE-S3-001-2016) Piezoelectric and pyroelectric materials and structures for energy harvesting (Invited)

C. R. Bowen*; 1. University of Bath, United Kingdom

10:40 AM

(MCARE-S3-002-2016) Flexible and high temperature piezoelectric composites for energy harvesting applications (Invited)

W. A. Groen*; 1. Technical University Delft, Netherlands

11:10 AM

(MCARE-S3-003-2016) Barium titanate-based materials for energy and related applications (Invited)

M. Deluca*; J. Krainer; E. Lackner; R. Wimmer-Teubenbacher; J. Spitaler; A. Köck; 1. Materials Center Leoben Forschung GmbH, Austria

S10: Batteries and Energy Storage

All solid-state Batteries I

Room: Salon E

Session Chairs: Palani Balaya, National University of Singapore; Mickael Dollé, Université de Montreal

10:00 AM

(MCARE-S10-001-2016) Advances Towards Solid State Batteries Using Garnet LLZO Electrolytes (Invited)

M. Doeff*; L. Cheng; 1. Lawrence Berkeley National Laboratory, USA

10:40 AM

(MCARE-S10-002-2016) Oxide-Based Solid State Electrolytes as Key Components for All-Solid-State Li-Ion Batteries (Invited)

M. J. Hoffmann*; T. Hupfer; E. C. Bucharsky; F. Lemke; G. Schell; A. Hintennach; 1. Karlsruhe Institute of Technology, Germany; 2. Daimler AG, Germany

11:20 AM

(MCARE-S10-003-2016) Bulk-Type All-Solid-State Lithium-Ion Batteries using Oxide Electrolytes (Invited)

T. Okumura*; T. Takeuchi; H. Kobayashi; 1. National Institute of Advanced Industrial and Technology (AIST), Japan

S11: Hydrogen Materials and Economy

Hydrogen Materials and Economy

Room: Salon G

Session Chairs: David Tamburello, Savannah River National Lab; Peter Pfeifer, University of Missouri

10:00 AM

(MCARE-S11-001-2016) Low-pressure storage of methane on high-surface-area carbon for natural gas vehicles: record performance in the lab and on a 40-liter prototype tank (Invited)

P. Pfeifer*; T. Rash; E. Knight; C. Schulz; D. Stalla; A. Gillespie; Y. Soo; 1. University of Missouri, USA

10:40 AM

(MCARE-S11-002-2016) Hydrogen extraction by a permselective vanadium alloy membrane from gas mixtures of hydrogen, nitrogen and ammonia

C. Nishimura*; J. Tsai; H. Kimura; H. Yoshinaga; S. Sakurai; 1. National Institute for Materials Science (NIMS), Japan; 2. Taiyo Koko Co. Ltd., Japan; 3. National Taipei University of Technology, Taiwan; 4. Suzuki Shokan Co. Ltd., Japan

11:00 AM

(MCARE-S11-003-2016) Metal-Dielectric Hybrid-Structured Film with Titanium Oxide for Enhanced Visible Light Absorption and Photo-Catalytic Applications

H. Kim*; J. Park; S. Nam; H. Kim; H. Choi; J. Baik; 1. Ulsan National Institute of Science and Technology, Republic of Korea; 2. Korea Advanced Institute of Science and Engineering (KAIST), Republic of Korea; 3. Korea University, Republic of Korea

11:20 AM

(MCARE-S11-004-2016) In-situ Adsorbent Growth (Invited)

D. A. Tamburello*; M. Sulic; D. L. Anton; B. J. Hardy; C. Corgnale; 1. Savannah River National Lab, USA; 2. Savannah River Consulting, USA

11:40 AM

(MCARE-S11-005-2016) Synergistic Effects of MWCNT and Nb₂O₅ on the Hydrogen Storage Characteristics of Li-nMg-B-N-H System

S. Srinivasan*; D. Demirocak; E. Stefanakos; Y. Goswami; 1. Florida Polytechnic University, USA; 2. Texas A&M University, USA; 3. University of South Florida, USA

12:00 PM

(MCARE-S11-006-2016) Kinetics and Thermodynamics of Hydrogen Sorption Studied by Manometric and Coupled Manometric/Calorimetric TechniquesK. Lilova*; L. Brown¹; 1. Setaram Inc., USA**S2: Spectral Conversion Materials for Energy Applications****Upconversion, Downconversion /Quantum Cutting and Luminescent Downshifting for Solar Cells II**

Room: Salon D

Session Chairs: Gunnar Westin, Uppsala University; Ruud Schropp, Eindhoven University of Technology (TU/e)

1:30 PM

(MCARE-S2-008-2016) Heterostructured quantum dots for solar energy applications (Invited)H. Zhao*; F. Rosei¹; 1. INRS, Canada

2:10 PM

(MCARE-S2-004-2016) Sol-gel derived frequency conversion coatings for solar cell applications (Invited)

R. M. Almeida*; 1. Instituto Superior Técnico /U Lisboa, Portugal

2:50 PM

Break

Upconversion, Downconversion /Quantum Cutting and Luminescent Downshifting for Solar Cells III

Room: Salon D

Session Chairs: Marta Quintanilla, CIC BiomaGUNE; Stefan Fischer, Lawrence Berkeley National Laboratory

3:10 PM

(MCARE-S2-005-2016) Co-Sensitized Upconversion (Invited)W. Zou¹; M. S. Pshenichnikov¹; J. Hummelen*; 1. University of Groningen, Netherlands

3:50 PM

(MCARE-S2-006-2016) Up-conversion in perovskite strontium stannate nanostructures for application in dye-sensitized solar cellV. Sahrawat²; A. Kumar*; 1. National Institute of Technology (NIT), Kurukshetra, India; 2. National Institute of Technology (NIT), India

4:10 PM

(MCARE-S2-007-2016) Glasses doped with trivalent rare-earth ions as photon downshifters for photovoltaic applications (Invited)F. Steudel¹; S. Loos²; B. Ahrens²; R. L. Leonard³; J. A. Johnson³; S. Schweizer*; 1. Fraunhofer IMWS, Germany; 2. South Westphalia University of Applied Sciences, Germany; 3. University of Tennessee Space Institute, USA**S3: Ferroelectrics and Multiferroics for Energy Applications****Single Phase Ferroelectrics and Multiferroics I**

Room: Salon F

Session Chair: Xavier Moya, University of Cambridge

1:30 PM

(MCARE-S3-005-2016) Design, Modeling and Experimental Values of Temperature Dependent Material Properties (Invited)

S. Tidrow*; 1. Alfred University, USA

2:10 PM

(MCARE-S3-006-2016) Towards functionality in fluorites: nonequilibrium structures in thin films and bulk ceramics (Invited)J. L. Jones*; C. Fancher¹; D. Hou¹; S. Jones¹; C. Chung¹; B. Johnson¹; 1. North Carolina State University, USA

2:40 PM

(MCARE-S3-007-2016) Multiferroic properties of holmium chromite and gadolinium chromiteS. Yin*; M. Jain¹; 1. University of Connecticut, USA

3:00 PM

Break

Single Phase Ferroelectrics and Multiferroics II

Room: Salon F

Session Chair: Steven Tidrow, Alfred University

3:20 PM

(MCARE-S3-008-2016) Structure- T_c relationships in BaTiO₃-based ferroelectric perovskites (Invited)P. Balachandran*; T. Lookman¹; D. Xue¹; 1. Los Alamos National Laboratory, USA

3:50 PM

(MCARE-S3-009-2016) Poling path in doped potassium sodium niobateP. Vilarinho*; R. Pinho¹; M. Costa¹; 1. University of Aveiro, Portugal

4:10 PM

(MCARE-S3-010-2016) Structure and electromechanical Properties of Li and Nb Co-doped BNT-BZ CeramicsA. Hussain*; A. Maqbool¹; R. Malik¹; J. Lee¹; T. Song¹; W. Kim¹; M. Kim¹; 1. Changwon National University, Republic of Korea

4:30 PM

(MCARE-S3-011-2016) Intrinsic magnetodielectric coupling in Fe and Fe-Nb substituted BaTiO₃ ceramicsS. Balasubramanian*; E. Rubavathi¹; V. Lakshmanan¹; 1. Manonmaniam Sundaranar University, India**Nanoscale Systems**

Room: Salon F

Session Chair: Jacob Jones, North Carolina State University

4:50 PM

(MCARE-S3-012-2016) Impedance analysis and modulus spectroscopy of Fe (III) containing strontium stannate nanoparticles

A. Kumar*; 1. National Institute of Technology (NIT), Kurukshetra, India

5:10 PM

(MCARE-S3-013-2016) Strain engineering in ferroelectric multilayers and superlatticesY. Yuzyuk*; R. Shakhovoy¹; V. Shirokov²; J. Belhadj³; M. El Marssi³; 1. Southern Federal University, Russian Federation; 2. Southern Scientific Center RAS, Russian Federation; 3. Université de Picardie Jules Verne, France**S8: Self-Power Generators****Piezoelectric Self-Power Generators I**

Room: Salon G

Session Chair: Sang-Woo Kim, Sungkyunkwan University

1:30 PM

(MCARE-S8-001-2016) Piezotronics in 2D materials (Invited)

W. Wu*; 1. Purdue University, USA

2:10 PM**(MCARE-S8-002-2016) Structural Approaches for Enhancing Output Power of Piezoelectric PVDF Generator (Invited)**W. Jung^{*}; C. Kang^{*}; 1. Korea Institute of Science and Technology, Republic of Korea**2:50 PM****Break****Piezoelectric Self-Power Generators II**

Room: Salon G

Session Chairs: Christian Falconi, University of Rome Tor Vergata; Chong-Yun Kang, Korea Institute of Science and Technology

3:20 PM**(MCARE-S8-003-2016) Soft Piezoelectric MEMS Technologies for Flow Energy Harvesting (Invited)**M. De Vittorio^{*}; 1. Istituto Italiano di Tecnologia, Italy**4:00 PM****(MCARE-S8-004-2016) Stretchable and Flexible Nanogenerators for Piezoelectric Energy Harvesting (Invited)**I. R. Voiculescu^{*}; 1. City College of New York, USA**4:40 PM****(MCARE-S8-005-2016) Key Material and System Parameters in Piezoelectric Vibration Energy Harvesting (Invited)**M. Kim^{*}; 1. Korea Research Institute of Standards and Science, Republic of Korea**S10: Batteries and Energy Storage****Lithium Batteries**

Room: Salon E

Session Chairs: Dany Carlier, ICMB-CNRS; Partha Mukherjee, Texas A&M University

1:30 PM**(MCARE-S10-004-2016) An active Rock Salt compound for high energy density Li-ion batteries (Invited)**V. Pralong^{*}; M. Freire¹; A. Maignan¹; C. Jordy²; D. Chateigner¹; N. Kosova³; O. Lebedev¹; 1. CNRS ENSICAEN, France; 2. SAFT, France; 3. Academy of sciences, Russian Federation**2:10 PM****(MCARE-S10-005-2016) Design architecture of high energy density low tortuosity battery electrode (Invited)**M. R. Amin^{*}; 1. Qatar Environment and Energy Institute, Hamad Bin Khalifa University, Qatar Foundation Qatar, Doha, Qatar**2:50 PM****(MCARE-S10-006-2016) Kinetic Study of Parasitic Reactions in Lithium-Ion Batteries: A Case Study on $\text{LiNi}_{0.6}\text{Mn}_{0.2}\text{Co}_{0.2}\text{O}_2$** X. Zeng^{*}; Y. Li¹; K. Amine¹; Z. Chen¹; 1. Argonne National Lab, USA**3:10 PM****(MCARE-S10-007-2016) Combustion-Mediated Route for Hollow Carbon Nanospheres with Excellent Electrochemical Properties**H. Nersisyan^{*}; C. Kim¹; J. Lee¹; 1. Chungnam national University, Republic of Korea**3:30 PM****(MCARE-S10-008-2016) Development of novel electrolyte additives for designed surface modification (Invited)**B. Lucht^{*}; 1. University of Rhode Island, USA**4:10 PM****(MCARE-S10-009-2016) Possible applications of new tailored electrolytes in different types of modern batteries (Invited)**M. Marcinek^{*}; L. Niedzicki¹; A. Bitner¹; P. Wiczorek¹; T. Trzeciak¹; M. Kalita¹; M. Dranka¹; Z. Zukowska¹; M. A. Muñoz-Márquez²; W. Wiczorek¹; 1. Warsaw University of Technology, Poland; 2. CIC Energigune, Spain**4:50 PM****(MCARE-S10-010-2016) Chemical and Thermal Control of Interfacial Stability in Lithium-ion Battery Electrodes (Invited)**C. T. Love^{*}; C. R. Becker²; S. M. Prokes¹; 1. U.S. Naval Research Laboratory, USA; 2. U.S. Army Research Laboratory, USA**5:30 PM****(MCARE-S10-011-2016) Fabrication and Characterization of LiFePO_4/N Thin Film Cathodes for Lithium Ion Batteries**K. Chiu^{*}; 1. Feng Chia University, Taiwan**Tuesday, April 19, 2016****Plenary Session II**

Room: Salon E

8:30 AM**(MCARE-PL-002-2016) Perovskite solar cells: A new paradigm in Energy sector**M. Nazeeruddin^{*}; 1. EPFL, Switzerland**9:30 AM****Break****S2: Spectral Conversion Materials for Energy Applications****Spectral Conversion for Photo-catalytic and Water-splitting Applications**

Room: Salon D

Session Chairs: Eva Hemmer, INRS; Marta Quintanilla, CIC BiomaGUNE

9:50 AM**(MCARE-S2-009-2016) Turning the sun into blue: enhancing photocatalytic activity by high effective NIR to UV-blue up-conversion with rare-earth doped materials (Invited)**J. Méndez-Ramos^{*}; L. Wondraczek²; N. Khaidukov²; P. Acosta-Mora¹; J. Ruiz-Morales¹; M. Borges¹; M. Sierra¹; P. Esparza¹; 1. Universidad de La Laguna, Spain; 2. University of Jena, Germany; 3. N.S. Kurnakov Institute of General and Inorganic Chemistry RAS, Russian Federation**10:30 AM****(MCARE-S2-010-2016) To what extent the plasmonic enhancement is effective in photocatalysis?**J. Augustynski^{*}; R. Solarska¹; K. Bienkowski¹; 1. CeNT, UW, Poland**10:50 AM****(MCARE-S2-011-2016) Heterojunction Metastructured Film of $\text{TiO}_2/\text{Cu}_2\text{O}$ with Enhanced Photoelectrochemical property and Photoelectrocatalytic Activity**J. Lee^{*}; H. Kim¹; J. Park¹; J. Baik¹; 1. Ulsan National Institute of Science and Technology, Republic of Korea**Plasmonic /Photonic Manipulation of Conversion Process**

Room: Salon D

Session Chairs: Eva Hemmer, INRS; Marta Quintanilla, CIC BiomaGUNE

11:10 AM**(MCARE-S2-012-2016) Photonic fiber arrays for light trapping in thin film photovoltaic cells (Invited)**J. Martorell^{*}; 1. ICFO-The Institute of Photonic Sciences, Spain

11:50 AM

(MCARE-S2-013-2016) Spectral concentration assisted by photonic crystals for upconversion in silicon solar cells

J. Marques-Hueso^{*}; R. Peretti²; R. Abargues³; B. Richards⁴; C. Seassal⁵; J. Martinez-Pastor²; 1. Heriot-Watt University, United Kingdom; 2. ETH, Switzerland; 3. University of Valencia, Spain; 4. KIT, Germany; 5. Ecole Centrale de Lyon, France

S3: Ferroelectrics and Multiferroics for Energy Applications**Composite Ferroelectrics and Multiferroics**

Room: Salon F

Session Chair: Jonathan Spanier, Drexel University

9:50 AM

(MCARE-S3-014-2016) All-oxide composites by Spark Plasma Sintering: a flexible approach towards giant dielectric properties (Invited)

C. Elissalde^{*}; M. Albino²; U. Chung³; J. Lesueur¹; B. Dominique¹; S. Mornet¹; C. Estournès²; M. Maglione¹; 1. ICMCB-CNRS, France; 2. Université du Maine, France; 3. CIRIMAT, France

10:30 AM

(MCARE-S3-015-2016) Magnetoelectric coupling in complex microstructures (Invited)

D. C. Lupascu^{*}; S. V. Vladimir¹; M. Etier¹; H. Trivedi¹; H. Wende¹; S. Salamon¹; J. Landers¹; M. Labusch¹; J. Schröder¹; 1. University of Duisburg-Essen, Germany

11:00 AM

(MCARE-S3-016-2016) Tuning Functionalities in Ferroic Nanocomposite Thin Films (Invited)

A. Chen^{*}; E. Enriquez¹; A. Eshghinejad²; W. Zhang³; S. Lee⁴; J. Li²; H. Wang³; J. MacManus-Driscoll¹; M. Fitzsimmons¹; Q. Jia¹; 1. Los Alamos National Lab, USA; 2. University of Washington, USA; 3. Texas A&M University, USA; 4. University of Cambridge, United Kingdom

11:30 AM

(MCARE-S3-017-2016) Nanocomposite Thin Films to Achieve High Magnetoelectric Coupling

M. Jain^{*}; 1. University of Connecticut, USA

11:50 AM

(MCARE-S3-018-2016) Characterization of (PZT) [PbZr_{0.52}Ti_{0.48}O₃]-epoxy-multi-walled carbon nanotube (MWCNT) composite piezoelectric films

S. Banerjee^{*}; K. Cook-Chennault²; 1. California State University, Fresno, USA; 2. Rutgers University, USA

S8: Self-Power Generators**Nanomaterials for Energy Harvesting**

Room: Salon G

Session Chairs: Husam Alshareef, King Abdullah University of Science and Technology; Jeong Min Baik, Ulsan National Institute of Science and Technology

9:50 AM

(MCARE-S8-007-2016) A ferroelectric dipole can it influence photochemistry (Invited)

S. Dunn^{*}; 1. QMUL, United Kingdom

10:30 AM

(MCARE-S8-008-2016) Coupling in-situ TEM and ex-situ analysis to understand heterogeneous sodiation of antimony (Invited)

D. Mitlin^{*}; 1. Clarkson University, USA

11:10 AM

(MCARE-S8-009-2016) Highly Flexible Solar Cells and Light-Emitting Diodes Using Organometal Hybrid Perovskites (Invited)

Z. Yu^{*}; 1. Florida State University, USA

S10: Batteries and Energy Storage**All Solid-state Batteries II**

Room: Salon E

Session Chairs: Stefan Adams, National University of Singapore; Mickael Dolle, University of Montreal

9:50 AM

(MCARE-S10-012-2016) Research of solid electrolyte for battery application (Invited)

Y. Kato^{*}; 1. Toyota Motor Europe, Belgium

10:30 AM

(MCARE-S10-013-2016) Formation of electrode-electrolyte interfaces in all-solid-state rechargeable lithium batteries (Invited)

A. Hayashi^{*}; M. Tatsumisago¹; 1. Osaka Prefecture University, Japan

11:10 AM

(MCARE-S10-014-2016) Cubic Li₇La₃Zr₂O₁₂ as a Solid Electrolyte

J. Wolfenstine^{*}; 1. US Army Research Laboratory, USA

11:30 AM

(MCARE-S10-015-2016) Towards all Solid State Batteries using Perovskite Solid Electrolytes

T. Bibienne^{*}; P. Alvares¹; F. Bardé²; F. Rosciano²; M. Dollé¹; 1. University of Montreal, Canada; 2. Toyota Motor Europe, Belgium

11:50 AM

(MCARE-S10-016-2016) Thin film Li₇La₃Zr₂O₁₂ as electrolyte for all-solid-state batteries

S. Lobe^{*}; H. Gehrke¹; C. Dellen¹; M. Finsterbusch¹; C. Tsai¹; S. Uhlenbruck¹; O. Guillon¹; 1. Forschungszentrum Juelich, Germany

S1: Functional Materials for Photoelectrochemical and Electrocatalytic Hydrogen Production**Functional Materials for Photoelectrochemical and Electrocatalytic Hydrogen Production**

Room: Salons A-C

Session Chair: Sanjay Mathur, University of Cologne

1:30 PM

(MCARE-S1-001-2016) Nanoengineered Films for Renewable Energy (Invited)

Y. Yang^{*}; 1. University of Central Florida, USA

2:10 PM

(MCARE-S1-002-2016) Morphological, dimensional, and interfacial effects on oxide semiconductor efficiency for solar water splitting (Invited)

L. Vayssieres^{*}; 1. Xian Jiaotong University, China

2:50 PM

(MCARE-S1-003-2016) The Origin of Electrochemical Activity of Cobalt Oxide Water Oxidation Catalytic Amorphous Thin Film

G. Kwon^{*}; H. Kim²; A. Mane²; J. Emery²; A. Martinson²; P. Stair²; D. Tiede¹; 1. Argonne National Laboratory, USA; 2. Northwestern University, USA; 3. Argonne National Lab, USA

3:10 PM

Break

3:30 PM

(MCARE-S1-004-2016) Photoelectrochemical Water Splitting via Molecular-Inorganic Hybrid System for Solar to Chemical Energy Conversion (Invited)

K. S. Joya^{*}; 1. University of Engineering and Technology (UET), Pakistan

4:10 PM**(MCARE-S1-005-2016) An insight into the influence of morphology and plasmonic silver nanoparticles on the photoelectrochemical activity of TiO₂ nanotube arrays (Invited)**

D. Padiyan*; 1. Manonmaniam Sundaranar University, India

4:50 PM**(MCARE-S1-006-2016) Complex thin and ultra-thin coatings for energy applications (Invited)**

G. Westin*; 1. Uppsala University, Sweden

5:30 PM**(MCARE-S1-007-2016) SrTiO₃-TiO₂ Eutectic Composite - a Candidate Material for Photoelectrochemical Hydrogen Production**

K. Wysmulek*; J. Sarl; K. Kolodziejak; P. Osewski; K. Orlinski; D. A. Pawlak; 1. Institute of Electronic Materials Technology, Poland; 2. Centre of New Technologies, Poland

5:50 PM**(MCARE-S1-008-2016) Photocatalytic degradation of Congo red under UV-light by MoS₂/Al₂O₃ composite produced by microwave method**

S. Vattikuti*; C. Byon; 1. Yeungnam University, Republic of Korea

6:10 PM**(MCARE-S1-009-2016) Photoelectrochemical Properties of TiO₂-WO₃ Self-Organized Eutectic Material**

K. Kolodziejak*; J. Sarl; K. Wysmulek; M. Bartsch; M. Niederberger; D. A. Pawlak; 1. ETH, Switzerland; 2. Institute of Electronic Materials Technology, Poland

S2: Spectral Conversion Materials for Energy Applications

Novel Upconversion and Downconversion Materials: Nanoparticles, Macro/Micro-sized Structures, Composites, Antenna for NIR Harvesting, Etc.

Room: Salon D

Session Chairs: Alberto Vomiero, Lulea University of Technology; Haiguang Zhao, INRS

1:40 PM**(MCARE-S2-014-2016) Rendering rare-earth photoluminescence via material design and modification: the consequences of structural and electronic alterations (Invited)**

G. Liu*; 1. Argonne National Lab, USA

2:20 PM**(MCARE-S2-015-2016) Hetero-metallic molecular approach to Ln-doped materials; from precursor to material (Invited)**

G. Westin*; 1. Uppsala University, Sweden

3:00 PM**Break**

Lanthanides, Dyes and Quantum Dots for Photovoltaic Applications

Room: Salon D

Session Chairs: Jose Marques-Hueso, Heriot-Watt University; Eva Hemmer, INRS

3:20 PM**(MCARE-S2-016-2016) Tuning nanomaterials in high-efficiency excitonic solar cells (Invited)**

A. Vomiero*; 1. Lulea University of Technology, Sweden

4:00 PM**(MCARE-S2-017-2016) Broadband absorbing Tm²⁺ based Luminescent Solar Concentrators without self-absorption losses (Invited)**

E. van der Kolk*; 1. Delft University of Technology, Netherlands

4:40 PM**(MCARE-S2-018-2016) Upconversion Quantum Yield in Lanthanide-Doped Nanoparticles: Going deeper into size, shape and host material dependencies**

M. Quintanilla*; E. Hemmer; J. Marques-Hueso; S. Rohani; R. Zamani; V. Roddatis; B. Richards; F. Vetrono; 1. CIC BiomaGUNE, Spain; 2. INRS, Canada; 3. Heriot-Watt University, United Kingdom; 4. Georg-August Universität, Germany; 5. Karlsruhe Institute of Technology, Germany

Application-oriented Approaches in Spectral Conversion

Room: Salon D

Session Chairs: Eva Hemmer, INRS; Jose Marques-Hueso, Heriot-Watt University

5:00 PM**(MCARE-S2-019-2016) Exploring the use of melanin pigments for solar energy conversion (Invited)**

C. Santato*; 1. Ecole Polytechnique de Montreal, Canada

S3: Ferroelectrics and Multiferroics for Energy Applications

Properties, Caloric Effects

Room: Salon F

Session Chair: Doru Lupascu, University of Duisburg-Essen

1:40 PM**(MCARE-S3-019-2016) Giant barocaloric effects in ferrielectric ammonium sulphate (Invited)**

X. Moya*; 1. University of Cambridge, United Kingdom

2:20 PM**(MCARE-S3-020-2016) Bulk ceramics Pb(Mg_{1/3}Nb_{2/3})O₃-PbTiO₃ as a working body for an electrocaloric cooling device (Invited)**

H. Uršič*; M. Vrabelj; Z. Kutnjak; U. Plaznik; A. Kitanovski; B. Rozic; V. Bobnar; L. Fulanovic; S. Drnovsek; A. Bencan; B. Malic; 1. Institute Jozef Stefan, Slovenia; 2. University of Ljubljana, Slovenia

2:50 PM**(MCARE-S3-021-2016) Ferroelectric core-shell ceramics for energy storage and electrocaloric applications**

M. Anoufa*; J. Kiat; 1. Labo SPMS, France

3:10 PM**Break**

Properties, Photovoltaic

Room: Salon F

Session Chair: Aiping Chen, Los Alamos National Lab

3:30 PM**(MCARE-S3-022-2016) Semiconducting Ferroelectric Photovoltaics (Invited)**

J. E. Spanier*; 1. Drexel University, USA

4:10 PM**(MCARE-S3-023-2016) Effect of ferroelectricity on solar light driven photocatalytic activity of BaTiO₃ -influence on the carrier separation and Stern layer formation**

S. Dunn*; 1. QMUL, United Kingdom

4:30 PM**(MCARE-S3-024-2016) Perovskite enhanced solid state ZnO solar cells**

S. Dunn*; 1. QMUL, United Kingdom

Round Table

Room: Salon F

Session Chair: Chris Bowen, University of Bath

4:50 PM**Opportunities and challenges for ferroelectrics and multiferroics in energy****S8: Self-Power Generators****Self-Powered Devices and Systems I**

Room: Salon G

Session Chair: Pooi See Lee, Nanyang Technological University

1:40 PM**(MCARE-S8-010-2016) Micro-fabricated Supercapacitors for On-Chip Energy Storage (Invited)**

H. N. Alshareef*; N. Kurra*; Q. Jiang*; 1. King Abdullah University of Science & Technology, Saudi Arabia

2:20 PM**(MCARE-S8-011-2016) Modelling of vertical-nanowire based devices for mechanical/electrical transduction (Invited)**

M. Mouis*; R. Tao*; M. Parmar*; G. Ardila*; L. Montes*; 1. IMEP-LAHC, France

3:00 PM**Break****Self-Powered Devices and Systems II**

Room: Salon G

Session Chairs: Mireille Mouis, CNRS, IMEP-LaHC; Miso Kim, Korea Research Institute of Standards and Science

3:30 PM**(MCARE-S8-012-2016) Towards self-powered flexible energy devices (Invited)**

P. Lee*; V. Bhavanasi*; K. Parida*; 1. Nanyang Technological University, Singapore

4:10 PM**(MCARE-S8-013-2016) Mesoporous Pores as Effective Dielectrics for Enhancing Triboelectric Nanogenerator Performance (Invited)**

J. Baik*; 1. Ulsan National Institute of Science and Technology, Republic of Korea

4:50 PM**(MCARE-S8-014-2016) Kinematic Designs for Sustainable and High-performance Triboelectric Nanogenerators (Invited)**

D. Choi*; 1. Kyung Hee University, Republic of Korea

5:30 PM**(MCARE-S8-015-2016) Importance of the μ -roughness for increasing triboelectric nanogenerator performances and lifetime (Invited)**

R. Hinchet*; S. Kim*; 1. SungKyunKwan University, Republic of Korea

S10: Batteries and Energy Storage**Batteries: Modeling and Mechanisms**

Room: Salon E

Session Chairs: Naoaki Yabuuchi, Tokyo Denki University; Anton Van der Ven, University of California, Santa Barbara

1:40 PM**(MCARE-S10-017-2016) Phase transformation mechanisms in the electrodes of Li, Na and Mg batteries (Invited)**

A. Van der Ven*; M. Radin*; D. Chang*; 1. University of California Santa Barbara, USA

2:20 PM**(MCARE-S10-018-2016) Mechano-Electro-Chemical (MEC) Coupling in Lithium Intercalation Compounds (Invited)**

Y. Qi*; C. James*; 1. Michigan State University, USA

3:00 PM**(MCARE-S10-019-2016) Migration Mechanism of Transition Metal Ions in $\text{LiNi}_{0.5}\text{Mn}_{0.5}\text{O}_4$**

G. Xu*; K. Amine*; Z. Chen*; 1. Argonne National Lab, USA

3:20 PM**(MCARE-S10-020-2016) Computational studies on diffusion of Li in oxides for rechargeable Li ion battery with infomatics (Invited)**

M. Nakayama*; R. Jalem*; 1. Nagoya Institute of Technology, Japan; 2. National Institute for Materials Science (NIMS), Japan

3:40 PM**(MCARE-S10-021-2016) Materials design guidelines for all-solid-state batteries (Invited)**

Y. E. Wang*; G. Ceder*; 1. Massachusetts Institute of Technology, USA; 2. University of California, Berkeley, USA

4:20 PM**(MCARE-S10-022-2016) How Electrode Processing Affects Li-ion Battery Performance?**

A. Mistry*; D. Juarez Robles*; P. P. Mukherjee*; 1. Texas A&M University, USA

4:40 PM**(MCARE-S10-023-2016) Understanding the voltage variation of lithium-manganese rich oxides from structural perspective**

Z. Chen*; K. Amine*; 1. Argonne National Lab, USA

5:00 PM**(MCARE-S10-024-2016) Correlations between microstructure, phase transformation, stress development and electrochemical behavior of electrode materials for Li-ion batteries (Invited)**

A. Mukhopadhyay*; 1. Indian Institute of Technology (IIT) Bombay, India

5:40 PM**(MCARE-S10-025-2016) Insights into Voltage Variations of Lithium Transition Metal Oxides during Cycling**

Y. Li*; Y. Liu*; G. Xu*; Y. Ren*; K. Amine*; Z. Chen*; 1. Argonne National Lab, USA

Posters**Poster Session**

Room: Water's Edge Ballroom

6:00 PM**(MCARE-S1-P001-2016) Preparation and hydrogen production characteristics of novel ZnO/carbon-based heterophotocatalyst**

S. Hwang*; H. Seo*; Y. Kim*; S. Lim*; 1. DGIIST, Republic of Korea

(MCARE-S2-P002-2016) Tuning Microstructure and Frequency Conversion Performance of Lanthanide Nanomaterial by Impurity Doping

Y. Wang*; 1. Fujian Institute of Research on the Structure of Matter, CAS, China

(MCARE-S2-P003-2016) Spectral properties of Er³⁺ ions in Gd₂O₃ matrix

Y. Kuznetsova^{*}; A. Zatsepin¹; 1. Ural Federal University, Russian Federation

(MCARE-S2-P004-2016) Near-UV → Red Down-Shifting Y₂O₃:Bi³⁺,Eu³⁺ Nanosheets for Solar Cells

Y. Iso^{*}; T. Matsunaga¹; Y. Kosuge¹; T. Isobe¹; 1. Keio University, Japan

(MCARE-S3-P005-2016) Phase transitions in compositionally graded ferroelectric superlattices

A. Razumnaya^{*}; Y. Tikhonov¹; Y. Yuzyuk¹; N. Ortega²; K. Ashok²; R. Katiyar²; 1. Southern Federal University, Russian Federation; 2. University of Puerto Rico, USA

(MCARE-S3-P006-2016) Quantitative local functional characterization at perovskite-spinel oxide interfaces in magnetoelectric composites

J. Ricote¹; I. San-Felipe¹; E. Vila¹; H. Amorin¹; W. Santa-Rosa²; M. Venet²; A. Castro¹; M. Alguero^{*}; 1. Instituto de Ciencia de Materiales de Madrid (ICMM), CSIC, Spain; 2. Universidade Federal de São Carlos, Brazil

(MCARE-S3-P007-2016) Poling effect on dielectric properties of lead-free Na_{0.4}K_{0.1}Bi_{0.5}TiO₃ relaxor ferroelectrics

V. Babu^{*}; B. Bagyalakshmi¹; S. Balasubramanian¹; 1. Manonmaniam Sundaranar University, India

(MCARE-S3-P008-2016) Electrical properties of BiFeO₃ thin films on different electrodes fabricated by Chemical Solution Deposition

P. Vilarinho^{*}; 1. University of Aveiro, Portugal

(MCARE-S3-P009-2016) The size and pressure effect on the magnetic and magnetocaloric property in HoCrO₃

S. Yin^{*}; M. Jain¹; 1. University of Connecticut, USA

(MCARE-S3-P010-2016) Novel lead free flexible composites for energy harvesting and sensor applications

W. A. Groen^{*}; 1. Technical University Delft, Netherlands

(MCARE-S4-P011-2016) Evaluation of precipitated Na₃Zr₂F₁₃ powder from the waste pickle acid

S. Han^{*}; 1. Chungnam National University, Republic of Korea

(MCARE-S4-P012-2016) Fabrication of SiC/SiC Joints for LWR Fuel Cladding Tubes by a Diffusion Bonding Method

Y. Jung^{*}; J. Park¹; H. Kim¹; D. Kim¹; W. Kim¹; 1. Korea Atomic Energy Research Institute, Republic of Korea

(MCARE-S4-P013-2016) Alkali Fluorides and Chlorides Characterized by TG-DSC-MS

E. Post^{*}; 1. NETZSCH Geraetebau GmbH, Germany

(MCARE-S5-P014-2016) Layered double hydroxide electrode materials for today's fuel cell technology: Structural and electrochemical investigations

M. A. Djebbi^{*}; 1. Institute of Analytical Science UMR CNRS 5280, University of Claude Bernard-Lyon 1, France

(MCARE-S5-P015-2016) Microstructural Investigation of LSM/YSZ Composite Anode Materials for Solid Oxide Electrolysis Cells

R. M. Cervera¹; C. Vaso^{*}; 1. University of the Philippines Diliman, Philippines

(MCARE-S6-P016-2016) SURMOF/CNC based Designer Solids for Photonic, Optical and Energy Applications

E. Redel^{*}; 1. KIT, Germany

(MCARE-S6-P017-2016) The combustion synthesis of FeTi alloy powders and the effect of additives

J. Choi^{*}; 1. Chung-nam University, Republic of Korea

(MCARE-S6-P018-2016) Electrowinning of Al-Sc alloys in CaF₂-NaF-Na₃AlF₆-Al₂O₃-Sc₂O₃ electrolyte

S. Kwon^{*}; 1. Chungnam National University, Republic of Korea

(MCARE-S7-P019-2016) Inverted hybrid solar cells based on metal oxide nanomaterials and P3HT

S. Seo^{*}; T. Mahmoudi¹; S. Lee¹; H. Yang¹; W. Rho¹; Y. Hahn¹; 1. Chonbuk National University, Republic of Korea

(MCARE-S7-P020-2016) Perovskite Solar Cells with Nanoimprinted Mesoporous TiO₂ Thin Films

H. Yang^{*}; W. Rho¹; S. Lee¹; S. Seo¹; Y. Hahn¹; 1. Chonbuk National University, Republic of Korea

(MCARE-S7-P021-2016) Noble Metals (Pt, Au, Ag) Doped Graphene for Photovoltaic Applications

T. Mahmoudi^{*}; S. Seo¹; Y. Hahn¹; 1. Chonbuk National University, Republic of Korea

(MCARE-S7-P022-2016) Enhanced electron transport on active layer with TiO₂ nanotube arrays in perovskite solar cells

W. Rho^{*}; H. Yang¹; S. Seo¹; S. Lee¹; Y. Hahn¹; 1. Chonbuk National University, Republic of Korea

(MCARE-S8-P023-2016) Composite flexible based on PZT/CNT/cellulose

R. M. Silva^{*}; B. D. Noremborg¹; L. Santana¹; O. Paniz¹; M. R. Gonçalves¹; V. G. Deon¹; N. L. Carreño¹; 1. Federal University of Pelotas, Brazil

(MCARE-S8-P024-2016) Flexible composite from hydrothermal synthesis

N. L. Carreño¹; V. G. Deon¹; R. M. Silva¹; A. G. Osório¹; M. F. Mesko¹; F. V. Motta²; R. M. Nascimento²; M. O. Orlandi²; 1. Federal University of Pelotas, Brazil; 2. Federal University of Rio Grande do Norte, Brazil; 3. Universidade Estadual Paulista, Brazil

(MCARE-S8-P025-2016) High Power Triboelectric Nanogenerator based on nanocomposite materials

H. Yoon^{*}; W. Seung¹; S. Kim¹; 1. Sungkyunkwan University, Republic of Korea

(MCARE-S8-P026-2016) Nanopatterned Yarn Based Wearable Triboelectric Nanogenerator

W. Seung^{*}; S. Kim¹; 1. Sungkyunkwan university, Republic of Korea

(MCARE-S8-P027-2016) Enhanced Triboelectric Nanogenerators based on the stretchable electrode

B. Ye^{*}; J. Chun¹; J. Baik¹; 1. Ulsan National Institute of Science and Technology (UNIST), Republic of Korea

(MCARE-S8-P028-2016) Nano-scale Mechanisms Contributing to Lead-Free Electro-mechanical Properties

P. Tung^{*}; J. Daniels¹; 1. University of New South Wales, Australia

(MCARE-S9-P029-2016) Enhancing thermoelectric performance of Ca(Sr)CoO ceramics through Ag-adding

J. Rodriguez^{*}; D. Garcia¹; 1. Universidad Nacional de Colombia, Colombia

(MCARE-S9-P030-2016) Thermal conductivity investigation of several half-Heusler compounds

G. Zhang^{*}; L. Chen¹; X. Zeng¹; J. Poon²; T. M. Tritt¹; 1. Clemson University, USA; 2. University of Virginia, USA

(MCARE-S10-P031-2016) Electrochemical Evaluation of Li₇La₃Zr₂O₁₂ Li-ion Conducting Solid Electrolyte

R. M. Cervera^{*}; R. Gamboa¹; S. Botin¹; 1. University of the Philippines Diliman, Philippines

(MCARE-S10-P032-2016) Silver based fast ion conducting glassy electrolyte: Promising material for solid state battery applications

R. Kosaraju^{*}; R. Emmadishetty²; A. Bojja²; 1. Osmania University College for Women, India; 2. Osmania University, India

(MCARE-S11-P033-2016) Preparation of highly porous carbon fibers from natural resources and their hydrogen storage characteristics

S. Lim^{*}; W. Choi¹; S. Hwang¹; 1. DGIST, Republic of Korea

(MCARE-S12-P034-2016) Surface wettability and optical properties of nanostructured ZnO/SiO₂ thin films by sol-gel method

E. Mehmandoust^{*}; R. Rostami²; M. Ghorbani²; M. Askari²; 1. University of Tehran, Islamic Republic of Iran; 2. Sharif University of Technology, Islamic Republic of Iran

(MCARE-S12-P035-2016) The modeling of Cold crucible induction heating for the metal 3d printing technology using Ti grade 5

Y. Kim^{*}; D. Kim¹; J. Lee¹; 1. Chungnam National University, Republic of Korea

Wednesday, April 20, 2016

Plenary Session III

Room: Salon E

8:30 AM

(MCARE-PL-003-2016) Next-generation Battery Chemistries: Materials Challenges and Prospects

A. Manthiram*; 1. University of Texas, Austin, USA

S4: Material Challenges in Nuclear Energy

Nuclear Energy I

Room: Salons A-C

Session Chairs: Yutai Katoh, Oak Ridge National Laboratory; Qing Huang, Ningbo Institute for Materials Technology and Engineering

9:50 AM

(MCARE-S4-001-2016) High temperature oxidation behavior of cladding materials for nuclear applications (Invited)

H. J. Seifert*; 1. Karlsruhe Institute of Technology, Germany

10:20 AM

(MCARE-S4-002-2016) Hydrothermal Corrosion of SiC Joints

T. Koyanagi*; Y. Katoh*; K. Terrani*; J. Kiggans*; Y. Kim*; T. Hinoki*; 1. Oak Ridge National Laboratory, USA; 2. GE Global Research, USA; 3. Kyoto University, Japan

10:40 AM

(MCARE-S4-003-2016) Instrumented Irradiation Creep Experiment with FeCrAl Alloys and SiC (Invited)

K. Terrani*; Y. Katoh*; Y. Yamamoto*; L. Snead*; T. Karlsen*; 1. Oak Ridge National Laboratory, USA; 2. Massachusetts Institute of Technology, USA; 3. Halden Reactor Project, Norway

11:10 AM

(MCARE-S4-004-2016) SiC/SiC composites processing for advanced nuclear reactors

C. Sauder*; J. Braun*; G. Loupiaz*; D. Bossu*; L. Briottet*; B. Riccetti*; 1. CEA, France

11:30 AM

(MCARE-S4-005-2016) Mechanical Properties of SiC/SiC Ceramic Matrix Composite Tubes for Accident-Tolerant Fuels

G. Singh*; Y. Katoh*; K. Terrani*; 1. Oak Ridge National Laboratory, USA

S6: Critical Materials for Energy

Critical Materials for Energy I

Room: Salon F

Session Chairs: Wei-Sheng Chen, National Cheng Kung University; Anja Waske, Leibniz-Institute for Solid State Materials Research

9:50 AM

(MCARE-S6-001-2016) Challenges and Opportunities in Recycling Rare Earth Materials (Invited)

R. T. Ott*; 1. Ames Laboratory (USDOE), USA

10:30 AM

(MCARE-S6-002-2016) Compressive creep strain of Fly ash based geopolymers and effect of activator solution to fly ash ratio on it (Invited)

M. R. Islam*; 1. Louisiana Tech University, USA

11:10 AM

(MCARE-S6-003-2016) Positioning to Win Government Research, Development, and Demonstration Funding

P. Winkler*; 1. Government Contracting Specialists, LLC, USA

11:30 AM

(MCARE-S6-004-2016) Role of raw materials towards the decarbonisation of the European energy system and evaluation of critical materials substitution paths

C. Pavel*; D. Blagoeva*; E. Tzimas*; 1. European Commission, Netherlands

11:50 AM

(MCARE-S6-005-2016) Corrosion behavior and surface characterization of Ta-W alloy coating layer by using MARC process

Y. Lee*; K. Kang*; K. Bae*; K. Park*; J. Lee*; 1. Chungnam National University, Republic of Korea; 2. Korea Institute of Energy Research, Republic of Korea; 3. Korea Institute of Industrial Technology, Republic of Korea

S7: Emerging Materials for Next Generation Photovoltaics

Next Generation Photovoltaics I

Room: Salon D

Session Chairs: Yoon-Bong Hahn, Chonbuk National University; Hanwei Gao, Florida State University

9:50 AM

(MCARE-S7-001-2016) A Solution Processed Solid State Heterojunction Device with Zero-Dimensional Organic-Inorganic Bismuth Halide Perovskite (CH₃NH₃)₃Bi₂I₉ Sheets

S. Oez*; J. C. Hebig*; E. Jung*; T. Singh*; A. Lepcha*; S. Olthof*; J. Flohre*; Y. Gao*; R. German*; K. Meerholz*; T. Kirchartz*; S. Mathur*; 1. Institute of Inorganic and Materials Chemistry, University of Cologne, Germany; 2. IEK-5 Photovoltaik, Forschungszentrum Jülich GmbH, Germany; 3. University of Cologne, Germany

10:10 AM

(MCARE-S7-002-2016) Perovskite Solar Cells: Towards Stability

Q. Jiang*; 1. Florida State University, USA

10:30 AM

(MCARE-S7-003-2016) Dielectric effects in perovskite solar cell materials

D. C. Lupascu*; G. Lackner*; I. Anusca*; S. V. Vladimir*; N. Andreeva*; M. Fiebig*; J. Lehmann*; B. Dkhil*; P. Gemeiner*; M. Sanlialp*; 1. University of Duisburg-Essen, Germany; 2. Saint-Petersburg State Polytechnical University, Russian Federation; 3. ETH Zurich, Switzerland; 4. CentraleSupélec, France

10:50 AM

(MCARE-S7-004-2016) Mixed-Halide Perovskites: Chlorine depletion and presence of metallic lead

M. Bär*; 1. Helmholtz-Zentrum Berlin, Germany

11:10 AM

(MCARE-S7-005-2016) Influence of GITC (guanidinium thiocyanate) on the performance of MAPbI₃ perovskite solar cells by two-step method

E. Jung*; S. Oez*; R. Bhattacharjee*; H. Wang*; S. Mathur*; 1. University of Cologne, Germany; 2. Queensland University of Technology, Australia

11:30 AM

(MCARE-S7-006-2016) Realization of Nozzle-Jet Printing Technique for Perovskite Solar Cells

Y. Wang*; H. Yang*; S. Seo*; W. Rho*; Y. Hahn*; 1. Chonbuk National University, Republic of Korea

S9: Direct Thermal to Electrical Energy Conversion Materials and Applications

Thermoelectric Materials I

Room: Salon G

Session Chair: Terry Tritt, Clemson University

9:50 AM

(MCARE-S9-001-2016) Thermal energy conversion via the spin Seebeck effect

S. Boona*; J. P. Heremans¹; 1. Ohio State University, USA

10:10 AM

(MCARE-S9-002-2016) Open-framework and other low thermal conductivity materials: Expanding our fundamental understanding in pursuit of technological applications (Invited)

G. S. Nolas*; 1. University of South Florida, USA

10:50 AM

(MCARE-S9-003-2016) Recent Progress in Oxide Thermoelectric Materials: n-Type SrTiO₃-based Ceramics (Invited)

A. Dehkordi*; 1. SunEdison, USA

11:30 AM

(MCARE-S9-004-2016) Multinary Chalcogenides: Potential Thermoelectric Materials with Polaronic-type Conduction

K. Wei*; A. R. Khabibullin¹; T. Stedman¹; L. M. Woods¹; G. S. Nolas¹; 1. University of South Florida, USA

S10: Batteries and Energy Storage

Li-air and Li-sulphur Batteries

Room: Salon E

Session Chairs: Valerie Pralong, CNRS ENSICAEN; Amartya Mukhopadhyay, IIT Bombay

9:50 AM

(MCARE-S10-026-2016) Fast-ion Conductor Design for Large-Scale Energy Storage Systems (Invited)

S. Adams*; 1. National University of Singapore, Singapore

10:30 AM

(MCARE-S10-027-2016) A Few Strategies for Sulfur Encapsulation in Li-S Battery (Invited)

A. J. Bhattacharyya*; 1. Indian Institute of Science, India

11:10 AM

(MCARE-S10-028-2016) Lithium-Sulfur batteries: materials for preventing polysulfides diffusion and mechanisms at interfaces (Invited)

R. Dedryvere*; R. Chellappan¹; A. Vizintin²; V. Lapornik²; D. Foix¹; R. Dominko²; 1. University of Pau - CNRS, France; 2. National Institute of Chemistry, Slovenia

11:50 AM

(MCARE-S10-029-2016) Physicochemical Evolution Behavior in the Li-air Battery Electrode

A. Mistry*; D. Juarez Robles¹; P. P. Mukherjee¹; 1. Texas A&M University, USA

S4: Material Challenges in Nuclear Energy

Nuclear Energy II

Room: Salons A-C

Session Chair: Jacob Eapen, North Carolina State University

1:40 PM

(MCARE-S4-006-2016) Joining of C/C Composites and SiC ceramics with Ti₃SiC₂ Interlayer by Electric Field Assisted Sintering Technique (Invited)

Q. Huang*; 1. Ningbo Institute for Materials Technology and Engineering, China

2:10 PM

(MCARE-S4-007-2016) Radiation Tolerance of Pressurelessly Processed Silicon Carbide Joints (Invited)

Y. Katoh*; T. Koyanagi¹; M. Ferraris²; 1. Oak Ridge National Laboratory, USA; 2. Politecnico di Torino, Italy

2:40 PM

(MCARE-S4-008-2016) Properties of commercial MAX phase Ti₃SiC₂ and Ti-Al-C ceramics after moderate dose neutron irradiation

C. Ang*; C. Shih¹; N. Cetiner¹; C. Silva¹; A. Campbell¹; S. Zinkle¹; Y. Katoh¹; 1. Oak Ridge National Laboratory, USA; 2. General Atomics, USA; 3. University of Tennessee, USA

3:00 PM

Break

3:20 PM

(MCARE-S4-009-2016) Topological Defects in Irradiated Graphite (Invited)

J. Eapen*; 1. North Carolina State University, USA

3:50 PM

(MCARE-S4-010-2016) Study the interfacial nanostructure and chemical bonding of the multi-layered graphene-reinforced alumina ceramic nanocomposites

I. Ahmad*; 1. King Saud University, Saudi Arabia

4:10 PM

(MCARE-S4-011-2016) Strengthening of Zry-4 Fuel Cladding Tubes using Oxide Particles by Laser Beam Treatment

Y. Jung*; D. Park¹; J. Park¹; J. Park¹; H. Kim¹; Y. Koo¹; 1. Korea Atomic Energy Research Institute, Republic of Korea

S6: Critical Materials for Energy

Critical Materials for Energy II

Room: Salon F

Session Chairs: Ryan Ott, Ames Laboratory (USDOE); Nobuhito Imanaka, Osaka University

1:40 PM

(MCARE-S6-006-2016) Ga-doped ZnO thin films from solar panel resources recycling technology (Invited)

W. Chen*; K. Chiu¹; Y. Wang¹; 1. National Cheng Kung University, Taiwan

2:20 PM

(MCARE-S6-007-2016) Electro reduction characteristic of zirconia by using copper oxide as additive

B. Yoo*; K. Park¹; J. Lee¹; 1. Chungnam National University, Republic of Korea; 2. Korea Institute of Industrial Technology, Republic of Korea

2:40 PM

(MCARE-S6-008-2016) Extraction behaviour of rare earths with liquid Mg

T. Kim*; B. Kim¹; S. Seo¹; K. Park¹; 1. Korea Institute of Industrial Technology, Republic of Korea

3:00 PM

Break

3:20 PM

(MCARE-S6-009-2016) Catalytic Combustion Type Carbon Monoxide Gas Sensor with Platinum, or Platinum-free Catalysts (Invited)

N. Imanaka*; 1. Osaka University, Japan

4:00 PM

(MCARE-S6-010-2016) RE-containing vs. RE-free materials for magnetocaloric refrigeration (Invited)

A. Waske*; B. Weise¹; M. Lee²; A. Gebert¹; 1. Leibniz-Institute for Solid State and Materials Research Dresden, Germany; 2. Korea Institute of Industrial Technology, Republic of Korea

4:40 PM**(MCARE-S6-011-2016) Fabrication of Nanostructured Mixed Metal Oxide Thin Films from Single Source Precursor for Technological Applications**M. A. Ehsan^{*}; A. Hakeem¹; T. Laoui¹; Z. Abdallah Yamani¹; 1. King Fahd University of Petroleum and Minerals, Saudi Arabia**5:00 PM****(MCARE-S6-012-2016) Diffusion mechanism of neodymium and dysprosium contained in REE magnet to liquid Mg**Y. Kim^{*}; T. Kim¹; B. Kim¹; K. Park¹; S. Seo¹; S. Nam¹; J. Lee¹; 1. Korea Institute of Industrial Technology, Republic of Korea**5:20 PM****(MCARE-S6-013-2016) Charge Stage in Electret by Nanosecond Pulse Power Technology for Energy Harvesting**T. Nakayama^{*}; K. Awaya¹; K. Nakata¹; H. Suematsu¹; K. Niihara¹; 1. Nagaoka Univ of Tech, Japan**S7: Emerging Materials for Next Generation Photovoltaics****Next Generation Photovoltaics II**

Room: Salon D

Session Chairs: Yoon-Bong Hahn, Chonbuk National University; Hanwei Gao, Florida State University

1:40 PM**(MCARE-S7-007-2016) Textured Microstructures for DSSCs using Microsphere Lithography and Acicular Particles**I. Ayan^{*}; P. A. Fuierer¹; 1. New Mexico Institute of Mining and Technology, USA**2:00 PM****(MCARE-S7-008-2016) Photo-enhancement of activity in spray-coated Cu₂SnSe₃ nanoparticle counter electrode for dye-sensitised solar cells**S. Dunn^{*}; 1. QMUL, United Kingdom**2:20 PM****(MCARE-S7-010-2016) Improved photovoltaic performance of inverted polymer solar cells through a sol-gel processed Al-doped ZnO anode buffer layer**T. Mahmoudi^{*}; S. Seo¹; Y. Hahn¹; 1. Chonbuk National University, Republic of Korea**2:40 PM****(MCARE-S7-011-2016) Defect annihilation and precipitate dissolution in N-type, Czochralski Si wafers by optical processing: enabling high efficiency solar cell fabrication**B. Sopor^{*}; 1. National Renewable Energy Laboratory, USA**S9: Direct Thermal to Electrical Energy Conversion Materials and Applications****Thermoelectric Materials II**

Room: Salon G

Session Chair: Jian He, Clemson University

1:40 PM**(MCARE-S9-005-2016) Lifting up the average thermoelectric figure of merit (Invited)**D. Wu¹; X. Liu¹; D. Feng¹; J. He^{*}; 1. South University of Science and Technology of China, China**2:20 PM****(MCARE-S9-006-2016) Novel properties of cage-like and earth-abundant thermoelectrics via theory and simulations (Invited)**L. M. Woods^{*}; 1. University of South Florida, USA**3:00 PM****Break****Thermoelectric Materials III**

Room: Salon G

Session Chair: George Nolas, University of South Florida

3:20 PM**(MCARE-S9-007-2016) Practical Design, Development and Validation of a Thermoelectric Power Generator (Invited)**T. C. Holgate^{*}; J. VanderVeer¹; T. E. Hammel¹; 1. Teledyne Energy Systems Inc, USA**4:00 PM****(MCARE-S9-008-2016) Cage substitution and guest atoms in type II Sn clathrates**A. R. Khabibullin^{*}; G. S. Nolas¹; L. M. Woods¹; 1. University of South Florida, USA**4:20 PM****(MCARE-S9-009-2016) Electron and Phonon Engineering in thermoelectrics**Y. Pei^{*}; 1. Tongji University, China**4:40 PM****(MCARE-S9-010-2016) Thermal Stability Measurements and Evolved Gas Analysis of Selected Thermoelectric Materials and Potential TE Standards**E. Post^{*}; 1. NETZSCH Geraetebau GmbH, Germany**5:00 PM****(MCARE-S9-011-2016) Thermal to Electric Energy Conversion: Structural Phase Transitions as a Voltage Pump**S. Tidrow^{*}; 1. Alfred University, USA**S10: Batteries and Energy Storage****Beyond Lithium Batteries and Supercapacitors**

Room: Salon E

Session Chairs: Raj Singh, Oklahoma State University; Reza Shahbazian-Yassar, University of Illinois at Chicago

1:40 PM**(MCARE-S10-030-2016) New Positive Electrode Materials for Rechargeable Li/Na Batteries (Invited)**N. Yabuuchi^{*}; 1. Tokyo Denki University, Japan**2:20 PM****(MCARE-S10-031-2016) NASICON Na₃V₂(PO₄)₃: a rich crystal chemistry (Invited)**J. Chotard^{*}; G. Rousse²; R. David¹; O. Menr  ³; F. Lal  re¹; Y. Deng¹; C. Masquelier¹; 1. University de Picardie Jules Verne, France; 2. Coll  ge de France, France; 3. UCCS, France**3:00 PM****(MCARE-S10-032-2016) Can we trust half-cells in Na based batteries? (Invited)**A. Ponrouch^{*}; 1. ICMAB - CSIC, Spain**3:40 PM****(MCARE-S10-033-2016) Manganese-based Layered Oxides as Cathode Materials for Na-ion Batteries (Invited)**M. Kwon¹; K. Lee^{*}; 1. Seoul National University, Republic of Korea**4:20 PM****(MCARE-S10-034-2016) Thermally and Electrochemically Driven Topotactical Transformations in Sodium Layered Oxides Na_xVO₂ (Invited)**M. Guignard^{*}; C. Didier¹; M. R. Suchomel²; D. Carlier¹; J. Darriet¹; C. Delmas¹; 1. ICMCB-CNRS, France; 2. Argonne National Lab, USA

5:00 PM**(MCARE-S10-035-2016) Non-aqueous semi-solid flow battery based on Na-ion chemistry (Invited)**

J. R. Morante*; 1. IREC, Catalanian Institute for Energy Research, Spain

5:20 PM**(MCARE-S10-036-2016) Recent Advances in Electrolytes for Magnesium Sulfur Batteries (Invited)**Z. Zhao-Karger*; M. Fichtner¹; 1. Karlsruhe Institute of Technology, Germany**5:40 PM****(MCARE-S10-037-2016) Prospects for Solid State Supercapacitors Based on Calcium Copper Titanium Oxide for Energy Storage Applications (Invited)**

R. N. Singh*; 1. Oklahoma State University, USA

6:00 PM**(MCARE-S10-038-2016) 3D printing of graphene aerogel**C. Zhou*; D. Lin¹; 1. Kansas State University, USA; 2. University at Buffalo, USA**Thursday, April 21, 2016****Plenary Session IV**

Room: Salon E

8:30 AM**(MCARE-PL-004-2016) Patenting Materials for Alternative & Renewable Energy: Challenges and Opportunities**

C. Paradies*; 1. Paradies Law, USA

S5: Materials Challenges in Fuel Cells**Materials Challenges in Fuel Cells**

Room: Salon D

Session Chair: Olivier Guillon, Forschungszentrum Juelich

9:50 AM**(MCARE-S5-001-2016) Processing and Properties of Hierarchical Porous and Multi-layered Ceramics for Energy Applications – Experiments and Simulations (Invited)**R. K. Bordia*; C. Martin²; 1. Clemson University, USA; 2. Université de Grenoble - Alpes, France**10:30 AM****(MCARE-S5-002-2016) Particle Atomic Layer Deposition for Synthesis of Fuel Cell Catalytic Material**W. W. McNary*; A. M. Lubers¹; A. W. Weimer¹; M. E. Maguire¹; D. Ludlow²; A. Drake¹; M. Faust³; M. Seipenbusch²; 1. University of Colorado, Boulder, USA; 2. Ludlow Electrochemical Hardware, USA; 3. Karlsruhe Institute of Technology, Germany**10:50 AM****(MCARE-S5-003-2016) Post-test analysis of a rechargeable oxide battery (ROB)**C. M. Berger¹; O. Tokariev¹; N. H. Menzler¹; M. Bram¹; O. Guillon*; 1. Forschungszentrum Jülich GmbH, Germany**11:10 AM****(MCARE-S5-004-2016) Proton-Conducting Ceramic Electrolyte Fuel Cell for the Conversion of Natural Gas to Electricity and Liquid Fuels**B. Balachandran*; T. H. Lee¹; S. E. Dorris¹; 1. Argonne National Laboratory, USA**S6: Critical Materials for Energy****Critical Materials for Energy III**

Room: Salon F

Session Chairs: Bum Sung Kim, KITECH; Michitaka Ohtaki, Kyushu University

9:50 AM**(MCARE-S6-014-2016) ZnO-based Oxide Thermoelectric Materials with Microstructure Control for Selective Phonon Scattering (Invited)**

M. Ohtaki*; 1. Kyushu University, Japan

10:30 AM**(MCARE-S6-015-2016) Two-step process for recycling used ZrF₄-containing pickling (Invited)**J. Lee*; B. Yoo¹; Y. Lee¹; S. Han¹; D. Park¹; H. Nersisyan¹; 1. Chungnam National University, Republic of Korea**11:10 AM****(MCARE-S6-016-2016) Effect of Flow Dynamics for the Synthesis of Cadmium Selenide Quantum Dots in a Microreactor**B. Kim*; D. Jenog¹; J. Park¹; T. Kim¹; T. Seong²; 1. Korea Institute of Industrial Technology, Republic of Korea; 2. Korea University, Republic of Korea**11:30 AM****(MCARE-S6-017-2016) Production of Potassium Manganese Oxide Nanowires with the Inclusion of Bird Feathers in the Central Membrane**

M. S. Solangi*; 1. United Energy Pakistan Limited, Pakistan

11:50 AM**(MCARE-S6-018-2016) Enhanced thermoelectric properties of p-type BiSbTe based alloys through the dispersion of nano-inclusions**B. Madavali¹; C. Lee¹; H. Kim²; J. Koo²; S. Hong*; 1. Kongju National University, Republic of Korea; 2. Aems Lab, Iowa State University, USA**S9: Direct Thermal to Electrical Energy Conversion Materials and Applications****Thermoelectric Materials IV**

Room: Salon G

Session Chair: Arash Dehkordi, SunEdison

9:50 AM**(MCARE-S9-012-2016) Design and optimization of high performance p-type half-Heusler thermoelectric materials with zT>1 (Invited)**

T. Zhu*; 1. Zhejiang University, China

10:30 AM**(MCARE-S9-013-2016) On the Role of NaBH₄ toward Enhancing Thermoelectric Performance of Bi₂Te₃ and SiGe (Invited)**J. He*; T. M. Tritt¹; 1. Clemson University, USA**11:10 AM****(MCARE-S9-014-2016) Probing the role of La Fillers and Sb vacancies in CoSb₃ Skutterudites**X. Zeng*; C. Hu²; J. He¹; J. Huang³; B. Sumpter²; H. Zhao¹; T. M. Tritt¹; 1. Clemson University, USA; 2. University of Minnesota-Twin cities, USA; 3. Oak Ridge National Lab, USA**11:30 AM****(MCARE-S9-015-2016) Characterization, Mechanical and Thermal Properties of Thermoelectric Materials and Nanocomposites**

K. Lilova*; 1. Setaram Inc., USA

11:50 AM

(MCARE-S9-016-2016) Development and performance of thermoelectric materials and modules (Invited)R. Funahashi*; T. Barbier¹; 1. National Institute of Advanced Industrial Science & Technology, Japan**S10: Batteries and Energy Storage****Battery Processing**

Room: Salons A-C

Session Chairs: Aninda Bhattacharyya, Indian Institute of Science; Kristina Lilova, Setaram Inc.

9:50 AM

(MCARE-S10-040-2016) Low-Cost Lithium-Ion Electrode Processing and Manufacturing Science (Invited)D. L. Wood*; J. Li¹; D. Mohanty¹; Z. Du¹; L. David¹; Y. Sheng¹; S. An²; C. Daniel¹; 1. Oak Ridge National Laboratory, USA; 2. University of Tennessee, USA

10:30 AM

(MCARE-S10-041-2016) New challenges to future electrochemical power devices for automotive application (Invited)

Y. Tabuchi*; 1. Nissan Motor Co., Japan

11:10 AM

(MCARE-S10-042-2016) Pre-lithiation of Freestanding Flexible Si Nanoparticles-Carbon Nanotubes Composite Anodes for Lithium Ion Batteries By Stabilized Lithium Metal PowderK. Yao*; J. P. Zheng¹; R. Liang¹; 1. Florida State University, USA

11:30 AM

(MCARE-S10-043-2016) Influence of morphology of $\text{Li}_4\text{Ti}_5\text{O}_{12}$ anode on lithium storage performanceS. N. Reddy*; V. Ramar¹; C. Wang¹; R. Desapogu¹; P. Balaya¹; 1. National University of Singapore, Singapore

11:50 AM

(MCARE-S10-044-2016) Thermal behavior, Thermal Runaway, Kinetic, and Surface Properties of Bulk and Nano Battery and Battery Elements Studied by Thermal Analysis and CalorimetryK. Lilova*; L. Brown¹; 1. Setaram Inc., USA**Advanced Characterization**

Room: Salon E

Session Chairs: Siegbert Schmid, University of Sydney; V. Yartys, Institute for Energy Technology

9:50 AM

(MCARE-S10-045-2016) Real-Time Observations of Electrochemical Reactions in Rechargeable Energy Storage Systems (Invited)

R. Shahbazian-Yassar*; 1. University of Illinois at Chicago, USA

10:10 AM

(MCARE-S10-046-2016) Comparative Analysis of *Ex-situ* and *Operando* X-ray Diffraction Experiments for Lithium Insertion Materials (Invited)

S. Schmid*; 1. The University of Sydney, Australia

10:50 AM

(MCARE-S10-047-2016) Structure and Electronic Structure of Battery Materials at Atomic Scale (Invited)

L. Gu*; 1. Institute of Physics, Chinese Academy of Sciences, China

11:30 AM

(MCARE-S10-048-2016) Evolution of Surface and Subsurface Phases on High-Voltage Aging of $\text{LiNi}_{0.8}\text{Co}_{0.15}\text{Al}_{0.05}\text{O}_2$ Cathode Materials-A STEM/EELS StudyP. Mukherjee*; S. Sallis²; L. Piper²; N. Pereira¹; G. G. Amatucci¹; F. Cosandey¹; 1. Rutgers University, USA; 2. Binghamton University, USA

11:50 AM

(MCARE-S10-049-2016) *In Operando* neutron diffraction study of lithium-ion and metal hydride batteries

V. A. Yartys*; 1. Institute for Energy Technology, Norway

Monday, April 18, 2016

Plenary Session I - ACerS-KICHe Distinguished

Lecture

Room: Salon E

8:40 AM

(MCARE-PL-001-2016) Energy harvesting with nanogenerators for realizing self-powered small electronics

S. Kim^{*1}; 1. Sungkyunkwan University, Republic of Korea

Energy harvesting systems based on piezoelectric and triboelectric nanomaterials are in great demand, as they can provide routes for the development of self-powered devices which are highly flexible, stretchable, mechanically durable, and can be used in a wide range of applications. Our recent research interest mainly focuses on the fabrication of piezoelectric and triboelectric nanogenerators based on various kinds of nanomaterials. Flexible nanogenerators exhibit good performances and are easy to integrate which make it the perfect candidate for many applications, and therefore crucial to develop. In this presentation, I firstly introduce the fundamentals and possible device applications of nanogenerators, including their basic operation modes. Then the different improvement parameters will be discussed. As main topics, I will present a couple of recent achievements regarding highly stretchable piezoelectric-pyroelectric hybrid nanogenerators, transparent flexible graphene triboelectric nanogenerators, textile-based wearable triboelectric nanogenerators, etc. The recent research and design efforts for enhancing power generation performance of nanogenerators to realize self powering of portable and wearable sensors and electronics will also be discussed in this talk.

S2: Spectral Conversion Materials for Energy Applications

Upconversion, Downconversion /Quantum Cutting and Luminescent Downshifting for Solar Cells I

Room: Salon D

Session Chairs: Eva Hemmer, INRS; Jose Marques-Hueso, Heriot-Watt University

10:00 AM

(MCARE-S2-001-2016) Upconverter Solar Cells: from Materials to Device Applications (Invited)

R. E. Schropp^{*1}; J. de Wild²; W. G. van Sark³; J. Feenstra⁴; J. Schermer⁴; 1. Eindhoven University of Technology (TU/e), Netherlands; 2. Luxembourg University, Luxembourg; 3. Utrecht University, Netherlands; 4. Radboud University, Netherlands

In single junction solar cells, the inability to absorb photons with an energy lower than the band gap and the thermalisation losses of excess photon energy together accounts for ~65% of the total energy losses. Spectral conversion of sunlight is a promising route to reduce these spectral mismatch losses. The advantage of spectral conversion is that it can be applied to existing solar cells. Whereas downconversion involves an optically active layer in front of the solar cell, with the risk that parasitic absorption occurs in this layer, upconversion is of special interest because the upconverter can be placed at the back of the cell. In this way the losses due to optical filtering are very small and in addition the isotropically emitted light at shorter wavelengths can be redirected to the solar cell by a mirror or a reflective white surface. The non-absorbed sub-bandgap photons passing through the cell get a second chance to be absorbed, after conversion to higher-energy photons. Thus it is relatively straightforward to demonstrate a positive contribution in upconverter solar cells. We will demonstrate and discuss experimental utilization of the concept

in two types of 1.8-eV bandgap semi-transparent solar cells; thin-film Si cells and InGaP cells, under broadband illumination using $\text{Er}^{3+}/\text{Yb}^{3+}$ upconverters.

10:40 AM

(MCARE-S2-002-2016) Upconversion of Sub-Bandgap Photons for Solar Energy Harvesting: Recent Progress, Obstacles, and Future Perspective (Invited)

S. Fischer^{*1}; 1. Lawrence Berkeley National Laboratory, USA

Upconversion of low-energy photons into high-energy photons increases the efficiency of photovoltaic devices by converting photons with energies below the absorption threshold of the solar cell into photons that can be utilized. Colloidal upconverter nanocrystals (UCNCs) are particularly interesting because they can be combined with plasmonic or photonic structures to boost their efficiency as well as combined with dyes or quantum confined structures to widen their narrow absorption range. However, practical applications of UCNCs are hindered by their low upconversion quantum yield (UCQY) and the high irradiances necessary to produce relevant upconversion luminescence. Achieving high UCQY under practically relevant irradiance remains a major challenge as the amount of radiation provided by the sun is rather low compared to the high laser powers typically used by scientist in their experiments. In this talk, an overview over the available materials and performances of different upconverter materials will be given and the present challenges will be discussed. The focus will be on UCNCs and how the UCQY can be significantly enhanced by still keeping the advantages of these nanomaterials.

11:20 AM

(MCARE-S2-003-2016) Modelling Energy Transfer in Lanthanide Doped (Nano)Crystals (Invited)

F. Rabouw¹; D. Yu²; A. Meijerink^{*1}; 1. Utrecht University, Netherlands; 2. Rutgers University, USA

Lanthanides have transformed the world of lighting in the past 40 years. In many lanthanide based luminescent materials energy transfer is involved. The well-known upconversion phosphor $\text{NaYF}_4:\text{Yb},\text{Er}$ relies on energy transfer from two Yb^{3+} ions to Er^{3+} . The opposite process of downconversion for the lanthanide couples ($\text{Er}^{3+}, \text{Yb}^{3+}$), ($\text{Tb}^{3+}, \text{Yb}^{3+}$) and ($\text{Pr}^{3+}, \text{Yb}^{3+}$) involves either two-step energy transfer or cooperative energy transfer. In the analysis of conversion efficiencies of up- and downconversion for solar cells it is crucial to model energy transfer in order to establish the internal quantum efficiency. In this presentation a short historical introduction to modelling energy transfer will be followed by an overview of recent developments, demonstrating the need for modelling using microscopic models based on actual distributions of lanthanide ions and distributions of donor-acceptor distances imposed by the crystal structure of the host. As an illustrative example, energy transfer from Ce^{3+} to Yb^{3+} will be discussed. In the literature cooperative energy transfer from Ce^{3+} to two Yb^{3+} ions has been reported but based on modelling we show that in fact the energy transfer is dominated by single step energy transfer via a metal-to-metal charge transfer state. Finally, an outlook into the future of modelling energy transfer will be given with a focus on spectral conversion for solar cells.

*Denotes Presenter

S3: Ferroelectrics and Multiferroics for Energy Applications

Ferroelectrics for Energy

Room: Salon F

Session Chair: Catherine Elissalde, ICMCB-CNRS

10:00 AM

(MCARE-S3-001-2016) Piezoelectric and pyroelectric materials and structures for energy harvesting (Invited)

C. R. Bowen^{*1}; 1. University of Bath, United Kingdom

The need for reduced power requirements for small electronic components, such as wireless sensor networks, has prompted renewed interest in recent years for energy harvesting technologies capable of capturing energy from ambient vibrations and heat. This presentation provides an overview of piezoelectric harvesting system along with the closely related sub-classes of pyroelectrics and ferroelectrics. These properties are, in many cases, present in the same material, providing the intriguing prospect of a material that can harvest energy from multiple sources including vibration and thermal fluctuations. Examples of bistable piezoelectric energy harvester are described where nonlinearity enables broadband operation, porous materials and pyroelectric harvesting where power is from temperature fluctuations. **Acknowledgement** The research leading to these results has received funding from the European Research Council under the European Union's Seventh Framework Programme (FP/2007-2013) / ERC Grant Agreement no. 320963 on Novel Energy Materials, Engineering Science and Integrated Systems (NEMESIS)

10:40 AM

(MCARE-S3-002-2016) Flexible and high temperature piezoelectric composites for energy harvesting applications (Invited)

W. A. Groen^{*1}; 1. Technical University Delft, Netherlands

Functional composites of electroceramic particles in a polymer matrix are valued for easy, low temperature processing and good mechanical properties. However, the piezoelectrical properties generally suffer due to limited connectivity of the electroceramic particles, especially at low ceramic volume fraction. Composites with enhanced properties compared to composites with randomly dispersed particles can be obtained by dielectrophoretic alignment of the particles during curing of the polymer matrix. Composites with oriented lead zirconium titanate, PZT, particles in an epoxy or polyurethane matrix can be used for an energy harvesting application inside an automobile tire. Higher energy output can be achieved by optimization of the filler material and matrix material. Flexible lead free piezoelectric composites have been developed on basis of potassium sodium lithium niobate (KLN) with silicone rubber. The piezoelectric properties of these structured 10 vol. % structured KLN-composites exceeds that of all values for such functional composites reported in the literature and is comparable to polymers based on PVDF. High temperature applications with composites up until 200°C are investigated on the basis of thermally stable polymers and lead titanate. Finally, pyroelectric composites will be discussed which has been developed by tuning the electrical conductivity of the polymer matrix.

11:10 AM

(MCARE-S3-003-2016) Barium titanate-based materials for energy and related applications (Invited)

M. Deluca^{*1}; J. Krainer¹; E. Lackner¹; R. Wimmer-Teubenbacher¹; J. Spitaler¹; A. Köck¹; 1. Materials Center Leoben Forschung GmbH, Austria

Barium titanate (BT)-based materials are nowadays very popular for energy-related applications. They are often used as replacement to lead-based counterparts due to increasingly strict environmental

regulations. Piezoelectric materials for energy harvesting or transducing applications, thermally stable dielectrics for energy storage, electrocaloric and greenhouse gas-sensing materials can all be produced from the BT material class upon suitable doping or the constitution of solid solutions. In this talk, BT-based materials will be introduced, with an emphasis on their complexity and the possible strategies to characterize and control the structural features at the basis of their excellent properties. Special attention will be given to BT-based relaxors, as the influence of the short-range structure on the macroscopic properties is far from being uncovered in this material class. It will be shown how a combination between experimental methods including Raman spectroscopy and X-ray diffraction, together with ab-initio modeling, can be very promising to fulfil this task. Finally, the use of BT in the emerging field of CO₂ gas sensors will be discussed. The versatility of BT and the methodologies needed to design its properties will be highlighted within the perspective of energy-related applications.

S10: Batteries and Energy Storage

All solid-state Batteries I

Room: Salon E

Session Chairs: Palani Balaya, National University of Singapore; Mickael Dollé, Université de Montreal

10:00 AM

(MCARE-S10-001-2016) Advances Towards Solid State Batteries Using Garnet LLZO Electrolytes (Invited)

M. Doeff^{*1}; L. Cheng¹; 1. Lawrence Berkeley National Laboratory, USA

The appeal of solid state batteries on paper is clear; ideal devices would be safer than current Li-ion batteries because there is no flammable liquid component to leak or catch fire, and energy densities are potentially much higher because the configuration allows the use of lithium metal instead of graphite anodes. There are, however, many technical challenges in building such devices and ensuring reasonable performance. While oxides based on the garnet structure (e.g., LiLa3Zr2O12 or LLZO) are among the most promising solid electrolytes for devices, based on their high conductivities and apparent stability against lithium, difficulties in densifying the materials and high interfacial resistances at lithium electrodes have precluded their use until now. Our recent research has been directed towards overcoming these obstacles. Classical ceramics processing techniques have been used to produce samples as thin as 200 microns, up to 94% dense, with excellent control over grain size and grain boundary chemistry. An array of advanced techniques including soft x-ray absorption spectroscopy (XAS) and synchrotron x-ray photoemission spectroscopy (XPS) has been used to understand the interfacial chemistry. This approach has resulted in the reduction of the interfacial impedance in Li/LLZO/Li cells to 37Ω-cm², the lowest ever reported. These advances ensure future viability of LLZO-containing solid-state batteries.

10:40 AM

(MCARE-S10-002-2016) Oxide-Based Solid State Electrolytes as Key Components for All-Solid-State Li-Ion Batteries (Invited)

M. J. Hoffmann^{*1}; T. Hupfer¹; E. C. Bucharsky¹; F. Lemke¹; G. Schell¹; A. Hintennach²; 1. Karlsruhe Institute for Technology, Germany; 2. Daimler AG, Germany

Lithium lanthan titanate (LLTO) and lithium titanium aluminum phosphate (LATP) are potential candidates as oxide solid state electrolytes with a high Li-ion conductivity. LATP with the composition Li_{1.3}Al_{0.3}Ti_{1.7}(PO₄)₃ was prepared by a modified sol gel method. Densification was achieved by field assisted sintering (FAST) as well as conventional pressureless sintering. LLTO were prepared by a standard mixed oxide route and pressureless densified. The resulting phase composition, crystal structure and theoretical density of both

phases were obtained from XRD analysis. Electrical properties, such as ionic conductivity, were determined by impedance spectroscopy in the frequency range from 1 Hz to 1 MHz. A maximum conductivity in the order of 10^{-3} S/cm at room temperature is obtained for phase-pure LATP compositions combined with a high relative density. However, strong anisotropy in thermal expansion causes microcracking in coarse-grained materials which finally leads to a reduction in ionic conductivity. The LLTO contains small quantities of Li-titanate as second phase and reveals an ionic conductivity of 10^{-3} for the grains and up to 10^{-4} for the grain boundaries. No significant influence of the second phase was detected, but grain growth enhances grain boundary conductivity by approximately one order of magnitude.

11:20 AM

(MCARE-S10-003-2016) Bulk-Type All-Solid-State Lithium-Ion Batteries using Oxide Electrolytes (Invited)

T. Okumura^{*1}; T. Takeuchi¹; H. Kobayashi¹; 1. National Institute of Advanced Industrial and Technology (AIST), Japan

Oxides are generally non-flammable, durable and non-toxic materials; high safety and reliability in a battery system is assured by the use of oxide as an electrolyte instead of the highly-reactive non-aqueous liquid. Indeed, a thin-film lithium-ion battery has been commercialized as energy storage parts of micro devices, in which electrode and electrolyte thin films are stacked by deposition techniques. To develop a thick bulk-type all-solid-state lithium-ion battery (BT-ASS-LIB) for applications such as electric vehicles, the thicknesses of stacked electrode and electrolyte layers need to be curtailed to several ten to hundred μm order. This can be achieved through powder technology. However, the good-contact interfaces should be prepared and also produces little ion-blocking impurities. Well-known lithium-ion conductive oxides based on the NASICON-type structures etc. possess high bulk conductivities of over 10^{-4} S cm^{-1} ; however, these oxides required sintering at high temperature beyond 1000 °C to facilitate good contact with the electrodes. In addition, most electrode materials produce impurities after high-temperature sintering. To address these issues, we assembled the BT-ASS-LIBs by the use of lithium-ion conductive oxides with low melting point and/or the use of low-temperature spark plasma sintering process, and investigated the battery performances in these simple batteries.

S11: Hydrogen Materials and Economy

Hydrogen Materials and Economy

Room: Salon G

Session Chairs: David Tamburello, Savannah River National Lab; Peter Pfeifer, University of Missouri

10:00 AM

(MCARE-S11-001-2016) Low-pressure storage of methane on high-surface-area carbon for natural gas vehicles: record performance in the lab and on a 40-liter prototype tank (Invited)

P. Pfeifer^{*1}; T. Rash¹; E. Knight¹; C. Schulz¹; D. Stalla¹; A. Gillespie¹; Y. Soo¹; 1. University of Missouri, USA

Under contract #500-08-022 from the California Energy Commission (2011-14), the University of Missouri has developed monolithic nanoporous carbon with a storage capacity of 0.13 kg methane/liter carbon and 0.26 kg methane/kg carbon at 35 bar and 25 C (http://www1.eere.energy.gov/cleancities/natural_gas_forum_meeting_oct11.html; Final Report in press (2015); U.S. Patents No. 8,691,177, 8,926,932). This is 4.5 times what a tank without carbon without carbon would hold at 35 bar and is world record volumetric storage capacity for adsorbed natural gas (ANG). The technology, showcased on a 40-liter conformable ANG tank, offers (i) reduced fueling costs because of low pressure (7 times lower than CNG,

250 bar); (ii) a tank that weighs 50% less than a CNG tank and has a 20% lower total volume; (iii) a rectangular tank geometry that can be integrated into the chassis of a vehicle, making NG vehicles an attractive alternative to gasoline and diesel vehicles. Data to be presented ranges from density of adsorbed methane films, 0.39-0.41 g/ml, comparable to the density of liquid methane at -161 C, to flow rates and pressure/temperature profiles for fast/slow fill and various discharge modes.

10:40 AM

(MCARE-S11-002-2016) Hydrogen extraction by a permselective vanadium alloy membrane from gas mixtures of hydrogen, nitrogen and ammonia

C. Nishimura^{*1}; J. Tsai³; H. Kimura⁴; H. Yoshinaga²; S. Sakurai²; 1. National Institute for Materials Science (NIMS), Japan; 2. Taiyo Koko Co. Ltd., Japan; 3. National Taipei University of Technology, Taiwan; 4. Suzuki Shokan Co. Ltd., Japan

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. There is a growing interest on non-porous membranes to be applied for hydrogen fueling stations in near future. 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. NIMS has accumulated experiences to develop vanadium alloys for hydrogen permselection. From 2014, we started a new project: Development of Innovative Hydrogen Production Technology from Energy Carriers Based on Vanadium Alloy Membranes, funded by JST-CREST. In this project, vanadium alloys optimized for hydrogen production process from energy carriers such as ammonia and methylecyclohexane will be developed for membrane separation. Here I present results of hydrogen permeation using vanadium alloy membranes from a gas mixture of hydrogen, nitrogen and ammonia. Permeation results with a gas mixture suggest enrichment of nitrogen and ammonia at the inlet surface when the flow rate of feed gas is low. Hydrogen permeability of vanadium alloy membrane was not degraded in a permeation test for 4 days at 573 K, with a gas mixture containing 1% ammonia.

11:00 AM

(MCARE-S11-003-2016) Metal-Dielectric Hybrid-Structured Film with Titanium Oxide for Enhanced Visible Light Absorption and Photo-Catalytic Applications

H. Kim^{*1}; J. Park¹; S. Nam²; H. Kim²; H. Choi³; J. Baik¹; 1. Ulsan National Institute of Science and Technology, Republic of Korea; 2. Korea Advanced Institute of Science and Engineering (KAIST), Republic of Korea; 3. Korea University, Republic of Korea

Two-dimensional metal-Dielectric hybrid-structure design based on ultrathin TiO₂ film for enhanced visible light absorption and photo-catalytic applications is reported, which mainly consists of three layers of Au film, TiO₂ film, and Au NPs. The Au and TiO₂ films are produced by using e-beam evaporation and atomic layer deposition in a carefully controlled way for minimizing surface roughness. As compared with bare TiO₂ film, the Au NPs/TiO₂/Au film significantly increased the photoactivity in the entire UV-visible region. The Au film increases the light absorption in the UV region with TiO₂ acting as an impedance-matching layer, while the Au NPs increase the light absorption in the visible region due to the plasmonic resonance effects, increasing the photocurrent under visible light. 3D finite-difference time-domain simulation results suggest that the Au film also plays an important role in enhancing the electrical field intensity at the interface between Au NPs and TiO₂ upon surface plasmon resonance excitation, thereby, contributing to the enhanced photoactivity of the film in the visible range. The current study will provide a new paradigm for designing two-dimensional plasmonic photoelectrodes to effectively harvest the entire UV-visible light for solar fuel production.

11:20 AM

(MCARE-S11-004-2016) In-situ Adsorbent Growth (Invited)

D. A. Tamburello^{*1}; M. Sulic²; D. L. Anton¹; B. J. Hardy¹; C. Corgnale²;
1. Savannah River National Lab, USA; 2. Savannah River Consulting, USA

Fully commercialized hydrogen-powered automobiles require advances in onboard storage. Metal-Organic Frameworks (MOFs) are crystalline materials composed of cage-like structures containing nano-scale pores, which improve gas adsorption over common adsorbents; however, MOFs have low bulk density and low thermal conductivity. Compaction can improve volumetric storage and thermal conductivity while reducing capacity but does not overcome the thermal contact resistance inherent within most solid/fluid heat exchangers (HX's). In-situ growth of an adsorbent onto a HX would be a solution to low volumetric density, thermal conductivity inefficiency, thermal contact issue, and potential HX manufacturing issues. This work presents separate in-situ growth studies: (1) HKUST-1 onto a carbon foam, KFOAM[®] (simplified HKUST1@KFOAM), and (2) MOF-5 onto aluminum tubing (simplified MOF5@Al). In both studies, the growth process was achieved with a viable adsorbent grown directly onto the HX. In the case of HKUST1@KFOAM, subsequent in-situ procedures indicate layered growth onto the substrate. For MOF5@Al, layering of the adsorbent occurred concurrently requiring no additional procedures. Analysis by powder X-ray diffraction (PXRD) demonstrates the crystallinity of the adsorbents, with peaks confirming the identity of functionalized material. Scanning electron micrographs show the adsorbents layered directly on the heat exchanger.

11:40 AM

(MCARE-S11-005-2016) Synergistic Effects of MWCNT and Nb₂O₅ on the Hydrogen Storage Characteristics of Li-nMg-B-N-H System

S. Srinivasan^{*1}; D. Demirocak²; E. Stefanakos³; Y. Goswami³; 1. Florida Polytechnic University, USA; 2. Texas A&M University, USA; 3. University of South Florida, USA

In this study, we have synthesized the complex hydrides (LiBH₄/LiNH₂/nanoMgH₂) as Li-nMg-B-N-H compounds for the reversible hydrogen storage at moderate temperature and pressure conditions. We have also examined its hydrogen storage characteristics with different dopants such as Multi Walled Carbon Nanotubes (MWCNT) and Nb₂O₅ nanoparticles in different concentration both plain and their combinations. From our TGA, TPD and PCT results, it is observed that an optimum concentration of 2wt%Nb₂O₅ and 10wt% MWCNT showed high hydrogen release characteristics when compared to pristine base compound and individual dopant counterparts. The structural, microstructural and surface behavior of undoped and doped Li-nMg-B-N-H samples have been compared and contrasted in this work.

12:00 PM

(MCARE-S11-006-2016) Kinetics and Thermodynamics of Hydrogen Sorption Studied by Manometric and Coupled Manometric/Calorimetric Techniques

K. Lilova^{*1}; L. Brown¹; 1. Setaram Inc., USA

Understanding the kinetics and the thermodynamics of adsorption/desorption is essential for the hydrogen storage applications. The gas sorption manometric Sievert's technique has proven to have many advantages for the evaluation of the ad- or ab- sorbed amount of gas by porous materials in a wide range of temperature and pressure. In addition, there is a total freedom in the size and shape of the sample holder, which allows coupling of techniques and in-situ measurements of various chemical and physical parameters. Coupling calorimetry and manometry results in a full characterization of the H₂ adsorption on solids. In addition to the adsorption isotherms and the derived isosteric heat, the differential heat of adsorption as a function of the adsorbed amounts can be obtained directly. Several

examples, including sorption on metal and MOFs will be presented to illustrate the methodology.

S2: Spectral Conversion Materials for Energy Applications

Upconversion, Downconversion /Quantum Cutting and Luminescent Downshifting for Solar Cells II

Room: Salon D

Session Chairs: Gunnar Westin, Uppsala University; Ruud Schropp, Eindhoven University of Technology (TU/e)

1:30 PM

(MCARE-S2-008-2016) Heterostructured quantum dots for solar energy applications (Invited)

H. Zhao^{*1}; F. Rosei¹; 1. INRS, Canada

In quantum dot (QD) based solar cells the photoconversion efficiency (PCE) is critically related to the ability of exciton generation after photon absorption and electron injection from photoexcited QDs to the wide bandgap semiconductor. In this talk, we focus on the synthesis of near infrared (NIR) colloidal core@shell QDs, the investigation of the photoelectron transfer rate from QDs to wide bandgap semiconducting mesoporous films using photoluminescence (PL) lifetime spectroscopy and further fabrication of solar cell. The various types QDs (bare QDs and core/shell QDs) were loaded into the mesoporous metal oxide thin film. The variation in core size and the shell thickness allows us to fine tune the electron injection rate. The results demonstrate the possibility of obtaining fast charge injection in NIR QDs stabilized by an external shell, with the aim of providing viable solutions to the stability issues typical of NIR QDs capped with pure organic ligand shells. In the end, all solution processed depleted bulk heterojunction solar cell devices based on NIR core@shell QDs and films of rutile TiO₂ nanorod arrays have been investigated. It was found that the maximum PCE of the solar cell up to ~2%. The stability and ease of processing in air together with the good performance of the PbS@CdS core@shell QDs, strongly suggest their high potential in solar cell applications.

2:10 PM

(MCARE-S2-004-2016) Sol-gel derived frequency conversion coatings for solar cell applications (Invited)

R. M. Almeida^{*1}; 1. Instituto Superior Técnico /U Lisboa, Portugal

High efficiency PV solar cells should absorb photons in the full solar spectrum, requiring up-conversion (UC) of sub-bandgap photons to avoid transparency and down-conversion (DC) of photons with energy above E_G to minimize thermalization losses. Although much work has already been done to develop new materials and geometries for up- and down-converters, the gains reported so far are still modest. Rare-earth (RE) doped phosphor layers may be deposited on solar cell materials to help achieve the above mentioned objectives and sol-gel (SG) processing is a low-cost technology which can be an interesting alternative to more established coating methods like CVD and PVD. RE-doped SG-derived active layers have been deposited by spin-coating onto Si substrates for frequency DC and UC, involving host matrices like aluminosilicate glasses, or yttria, YAG and titania ceramics and active elements like Er, Tb, Yb and Tm. These films have been characterized by spectroscopic ellipsometry, FTIR and Raman spectroscopies, XRD, SEM and photoluminescence spectroscopy. The combination of such coatings with 1-D photonic crystals, modelled by the Transfer Matrix Method, has also been investigated in connection with an improved control of the different RE light emissions. The advantages and drawbacks of this promising technology and its future perspectives will be discussed, compared to other possible alternatives.

Upconversion, Downconversion /Quantum Cutting and Luminescent Downshifting for Solar Cells III

Room: Salon D

Session Chairs: Marta Quintanilla, CIC BiomaGUNE; Stefan Fischer, Lawrence Berkeley National Laboratory

3:10 PM

(MCARE-S2-005-2016) Co-Sensitized Upconversion (Invited)

W. Zou¹; M. S. Pshenichnikov¹; J. Hummelen^{*1}; 1. University of Groningen, Netherlands

We report on our discovery of efficient broadband near-IR light up-conversion. Photon upconversion of the (near)infrared (NIR) photons is a promising way to go past the Shockley-Queisser limit that sets up the maximal efficiency of 32% to a single junction solar cell. However, the practical applicability of the most efficient upconversion materials known to date at moderate light intensities (i.e. below 1000 Suns) is limited by the extremely weak and narrow-band (N)IR absorption. First and inspired by a natural design of photosynthetic complexes, we introduced the novel concept of an upconversion material in which an organic (N)IR dye is used as an antenna for β -NaYF₄:Yb,Er nanoparticles (NPs) where the upconversion occurs. The overall upconversion efficiency of the dye-sensitized NPs was dramatically enhanced (by a factor of ~3300) as a result of increased absorptivity and overall broadening of the absorption spectrum of the upconverter. More recently, we showed that this dye-sensitized upconversion can be readily extended to cover any desired part of the solar spectrum by applying a set of different dye molecules with overlapping absorption spectra, acting as an extremely broadband antenna system, connected to a suitable upconverter. We will now present the results on co-sensitized upconversion with two types of antenna molecules, leading to a further enhancement of upconversion.

3:50 PM

(MCARE-S2-006-2016) Up-conversion in perovskite strontium stannate nanostructures for application in dye-sensitized solar cell

V. Sahrawat²; A. Kumar^{*1}; 1. National Institute of Technology (NIT), Kurukshetra, India; 2. National Institute of Technology (NIT), India

The light to electricity conversion efficiency of dye sensitized solar cells (DSSCs) is not only decided by the dye molecules, semiconducting material and redox shuttle selection, but also depends on particle size and size distribution of the semiconducting photo-anode. In this work, a simple, eco-friendly facile wet chemical nitrate precursor route for the synthesis of pristine and alkaline earth metal co-doped (Er and Yb in ratio 10/90,15/85 and 20/80) nano-crystalline (~ 15-25 nm) SrSnO₃, which is room temperature n-type wide band gap (~ 4.1 eV) orthorhombic perovskite semiconductor, has been utilized. The obtained rare earth alkaline doped materials have been used as up-conversion semiconductor photo-anode in DSSC. The particle sizes of synthesized nanostructures were estimated to be in the range of 15-25 nm. The increment in band gap of SrSnO₃ was observed with the increase in Er and Yb content. The perovskite SrSnO₃ samples exhibited strong emission around 365 nm following band-gap excitation by 290 nm. Further, Er/Yb doped samples have shown strong emission at 550 nm with the excitation of wavelength of 980 nm. The resistivity values decreased with increase in the dopants Er and Yb concentration due to enhancement in charge carrier concentration. The DSSC device has been successfully fabricated and tested for its impedance and current voltage (I-V) behavior.

4:10 PM

(MCARE-S2-007-2016) Glasses doped with trivalent rare-earth ions as photon downshifters for photovoltaic applications (Invited)

F. Steudel¹; S. Loos²; B. Ahrens²; R. L. Leonard³; J. A. Johnson³; S. Schweizer^{*1}; 1. Fraunhofer IMWS, Germany; 2. South Westphalia University of Applied Sciences, Germany; 3. University of Tennessee Space Institute, USA

Rare-earth (RE) doped glasses are investigated for their potential as photon downshifting covers for CdTe solar cells. Two glass matrices are analyzed: borate glass and fluorozirconate-based (FZ) glass. Both glasses are single- or double-doped with the trivalent rare-earth ions Sm³⁺, Eu³⁺, and Tb³⁺, enabling intense luminescence in the red (Sm³⁺ and Eu³⁺) and green (Tb³⁺) spectral ranges upon excitation in the ultraviolet and blue spectral range. The RE concentrations are varied over a broad range to optimize for optical absorption and luminescence efficiency. To evaluate their potential as photon downshifting covers, the gain in short-circuit current density of CdTe solar cells with different thicknesses of the CdS buffer layer is calculated for each glass. Though the single-doped glasses reveal a slight increase in short-circuit current density, the double-doped glasses allow for greater efficiency gains since a significantly broader spectral range for absorption exists. Compared to borate glass, Sm³⁺ and Tb³⁺ single-doped FZ-based glasses provide a larger gain due to greater quantum efficiencies in this system. In contrast, for Eu³⁺ doping, the gain for borate glass is significantly greater than for FZ-based glass due to non-usable emissions in the blue spectral range in the case of FZ-based glass.

S3: Ferroelectrics and Multiferroics for Energy Applications

Single Phase Ferroelectrics and Multiferroics I

Room: Salon F

Session Chair: Xavier Moya, University of Cambridge

1:30 PM

(MCARE-S3-005-2016) Design, Modeling and Experimental Values of Temperature Dependent Material Properties (Invited)

S. Tidrow^{*1}; 1. Alfred University, USA

Through transformation into ionic radii space, use of physical constraints, planar and volume, and use of the Clausius-Mossotti relation, coordination and temperature dependent "effective" ion properties, radii and polarizability, have been deduced that within a relatively new theoretic framework significantly outperforms Goldschmidt's tolerance factor for a priori predicting room temperature material properties: structure; lattice parameter; and volume. Here, we use the theory to show that the relatively new theoretic framework can be used to model such improved material parameters: structure; lattice parameter; and volume; structural phase transition temperature; over a wide temperature range. Additionally, we specifically simulate temperature dependent properties: lattice parameter and volume, dielectric constant; and, structural phase transition temperature; of a significant number of, both Pb and non-Pb based, ferroelectric and/or anti-ferroelectric materials including their solid solutions.

2:10 PM

(MCARE-S3-006-2016) Towards functionality in fluorites: nonequilibrium structures in thin films and bulk ceramics (Invited)

J. L. Jones^{*1}; C. Fancher¹; D. Hou¹; S. Jones¹; C. Chung¹; B. Johnson¹; 1. North Carolina State University, USA

In 2011, HfO₂-based thin film capacitors were shown to exhibit ferroelectric behavior when crystallized with certain elements (e.g., Si, Y, Zr, and Gd). The ferroelectric behavior is only observed when

the materials are processed in specific conditions, for example, unique stress states induced by special annealing procedures. A non-centrosymmetric and polar space group is suspected in the films, though no rigorous crystallographic analyses of the materials has been published. In this work, we synthesized doped HfO₂ ceramics and powders in order to study the structures and phase stability using X-ray powder diffraction and structure inversion methods (i.e., the Rietveld method). Our results demonstrate that dopants (Si, Gd, Y, and Zr) substitute for Hf and, in some cases, can create non-equilibrium structures. The phase evolution of Si-doped HfO₂ non-equilibrium structure was determined as a function of calcination temperature. The HfSiO₄ secondary phase is ultimately precipitated with increased temperature. In addition, X-ray diffraction patterns were measured on Si, Gd, Y, and Zr doped HfO₂ under high pressures up to 30 GPa. The observed pressure-induced sequence confirmed the structures predicted by a computational model published by other investigators. Overall, the results point towards paths to polar phases and ferroelectricity in HfO₂-based materials.

2:40 PM

(MCARE-S3-007-2016) Multiferroic properties of holmium chromite and gadolinium chromite

S. Yin^{*1}; M. Jain¹; 1. University of Connecticut, USA

In this work, HoCrO₃ and GdCrO₃ powders and thin films were synthesized via a solution route. The phase purity and structural properties were examined by Raman spectroscopy and Rietveld refinement of the x-ray diffraction data. The dc magnetic measurement indicates that the ordering temperatures of Cr³⁺ are 140 K and 170 K for HoCrO₃ and GdCrO₃, respectively. By fitting the temperature dependent susceptibility data of the powder samples in the paramagnetic region with the Curie-Weiss fit, the effective magnetic moment were determined and in good agreement with theoretically calculated values. The isothermal magnetization measurements were also performed to obtain the magnetic behavior and temperature dependence of coercive field and remnant magnetization data. Further, the magnetocaloric properties of HoCrO₃ and GdCrO₃ powders samples were studied, indicating their potential for applications in magnetic refrigeration. The structural, magnetic, and dielectric data of these samples will be presented in details.

Single Phase Ferroelectrics and Multiferroics II

Room: Salon F

Session Chair: Steven Tidrow, Alfred University

3:20 PM

(MCARE-S3-008-2016) Structure-T_C relationships in BaTiO₃-based ferroelectric perovskites (Invited)

P. Balachandran^{*1}; T. Lookman¹; D. Xue¹; 1. Los Alamos National Laboratory, USA

One of the key impediments to the development of BaTiO₃ based materials as a candidate to replace toxic-Pb based functional materials is their relatively low ferroelectric Curie temperature (T_C). Amongst many potential routes that are available to modify the T_C, ionic substitutions at the Ba- and Ti-sites remain the most common approach. Here, we perform density functional theory (DFT) calculations on a series of ATiO₃ and BaBO₃ perovskites, where A=Ba, Ca, Sr, Pb, Cd, Sn and Mg and B=Ti, Zr, Hf and Sn. Our objective is to study the relative role of A- and B-cations in impacting the T_C of the tetragonal (P4mm) and rhombohedral (R3m) ferroelectric phases in the BaTiO₃ based solid-solutions, respectively. Using symmetry-mode analysis, we obtain a quantitative description of the relative contributions of various divalent (A) and tetravalent (B) cations to the ferroelectric distortions. Our results show that Ca, Pb, Cd, Sn and Mg have large mode amplitudes for ferroelectric distortion in the tetragonal phase relative to Ba, while Sr suppresses it. On the other hand, Zr, Hf, and Sn tetravalent cations severely suppresses

the ferroelectric distortion in the rhombohedral phase relative to Ti. We correlate the calculated mode strengths to the experimentally measured T_C for known systems using machine learning and uncover trends that provides insights in the design of high performance BaTiO₃-based piezoelectrics

3:50 PM

(MCARE-S3-009-2016) Poling path in doped potassium sodium niobate

P. Vilarinho^{*1}; R. Pinho¹; M. Costa¹; 1. University of Aveiro, Portugal

Potassium sodium niobate (KNN) is one of the most promising lead-free systems. To maximize the piezoelectric properties of piezoceramics the alignment of ferroelectric domains is required via a poling process. In this work, the effect of the poling path on the dielectric, piezoelectric and ferroelectric properties, of (K_{0.49}Na_{0.49}Li_{0.02})(Nb_{0.985}Cu_{0.015})O₃ (KNNLC) is presented and discussed. Our results show that: i) the dielectric constant at room temperature increases from 179 for unpoled KNNLC ceramics to 234 for poled ones (40 kV per cm, 100 degrees C and 30 min); ii) the Curie temperature do not change after poling (T_C = 396 degree C); iii) the piezoelectric coefficient increases ~ 40% from d₃₃ = 56 pC per N to d₃₃ = 91 pC per N with poling temperature; iv) P_r increases from 2.6 μC per cm² to 18.2 μC per cm², for unpoled KNNLC ceramics and KNNLC ceramics poled at 40 kV per cm, 30 min and 100 degree C, respectively and v) the pinched ferroelectric loops of unpoled KNNLC ceramics disappear after poling at 100 degree C. The mechanism behind the relations of poling path and the defect structure of doped KNN is presented.

4:10 PM

(MCARE-S3-010-2016) Structure and electromechanical Properties of Li and Nb Co-doped BNT-BZ Ceramics

A. Hussain^{*1}; A. Maqbool¹; R. Malik¹; J. Lee¹; T. Song¹; W. Kim¹; M. Kim¹; 1. Changwon National University, Republic of Korea

In this work, lead-free bulk 0.95[Bi_{0.5}Na_(0.5-x)Li_xTi_(1-y)Nb_yO₃]-0.05BaZrO₃ (BNLTN-BZ, with x, y = 0-0.03) ceramics were prepared by a conventional solid-state reaction method. The effect of Li and Nb co-doping on the crystal structure, microstructure, dielectric, ferroelectric and electric field induced strain behavior of BNT-BZ ceramic was investigated. X-ray diffraction patterns revealed the formation of single phase perovskite structure in the studied composition range. However, with increasing co-doping in the Li and Nb concentration, the maximum dielectric constant decreased and the dielectric maximum temperature (T_m) shifted towards lower temperature. The field induced strain response of BNLTN-BZ increases from 0.18% for x, y = 0 to 0.38% for x, y = 0.01, at an applied field of 7 kV/mm. The corresponding dynamic piezoelectric coefficient for these composition were (S_{max}/E_{max} = 257 pm/V) and (S_{max}/E_{max} = 542 pm/V), respectively. These results suggest that the BNLTN-BZ ceramic can be considered as a promising candidate material for piezoelectric application.

4:30 PM

(MCARE-S3-011-2016) Intrinsic magnetodielectric coupling in Fe and Fe-Nb substituted BaTiO₃ ceramics

S. Balasubramanian^{*1}; E. Rubavathi¹; V. Lakshmanan¹; 1. Manonmaniam Sundaranar University, India

Multiferroic materials offer potential applications in energy harvesting technology components such as transducers, transformers and power amplifiers. Magnetism successfully imposed on lead-free perovskite ferroelectric materials which provide a way to increase cross-coupling coefficients as against leaky single-phase natural multiferroic materials. Transition metal substituted BaTiO₃ exhibits coexistence of polarisation and magnetisation. Present work focus on magnetodielectric (MD) measurements on Fe (x = 0, 0.05 and x=0.1) and Fe & Nb (x = 0, 0.05 and x=0.1) substituted BaTiO₃. Fe substitution leads to oxygen vacancies which stabilise

hexagonal and tetragonal structures whereas charge-compensated Fe-Nb substitution leads to cubic phase at higher mole fractions. Density, lattice parameter and phase volume fractions are calculated for all mole fractions. Both the substitutions lead to leaky P-E loops and saturated M-H loops and remnant polarisation and magnetisation decreases. MD measurements were carried out as a function of frequency (10^{-1} to 10^6 Hz) and magnetic field (0 – 1 Tesla). Parallel and perpendicular geometry of **E** and **H** showed no variation. Extrinsic contribution occurs up to 10 kHz. Large intrinsic MD constant of 3.7% is measured for Fe substitution while that of Fe-Nb substituted is 6%. Large dc magnetoresistance confirms extrinsic contribution to MD constant.

Nanoscale Systems

Room: Salon F

Session Chair: Jacob Jones, North Carolina State University

4:50 PM

(MCARE-S3-012-2016) Impedance analysis and modulus spectroscopy of Fe (III) containing strontium stannate nanoparticles

A. Kumar^{*1}; 1. National Institute of Technology (NIT), Kurukshetra, India

We report the sol-gel synthesis of pristine and Fe containing perovskite strontium stannate nanoparticles, stabilized by cetyl trimethyl ammonium bromide (CTAB). X-ray diffraction data and selected area diffraction (SAED) patterns of pristine and Fe doped strontium stannate nanoparticles reveal the formation of orthorhombic phase with pbnm space symmetry. The high resolution transmission electron microscopic data shows the formation of nanoparticles having particle size of 20 nm. Raman spectra of pristine and Fe doped strontium stannate nanoparticles depict the peaks at 220, 256, 306, 404, 452 and 561 cm^{-1} corresponding to Sn-O and O-Sn-O stretching. The band gap values of strontium stannate nanoparticles were found to decrease with increase in the Fe content, due to the Fe³⁺ induced defect levels near the conduction band. The photoluminescence spectra confirm the red shift of band emission peak centered 370 nm. The dc resistivity of pristine and Fe doped SrSnO₃ is found to decrease with increase in Fe concentration. The variation of impedance (Z and Z''), conductivity and electric modulus (M and M'') of pristine and Fe doped strontium stannate nanoparticles as a function of frequency (20 Hz to 2 MHz) at different temperatures (310-410 K) has been studied.

5:10 PM

(MCARE-S3-013-2016) Strain engineering in ferroelectric multilayers and superlattices

Y. Yuzyuk^{*1}; R. Shakhovoy¹; V. Shirokov²; J. Belhadi³; M. El Marssi³; 1. Southern Federal University, Russian Federation; 2. Southern Scientific Center RAS, Russian Federation; 3. Université de Picardie Jules Verne, France

Two sets of symmetric ferroelectric/paraelectric $[\text{BaTiO}_3]_{(1-x)\Lambda}/[\text{BaZrO}_3]_{x\Lambda}$ superlattices (SL) with different modulation periods Λ , and asymmetric SLs with varied composition $15 \leq x \leq 0.85$ and fixed modulation period Λ were epitaxially grown by PLD on MgO substrates and were studied by means of x-ray diffraction and a Raman spectroscopy. We showed that the large strain in SLs induced ferroelectricity in BaZrO₃ (BZ) layers with polar axis normal to the substrate, while BaTiO₃ (BT) layers exhibit in-plane polar orientation. XRD and Raman spectroscopy revealed lattice distortions due to the misfit strain generated by the large lattice mismatch between the alternating BZ and BT layers. This strain is responsible for the significant upward frequency shift of the $E(\text{TO})$ soft mode. The temperature-dependent Raman spectra revealed giant shift of the ferroelectric phase transition up to 723 K in asymmetric SLs. The experimental results corroborate with the “temperature-misfit strain” phase diagram, constructed using a phenomenological approach. The temperature of the ferroelectric phase transition in

the BT/BZ superlattices depends on the distortion of the BT layers, which can be tuned by varying the periodicity in the SL or by changing the volume fraction of the BT layers at a fixed periodicity. We demonstrate the route of strain engineering in SLs with a stable ferroelectric phase in the desired temperature range.

S8: Self-Power Generators

Piezoelectric Self-Power Generators I

Room: Salon G

Session Chair: Sang-Woo Kim, Sungkyunkwan University

1:30 PM

(MCARE-S8-001-2016) Piezotronics in 2D materials (Invited)

W. Wu^{*1}; 1. Purdue University, USA

Monolayer MoS₂ and other TMDCs have been theoretically predicted to exhibit piezoelectricity due to the strain induced lattice distortion and associated ion charge polarization, suggesting possible applications of these 2D nanomaterials in nano-scale electromechanical devices that take advantage of their outstanding semiconducting and mechanical properties. Recently, the first experimental observation of piezoelectricity in single atomic layer 2D MoS₂ and its application in mechanical energy harvesting and piezotronic sensing was demonstrated. Cyclic stretching and releasing of odd-layer MoS₂ flakes produces oscillating electrical outputs, which converts mechanical energy into electricity. More significantly, transport measurements show a strong piezotronic effect in single-layer MoS₂, but not in bilayer and bulk MoS₂. The coupling between piezoelectricity and semiconducting properties in two-dimensional nanomaterials may enable the development of applications in powering nanodevices, adaptive bioprobes and tunable/stretchable electronics/optoelectronics. **Acknowledgments** The author is grateful to Prof. Zhong Lin Wang and sincerely thanks Prof. Wang and his group at Georgia Tech for their generous support and significant contributions to the work presented here. The author gratefully thanks the College of Engineering and School of Industrial Engineering at Purdue for the start-up support.

2:10 PM

(MCARE-S8-002-2016) Structural Approaches for Enhancing Output Power of Piezoelectric PVDF Generator (Invited)

W. Jung^{*}; C. Kang^{*1}; 1. Korea Institute of Science and Technology, Republic of Korea

Flexible piezoelectric generators have attracted great attention in recent years for their possible applications in mechanical energy scavenging devices because of portable, wearable, and implantable electronics. Key issues for realizing a flexible piezoelectric generator contain the insufficient output power generation and the poor efficiency at the low-frequency. Here we proposed new concepts of the structural approaches to enhance output power of the flexible piezoelectric generator using Polyvinylidene fluoride (PVDF): use of a substrate, curved structure, and optimization of aspect ratio of the generator for maximizing output power density. Through these approaches induced stress and output voltage of the generator are analysed by FEM modelling and demonstrated them by experiments. Considering these results for the optimization of the generator we fabricated a multi-layered flexible curved generator, which produces ~200V of the peak output voltage and ~2.7 mA of the peak output current. The output power density of the generator reaches ~17 mW/cm^2 , which is enable to powerfully drive various commercial electronics as a power source. Furthermore, it successfully demonstrated this power source can light up 952 LED bulbs. This conceptual technology will open a new avenue for realization of self-powered systems such as portable and wearable electronics.

Piezoelectric Self-Power Generators II

Room: Salon G

Session Chairs: Christian Falconi, University of Rome Tor Vergata;
Chong-Yun Kang, Korea Institute of Science and Technology

3:20 PM

(MCARE-S8-003-2016) Soft Piezoelectric MEMS Technologies for Flow Energy Harvesting (Invited)

M. De Vittorio^{*1}; 1. Istituto Italiano di Tecnologia, Italy

While wind and fluid flow represent some of the most attractive renewable energy sources, wind turbines technologies exhibit major drawbacks in terms of visual, noise and environmental impact and cut-in wind speed higher than 3 m s⁻¹. In this presentation it will be shown that small flags, made by piezoelectric thin film on flexible polymers and whose shape resembles the dry leaves of trees, can efficiently act as harvesters of energy at extremely low wind or flow speed, such as from a gentle blow or breath. Piezoelectricity on flexible polymers is achieved by depositing a thin film of piezoelectric aluminium nitride (AlN), sandwiched between metal electrodes and deposited on Kapton substrates with columnar grains coherent through the polycrystalline layers. The prototype flags have a natural curling due to the release of the residual stress of the layers. While the curling is essential for the activation of the maximum flag oscillation, this system is so elastic and light that oscillations start at a cut-in flow speed of 0.1 m s⁻¹. Starting from tens of mVs, the voltage increases above 1 V when the flag is flattened and parallel to the fluid flow lines, with a generated power of mWs cm⁻³. It will also be shown that the same technology, by virtue of its soft and conformable structure can act as a piezoelectric skin or wearable device, scavenging electrical energy from human motion.

4:00 PM

(MCARE-S8-004-2016) Stretchable and Flexible Nanogenerators for Piezoelectric Energy Harvesting (Invited)

I. R. Voiculescu^{*1}; 1. City College of New York, USA

This is an invited presentation that will cover current research in the area of stretchable and flexible nanogenerators for piezoelectric energy harvesting. Using piezoelectric materials for mechanical energy harvesting has received attention because of the direct conversions process and the feasibility for integrated applications. Traditionally, PZT has been the material used for mechanical energy harvesting. Nevertheless, the brittle nature of PZT ceramic gives rise to issues such as reliability, and durability for long-term sustainable operations. Recently, several groups have demonstrated flexible PZT ribbon based generator for mechanical energy harvesting, which shows highly improved mechanical properties compared to bulk thin-films due to reduced dimensions. The author will present current research developed by several scientists in the area of stretchable and flexible nanogenerators. Piezoelectric devices fabricated from ZnO and PZT nanoribbons with different configurations will be discussed. Different stretchable and flexible nanogenerators based on ZnO nanowires will be also discussed. A flexible and implantable nanogenerator fabricated from PZT nanoribbons, intended to harvest energy from the motions of the heart, lung or diaphragm will be also presented. Piezoelectric materials are the ideal components for energy harvesting devices used for powering implantable devices.

4:40 PM

(MCARE-S8-005-2016) Key Material and System Parameters in Piezoelectric Vibration Energy Harvesting (Invited)

M. Kim^{*1}; 1. Korea Research Institute of Standards and Science, Republic of Korea

Piezoelectric vibration energy harvesters (PVEHs) at multi-scales have received considerable attention as an enabling technology for self-powered electronic devices. A key challenge has been insufficient power and voltage generation for practical applications,

which necessitates creative and disruptive materials and structure design at various scales. With this purpose in mind, key material and system parameters that affect the PVEH performance metrics are thoroughly identified through a systematic sensitivity analysis. This helps construction of both design and testing parameters, allowing us to achieve optimal device design with enhanced PVEH performance. Furthermore, study on the correlation of material and system parameters contributes to knowledge for fundamental understanding of conversion mechanisms in PVEH systems, which in turn provides guidelines of optimal parameter tuning to maximize the performance of the given device.

S10: Batteries and Energy Storage

Lithium Batteries

Room: Salon E

Session Chairs: Dany Carlier, ICMB-CNRS; Partha Mukherjee, Texas A&M University

1:30 PM

(MCARE-S10-004-2016) An active Rock Salt compound for high energy density Li-ion batteries (Invited)

V. Pralong^{*1}; M. Freire¹; A. Maignan¹; C. Jordy²; D. Chateigner¹; N. Kosova³; O. Lebedev¹; 1. CNRS ENSICAEN, France; 2. SAFT, France; 3. Academy of sciences, Russian Federation

The design of new materials that provide high energy densities and long cycle life together with being economic and environmental benign is crucial for the energy storage. Therefore, the soft chemistry used to prepare the original frameworks, new structures is in perfect appropriateness with such a target. We will discuss our strategies to generate original framework showing ionic conductivity. Our approach is based on topotactic reactions starting from existing ionic conductors with a compact anionic framework. We will show that the lithium/sodium insertion leads to new rock salt type structure. The examples will be based on vanadium, titanium, molybdenum and manganese type oxides. Regarding the latter one, we will report for the first time the synthesis, structural and electrochemical characterizations of a new non-lamellar oxide based on manganese oxide with the highest capacity observed ever before in the Li-Mn-O system. This new patented material with a disordered rock salt structure shows a discharge capacity of 300 mAh/g. The structure-properties relationships are studied and the possibility to use these materials as electrode materials for power generation systems is discussed.

2:10 PM

(MCARE-S10-005-2016) Design architecture of high energy density low tortuosity battery electrode (Invited)

M. R. Amin^{*1}; 1. Qatar Environment and Energy Institute, Hamad Bin Khalifa University, Qatar Foundation Qatar, Doha, Qatar

The high battery price and safety issues are major concern for available use of electric vehicle (EV). An EV battery based on the best Li-ion cells cannot reach an energy density higher than 150–200 Wh kg⁻¹. On the other hand high inactive materials content of current nonaqueous battery designs contributes directly to high battery cost and reduces specific energy and energy density. Area specific capacity, which is perhaps the most objective measure of design performance, cannot be increased arbitrarily by increasing electrode thickness and/or density, due to kinetic limitations. Thus, higher usable energy at practical C-rates can be achieved from thick, dense electrodes if the topology of the pore structure is tailored to lower tortuosity. Here we report on the fabrication and electrochemical testing of thick, dense, low tortuosity electrodes by the freeze-casting of aqueous suspensions followed by drying/sintering. This shaping technique allows design of oriented and interconnected structures that have a low tortuosity and high ionic transport. The

electrochemical performance of the fabricated electrodes in half cells exhibits high areal capacity. The hybrid pulse power characterization (HPPC) and dynamic stressed test (DST) were performed. We also report on the characterization of electronic and ionic conductivity in several candidate cathodes as a function of temperature and lithium content.

2:50 PM

(MCARE-S10-006-2016) Kinetic Study of Parasitic Reactions in Lithium-Ion Batteries: A Case Study on $\text{LiNi}_{0.6}\text{Mn}_{0.2}\text{Co}_{0.2}\text{O}_2$

X. Zeng^{*1}; Y. Li¹; K. Amine¹; Z. Chen¹; 1. Argonne National Lab, USA

The global R&D effort has been driven by the growing application of high energy-density lithium-ion batteries to electrify the transportation system and achieve significant reduction on non-renewable fuels consumption and greenhouse gas emission. However, high initial energy-density still generally be obtained with the price of a reduction on battery safety and life, both of which are fundamentally connected to the parasitic reactions between the active electrode materials and the non-aqueous electrolyte at various temperatures. A fundamental study of parasitic reactions can not only help to select a proper improving strategy, but also substantially shorten the electrochemical validating process. A home-built high-precision leakage current measuring system was deployed to investigate the parasitic reaction kinetics between $\text{LiNi}_{0.6}\text{Mn}_{0.2}\text{Co}_{0.2}\text{O}_2$ and conventional carbonate electrolyte. The parasitic reaction rate was found strongly dependent on the cathode upper cutoff potential. The kinetic data also indicated a significant change of reaction mode at ~ 4.5 V vs. Li^+/Li . It demonstrated that the kinetic study could be crucial in developing advanced electrode materials with a fundamental balance between energy density and battery life.

3:10 PM

(MCARE-S10-007-2016) Combustion-Mediated Route for Hollow Carbon Nanospheres with Excellent Electrochemical Properties

H. Nersisyan^{*1}; C. Kim¹; J. Lee¹; 1. Chungnam national University, Republic of Korea

We have developed the combustion synthesis of hollow carbon nanospheres based on metathesis (exchange) reaction between sodium azide and halogen polymer (polyvinylchloride- $(\text{CH}_2\text{-CHCl})_n$ or polytetrafluoroethylene- $(\text{C}_2\text{F}_4)_n$). The metathesis reaction was driven by thermal heat from the exothermic recombination of Na^+ and Cl^- ions or Na^+ and F^- ions into NaCl or NaF salt. Thermocouple measurements indicated that reaction temperatures of 1320 and 1750 °C were reached using $(\text{CH}_2\text{-CHCl})_n$ and $(\text{C}_2\text{F}_4)_n$ polymers, respectively. The FESEM analysis indicated the self-templated formation of core-shell nanostructures, where the core is sodium salt (NaCl or NaF) nanoparticles and the shell is carbon. Hollow carbon nanospheres were successfully prepared after water purification of the reaction product. By virtue of the structural advantages, the hollow carbon spheres had excellent electrochemical properties for use as a potential anode material for lithium-ion batteries, including high capacity, remarkable cyclability, and superior rate capability.

3:30 PM

(MCARE-S10-008-2016) Development of novel electrolyte additives for designed surface modification (Invited)

B. Lucht^{*1}; 1. University of Rhode Island, USA

An investigation of the effect of electrolyte on performance of in lithium ion batteries will be presented. The electrochemical performance of common electrolyte formulations will be discussed along with detailed ex-situ surface analysis of the cycled electrodes. The ex-situ analysis allows the development of an understanding of the role of the electrolyte and common additives in the structure of interfacial electrode films on both the anode (solid electrolyte interphase, SEI) and on the cathode. Correlation of the structure of the surface films with the performance limiting reactions in lithium ion batteries affords insight into the mechanism of interfacial film formation and

function. The mechanistic insight is used to systematically develop novel additives designed for specific electrode surface modification to afford optimized electrochemical performance. The electrochemical performance and ex-situ surface analysis of electrodes cycled with novel Additives for Designed Surface Modification (ADSM) will be presented.

4:10 PM

(MCARE-S10-009-2016) Possible applications of new tailored electrolytes in different types of modern batteries (Invited)

M. Marcinek^{*1}; L. Niedzicki¹; A. Bitner¹; P. Wiczorek¹; T. Trzeciak¹; M. Kalita¹; M. Dranka¹; Z. Zukowska¹; M. A. Muñoz-Márquez²; W. Wiczorek¹; 1. Warsaw University of Technology, Poland; 2. CIC Energigune, Spain

Market development of mobile devices, EVs and power plants requires a constant need for energy storage systems with better performance, low cost, safer and environmental friendly. New positive/negative electrode materials are designed and studied in many university and industrial laboratories which sometimes do not work well with commercially available electrolytes. In this lecture we present lines of new lithium electrolytes and their sodium analogues as an alternative candidates for battery components based on the concept of tailoring new salts having relatively large anions with delocalized charge. New salts can be used in liquid as well as polymeric electrolytes based on low/ high molecular weight systems. They exhibit limitations in the formation of nonconductive ionic associates and in turn the improvement in the conductivity and cation transference numbers. The lecture will be illustrated by examples of application of newly designed electrolytes in preliminary cells with novel electrode materials and discussion on possible extension of its use in sodium or sulphur systems. Acknowledgements: Some of the experiments were financed by Sirbatt and EuroLiion FP7 European Projects.

4:50 PM

(MCARE-S10-010-2016) Chemical and Thermal Control of Interfacial Stability in Lithium-ion Battery Electrodes (Invited)

C. T. Love^{*1}; C. R. Becker²; S. M. Prokes¹; 1. U.S. Naval Research Laboratory, USA; 2. U.S. Army Research Laboratory, USA

The performance and safety of energy storage devices are controlled by the efficiency and stability of the processes occurring at the electrode/electrolyte interfaces. In this talk we discuss how the anode surface chemistry present locally at the electrode/electrolyte interface influences the long-term cycling performance of silicon anode materials as well as how environmental aspects, such as temperature, slow mass transport through liquid electrolytes leading to lithium plating and dendrite formation on anode surface. Specifically, we utilize in-situ optical microscopy to image the nucleation and growth of detrimental lithium dendrites on the surface of graphite anodes at low temperature; and in-situ atomic force microscopy to understand the role of nanoscale atomic layer deposition of Al_2O_3 coatings on nanostructured silicon materials to mitigate deleterious surface reactions affecting electrochemical performance. The results offer new insights into the mechanisms responsible for increased electrochemical performance with chemical control of the interface as well as suggest thermal boundaries for the safe recharge of lithium-ion batteries.

5:30 PM

(MCARE-S10-011-2016) Fabrication and Characterization of $\text{LiFePO}_x\text{N}_y$ Thin Film Cathodes for Lithium Ion Batteries

K. Chiu^{*1}; 1. Feng Chia University, Taiwan

Nitrogen doping into LiFePO_4 were studied by many researchers using molecular modeling. Theoretically, the nitrogen doped $\text{LiFePO}_x\text{N}_y$ would show lower electrical resistivity as well as higher ionic conductivity. However, the modeled results have not been proved experimentally. There is no report on the real synthesis and

systematical analysis of such material. The current study reveals fabrication and characterization of $\text{LiFePO}_x\text{N}_y$. $\text{LiFePO}_x\text{N}_y$ films were deposited under various N_2/Ar flow ratios. No carbon additives were added. The amounts of nitrogen doping increased with the N_2/Ar flow ratios. Enhanced LiO_6N vibration signals were recorded by Fourier transform infrared spectroscopy. The binding energy bands of different coordinated N-P bonds were found and characterized by X-ray photoelectron spectroscopy (XPS). The crystal lattice distortion or defects in Li-O and Fe-O sites were also characterized. It has been found that nitrogen doping has elevated the conductivity to $10^4 \text{ S}\cdot\text{cm}^{-1}$. Charge-discharge and cyclic voltammetry curves revealed a reversible capacity of $140 \text{ mAh}\cdot\text{g}^{-1}$ at 0.2 C. The $\text{LiFePO}_x\text{N}_y$ films were charged-discharged for 100 cycles at 1C, and capacity retention of 97 % has been achieved.

Tuesday, April 19, 2016

Plenary Session II

Room: Salon E

8:30 AM

(MCARE-PL-002-2016) Perovskite solar cells: A new paradigm in Energy sector

M. Nazeeruddin^{*1}; 1. EPFL, Switzerland

Methylammonium lead triiodide perovskite solar cells have emerged as credible contenders to conventional p-n junction photovoltaic devices. Perovskite material involves low cost precursors, capable of being processed via a variety of scalable methods and deliver high power conversion efficiencies comparable to thin film and crystalline silicon solar cells. Using $\text{CH}_3\text{NH}_3\text{PbI}_3$ perovskite as an absorber layer and molecularly engineered functional hole transport material, power conversion efficiencies (PCE) over 20% were obtained. However, a fundamental understanding of the working principle of perovskite solar cells, and stability of the material is still lacking. In addition, an anomalous hysteresis behavior in the current-voltage characteristics is often reported in perovskite solar cells possibly related to ion migration and imbalanced extraction of charges. In this talk we present various deposition methods for perovskite absorbing layer, and the synthesis and characterization of novel hole transporting materials to address the stability and hysteresis behavior.

Nazeeruddin has been named Thomson Reuters "Highly Cited Researcher" and one of the 19 scientists identified by Thomson Reuters as The World's Most Influential Scientific Minds 2015 from all scientific domains.

S2: Spectral Conversion Materials for Energy Applications

Spectral Conversion for Photo-catalytic and Water-splitting Applications

Room: Salon D

Session Chairs: Eva Hemmer, INRS; Marta Quintanilla, CIC BiomaGUNE

9:50 AM

(MCARE-S2-009-2016) Turning the sun into blue: enhancing photocatalytic activity by high effective NIR to UV-blue up-conversion with rare-earth doped materials (Invited)

J. Méndez-Ramos^{*1}; L. Wondraczek²; N. Khaidukov³; P. Acosta-Mora¹; J. Ruiz-Morales¹; M. Borges¹; M. Sierra¹; P. Esparza¹; 1. Universidad de La Laguna, Spain; 2. University of Jena, Germany; 3. N.S. Kurnakov Institute of General and Inorganic Chemistry RAS, Russian Federation

Here we explore the ground-breaking photonic approach for enhancing photocatalytic activity through solar energy harvesting,

which bases on up-conversion luminescence processes in rare-earth (RE) doped materials in order to satisfy large band-gap requirements of main water-splitting semiconductor electrodes by transforming unused long-wavelength solar radiation into useful UV-blue light, aimed at increasing the efficiency in solar-driven H_2 generation, solar fuels, CO_2 storage and fine chemicals production. Thus we have synthesized and comparatively studied a series of RE-doped luminescent materials including: fluoride ZBLAN glasses, nano-glass-ceramics, nano-particles, hydrothermal KYF_4 and K_2YF_5 crystals and novel organic resins, for an endless range of technological applications in coatings targeted to module-scale solar-chemical energy harvesting devices. Our approach focuses on optimizing the incident radiation, turning sunlight into blue. Up-conversion wavelength *SHIFT happens*, there is *plenty of energy at the bottom*. We envisage a semi-industrial exploitation for sustainable H_2 production by means of solar seawater splitting within the existing traditional solar salt flats, as a system of shallow seawater pools operating like slurry-type photo-reactors, available in Canary Islands, ideal host territory for a renewal energy community.

10:30 AM

(MCARE-S2-010-2016) To what extent the plasmonic enhancement is effective in photocatalysis?

J. Augustynski^{*1}; R. Solarska¹; K. Bienkowski¹; 1. CeNT, UW, Poland

Implementation of various plasmonic metallic nanostructures, most frequently including gold or silver nanoparticles to enhance light absorption either in photocatalytic or in photo-electrochemical systems is receiving recently a broad attention. Strong localized electromagnetic fields induced by irradiated metallic nanostructures, deposited at the surface of semiconductors, lead, in particular, to greatly enhanced optical absorption and electron-hole generation reported both for the photocatalysts and photoelectrodes. Although a large number of reports show an extension of photo-activity of photocatalyst, such as e.g. TiO_2 , to over band-gap frequencies, attributed to hot electron injection into the semiconductor with the formation of holes in the metal particles, the evoked mechanism remains unclear. On the other hand, overlapping between the semiconductor and the metal particles absorbance does lead to large enhancement of the photocurrents due to localized electromagnetic field effect, as observed for water splitting at hybrid Au/WO_3 or Ag/WO_3 photoanodes.

10:50 AM

(MCARE-S2-011-2016) Heterojunction Metastructured Film of $\text{TiO}_2/\text{Cu}_2\text{O}$ with Enhanced Photoelectrochemical property and Photoelectrocatalytic Activity

J. Lee^{*1}; H. Kim¹; J. Park¹; J. Baik¹; 1. Ulsan National Institute of Science and Technology, Republic of Korea

p-n heterostructure design based on $\text{Cu}_2\text{O}/\text{TiO}_2$ film for enhanced photoelectrochemical and photoelectrocatalytic activities is reported, which mainly consists of four layers of Au film, TiO_2 film, Cu_2O film, and Au NPs. p-type Cu_2O film and n-type TiO_2 film are produced by using electrodeposition and atomic layer deposition. The Cu_2O film formed by electrodeposition was obtained high carrier concentration, which resulted in large internal electric field between Cu_2O and TiO_2 interface. Thus, photo-generated charge carriers were efficiently led to charge separation. The Au NPs/ $\text{Cu}_2\text{O}/\text{TiO}_2/\text{Au}$ film shows a remarkable enhancement in the photocurrent density in the UV-visible region, compared with bare TiO_2 film. Metal-hetero junction structure effectively absorbed visible light by the surface plasmon resonance and efficiently separated electron-hole pairs in the photoelectrode.

Plasmonic /Photonic Manipulation of Conversion Processes

Room: Salon D

Session Chairs: Eva Hemmer, INRS; Marta Quintanilla, CIC BiomaGUNE

11:10 AM

(MCARE-S2-012-2016) Photonic fiber arrays for light trapping in thin film photovoltaic cells (Invited)

J. Martorell^{*1}; 1. ICFO-The Institute of Photonic Sciences, Spain

Research in thin film solar cells triggered when it was proposed as a low cost alternative to the silicon based PV technology. However, the low material crystallinity in the majority of thin film cells combined with extremely thin active layers prevents in many cases an efficient sunlight harvesting as well as stable cell operation. To obtain the maximum possible light harvesting efficiency in in such thin film devices, light incidence must be achieved simultaneously to light trapping in an orthogonal direction. Indeed the most effective sunlight harvesting would require a bending of the incident light propagation path followed by a trapping within the active material layer. In here, I will consider configurations to effectively reach such, to some extend contradictory, behavior for the light propagation. Special attention will be given to light harvesting and photovoltaic performance of thin film solar cells deposited on the back side of Photonic Fiber Plate. In such periodically ordered system an ergodic light propagation resulting from a chaotic photon trajectory is achieved when the adjacent fibers are interpenetrated. Finally, prospects for a stable operation in thin film organic solar cells will be discussed.

11:50 AM

(MCARE-S2-013-2016) Spectral concentration assisted by photonic crystals for upconversion in silicon solar cells

J. Marques-Hueso^{*1}; R. Peretti²; R. Abargues³; B. Richards⁴; C. Seassal⁵; J. Martinez-Pastor³; 1. Heriot-Watt University, United Kingdom; 2. ETH, Switzerland; 3. University of Valencia, Spain; 4. KIT, Germany; 5. Ecole Centrale de Lyon, France

A challenge for the implementation of up-converters into silicon solar cells is the limited absorption bandwidth of conventional erbium-doped materials, which is usually extended from 1470 to 1580 nm. This accounts for 24.5 W m^{-2} . This could ideally be increased up to 87.7 W m^{-2} via spectral concentration, which in turn could increase the upconversion efficiency by a maximal factor 13 due to its non-linear nature. Infrared luminescent down-shifters, such as quantum dots, could increase the amount of available energy for the upconverter. However, it is difficult to tailor the absorption and emission of the quantum emitters. This work researches the use of photonic crystals for reshaping the emission spectrum of the quantum dots (QD) to thus achieve a better match with the absorbance of the erbium. This strategy has allowed a spectral concentration of the QD emission of 67%, an increase of the match of the QD emission and the erbium absorption of 158%, and a vertical emission enhancement of nearly a factor 7. These results suggest that spectral concentration is a technique that has scope to be significantly improved and provide a large energy gain for UC photovoltaics.

S3: Ferroelectrics and Multiferroics for Energy Applications

Composite Ferroelectrics and Multiferroics

Room: Salon F

Session Chair: Jonathan Spanier, Drexel University

9:50 AM

(MCARE-S3-014-2016) All-oxide composites by Spark Plasma Sintering: a flexible approach towards giant dielectric properties (Invited)

C. Elissalde^{*1}; M. Albino²; U. Chung¹; J. Lesueur¹; B. Dominique¹; S. Mornet¹; C. Estournès³; M. Maglione³; 1. ICMCB-CNRS, France; 2. Université du Maine, France; 3. CIRIMAT, France

Integration for electronics and high density storage applications raise a growing interest towards materials exhibiting colossal dielectric permittivity and moderate dielectric losses. Such properties were recently reported in (Nb+In) co-doped TiO₂ ceramics and ascribed to defects engineering. Charged interfaces in ferroelectric materials play also a central role in raising artificially the dielectric parameters towards huge ranges. Focusing on BaTiO₃ ceramics, giant parameters can be obtained by appropriate substitutions or decreasing grain size using fast sintering process such as Spark Plasma Sintering. In all cases giant effective dielectric properties are related to the localization of free electronic charges at interfaces. An accurate control of properties requires to fix the reduction level of titanium due to high density of oxygen vacancies. Our strategy lies in the elaboration by SPS of all-oxide composites (Ba_xSr_{1-x}TiO₃ combined with SiO₂, TiO₂, ZrO₂) with different architectures (core@shell, multilayer, random 3D mixing). We took advantage of the SPS capabilities in terms of short sintering cycles and current effects to elaborate dense composites with adjustable dielectric properties. The specific SPS conditions enable the control of both the interface between the two components and the reduction level leading to interface-driven dielectric properties.

10:30 AM

(MCARE-S3-015-2016) Magnetoelectric coupling in complex microstructures (Invited)

D. C. Lupascu^{*1}; S. V. Vladimir¹; M. Etier¹; H. Trivedi¹; H. Wende¹; S. Salamon¹; J. Landers¹; M. Labusch¹; J. Schröder¹; 1. University of Duisburg-Essen, Germany

Composites are able to provide the highest magnetoelectric coupling coefficients known. This is due to the much higher piezoelectric and magnetostrictive effects in single phases compared to coupled effects in intrinsic multiferroics. Many systems rely on mechanical coupling at the interface. In this contribution we will outline the effect of complex microstructures on the effective coupling coefficients. Particular attention will be devoted to the differences between 2-2, 1-3 and 0-3 connectivities. In the different cases the experimental determination of the direct and converse coupling coefficients may yield significantly different results. We will explain these effects in the context of a thermodynamic analysis and the assignment of the correct conversion between these coefficients in the context of dielectric constant and partial conductivity. The importance of differences of the coupling at the microstructure level will be analyzed using piezoforce microscopic experiments and FEM modelling. Support through DFG in the Forschergruppe 1509 and the EU in the FP7 Marie Curie Initial Training Network "Nanomotion" (grant agreement no. 290158) are acknowledged.

11:00 AM

(MCARE-S3-016-2016) Tuning Functionalities in Ferroic Nanocomposite Thin Films (Invited)

A. Chen^{*1}; E. Enriquez¹; A. Eshghinejad²; W. Zhang³; S. Lee⁴; J. Li²; H. Wang³; J. MacManus-Driscoll³; M. Fitzsimmons³; Q. Jia¹; 1. Los Alamos National Lab, USA; 2. University of Washington, USA; 3. Texas A&M University, USA; 4. University of Cambridge, United Kingdom

Owing to the unique interface coupling and vertical interfacial strain, vertical heteroepitaxial nanocomposite films can be used to design enhanced and/or novel functionalities. In this presentation, we will discuss our efforts to design, synthesize and characterize a variety of epitaxial nanocomposite thin films in both lateral and vertical fashions. Using controlled synthesis and advanced probing techniques, we are able to manipulate the nanoscale thin films growth and understand the underlying physics of the emergent phenomena at heterointerfaces. For example, we observed induced interface magnetism in BiFeO₃ (BFO) layer in the La_{0.7}Sr_{0.3}MnO₃/BiFeO₃ superlattices. In addition, we will use vertically aligned epitaxial nanocomposites (such as La_{0.7}Sr_{0.3}MnO₃:ZnO, BaTiO₃:CoFe₂O₄, etc) to illustrate the effect of interface/strain on the functionalities including magnetoresistance and magnetoelectric coupling. The interface and strain are key factors to tune functionalities in nanocomposite thin films.

11:30 AM

(MCARE-S3-017-2016) Nanocomposite Thin Films to Achieve High Magnetoelectric Coupling

M. Jain^{*1}; 1. University of Connecticut, USA

Solution synthesis methods allow low-cost and large area fabrication of thin films, nanoparticles, and biphasic nanocomposites of many functional and multifunctional materials. Magnetoelectric (ME) multiferroic material, which exhibit some magnetic and electric orders, are of great interest for memory and sensing applications. In biphasic nanocomposites, concentration and connectivity of the two phases play an important role in defining their physical properties. In this talk, structural, microstructural, ferroelectric and magnetoelectric properties of biphasic ME multiferroic nanocomposite films will be presented. For magnetic phase, CoFe₂O₄ nanoparticles or nanophase were incorporated in the piezoelectric PbZr_{0.52}Ti_{0.48}O₃ matrix in order to observe the ME coupling that is mediated through mechanical strain at the interfaces between the two phases. The results with a couple of concentrations will be presented in details.

11:50 AM

(MCARE-S3-018-2016) Characterization of (PZT) [PbZr_{0.52}Ti_{0.48}O₃]-epoxy-multi-walled carbon nanotube (MWCNT) composite piezoelectric films

S. Banerjee^{*1}; K. Cook-Chennault²; 1. California State University, Fresno, USA; 2. Rutgers University, USA

Three-phase lead zirconate titanate (PZT) [PbZr_{0.52}Ti_{0.48}O₃]-epoxy-multi-walled carbon nanotube (MWCNT) composite films were prepared, where the volume fraction of PZT was held constant at 30%, while the volume fraction of the MWCNTs was varied from 0.1% - 10%. The samples were poled using either an electrode-contact or contactless (Corona) poling technique. The piezoelectric strain coefficients (d_{33}), dielectric constant (ϵ'), and dielectric loss tangent ($\tan \delta$) of the samples were measured, and compared as a function of poling technique. The highest values for dielectric constant and piezoelectric strain coefficients were 465.82 and 18.87 pC/N for MWCNT volume fractions of 10% and 6% respectively, and were obtained for samples that were poled using the Corona contactless method. The impedance and dielectric spectra of the composites were recorded over a frequency range of 100Hz-20MHz. The fractured surface morphology and distribution of the PZT particles and MWCNTs were observed with the aid of Electron Dispersion Spectroscopy (EDS) and a Scanning Electron Microscope (SEM) which show the inclusions embedded in the Epoxy matrix.

The surface morphology of the MWCNTs was observed with the aid of a field emission Transmission Electron Microscope (TEM).

S8: Self-Power Generators

Nanomaterials for Energy Harvesting

Room: Salon G

Session Chairs: Husam Alshareef, King Abdullah University of Science and Technology; Jeong Min Baik, Ulsan National Institute of Science and Technology

9:50 AM

(MCARE-S8-007-2016) A ferroelectric dipole can influence photochemistry (Invited)

S. Dunn^{*1}; 1. QMUL, United Kingdom

There has been growing interest in the use for non-centrosymmetric systems for energy harvesting applications. These include kinetic to electric and photonic to chemical or electric. To date there has been a focus on using a ferroelectric material as a photocatalyst where the domain structure determines the band structure. We recently showed that the photocatalytic performance of BaTiO₃ can be enhanced to match that of TiO₂ by depositing nanostructured silver. I'll discuss a variety of techniques and mechanisms that indicate the dipole of the ferroelectric has a strong influence on the photochemistry. Using dye degradation, transient absorption spectroscopy and carbon dioxide remediation I'll that carrier dynamics for a range of ferroelectric single crystal substrates are significant to increase performance. By probing BaTiO₃ below and through the Curie temperature we show an influence on dipole on recombination with BaTiO₃ having a carrier lifetime exceeding 1 second at room temperature. This indicates that the dipole has an impact on recombination of photoinduced carriers. This data presenting a thermal trend consistent with changes in the crystal structure and associated changes in remnant polarization will be related to the body of work on ferroelectric materials and highlights the interest in polar systems for photo energy conversion.

10:30 AM

(MCARE-S8-008-2016) Coupling in-situ TEM and ex-situ analysis to understand heterogeneous sodiation of antimony (Invited)

D. Mitlin^{*1}; 1. Clarkson University, USA

We employed an in-situ electrochemical cell in the transmission electron microscope (TEM) together with ex-situ time-of-flight, secondary-ion mass spectrometry (TOF-SIMS) depth profiling, and FIB - helium ion scanning microscope (HIM) imaging to analyze Na storage in Sb thin films. TOF-SIMS analysis indicates that sodiation does not proceed uniformly, leading to local volumetric expansion gradients and major intrinsic stress in the structure. In-situ TEM shows time-dependent buckling and localized separation of the sodiated films from their TiN-Ge nanowire support, which is a mechanism of stress-relaxation. Localized horizontal fracture does not occur directly at the interface, but rather at a short distance away within the bulk of the Sb. HIM images of FIB cross-sections taken from sodiated half-cells, electrically disconnected and aged at room temperature, demonstrate non-uniform film swelling and the onset of analogous through-bulk separation. TOF-SIMS highlights time-dependent segregation of Na within the structure, both to the film-current collector interface and to the film surface where a solid electrolyte interphase (SEI) exists, agreeing with the electrochemical impedance results that show time-dependent increase of the films' charge transfer resistance. We propose that Na segregation serves as a secondary source of stress relief, which occurs over somewhat longer time scales.

11:10 AM

(MCARE-S8-009-2016) Highly Flexible Solar Cells and Light-Emitting Diodes Using Organometal Hybrid Perovskites (Invited)Z. Yu^{*1}; 1. Florida State University, USA

Recently, astounding optoelectronic properties have been discovered in organometal hybrid perovskites, especially in a group of methyl ammonium lead halide compounds. Such materials have a general ABX_3 chemical formula, in which A is a cesium (Cs^+) or an aliphatic ammonium (RNH_3^+) cation, B is a divalent Pb^{2+} or Sn^{2+} cation and X is an anion such as Cl, Br⁻ or I⁻. Their crystal structures resemble the one commonly found in $BaTiO_3$. The hybrid perovskites can be processed like polymeric semiconductor materials using solution processes into large area thin films on arbitrary substrates, meanwhile, they can be crystallized into three-dimensional periodic structures like conventional inorganic semiconductors exhibiting superior charge transportation properties. In this talk, highly flexible solar cells and light-emitting diodes using organometal hybrid perovskites will be discussed. Such devices can be bent to a radius of curvature of 5mm without affecting the device properties.

S10: Batteries and Energy Storage**All Solid-state Batteries II**

Room: Salon E

Session Chairs: Stefan Adams, National University of Singapore;

Mickael Dolle, University of Montreal

9:50 AM

(MCARE-S10-012-2016) Research of solid electrolyte for battery application (Invited)Y. Kato^{*1}; 1. Toyota Motor Europe, Belgium

Large-scale batteries are in high demand for applications such as plug-in electric hybrid or electric vehicles, and smart electric power grids. The all-solid-state battery is the most promising candidate for future battery systems, due to the high energy density obtained by direct-series-stacking of the battery cells. However, the low power characteristics of the all-solid-state battery, due to higher cell-resistivity than conventional liquid electrolyte batteries, still remain as an unsolved issue. Therefore, a solid electrolyte having high ionic conductivity comparable to those of liquid electrolytes have been desired for realizing all-solid-state battery in large-scale. Some notable progress has been made in this field, and significant research efforts have recently discovered a novel superionic conductor, $Li_{10}GeP_2S_{12}$ (LGPS), in the $Li_xGeS_4-Li_3PS_4$ quasi-binary system. The material research for solid electrolyte has been conducted based on the LGPS crystal structure and around its composition. We will present our recent results focusing on this type of materials.

10:30 AM

(MCARE-S10-013-2016) Formation of electrode-electrolyte interfaces in all-solid-state rechargeable lithium batteries (Invited)A. Hayashi^{*1}; M. Tatsumisago¹; 1. Osaka Prefecture University, Japan

Development of all-solid-state rechargeable lithium batteries with inorganic solid electrolytes attracts much attention because of their high safety and high energy density. Sulfide and oxide glass-ceramic electrolytes with high conductivity have been developed. Glass electrolytes are useful as a precursor for stabilizing metastable crystalline phases with high conductivity. The prepared glass-ceramics in the sulfide system $Li_2S-P_2S_5$ and oxide system $Li_3BO_3-Li_2SO_4$ respectively show the conductivity of 10^{-2} and 10^{-5} S cm^{-1} at 25°C. These sulfide and oxide electrolytes have good mechanical properties for application to solid-state batteries. Formation of favorable solid-solid interfaces between electrode and electrolyte is important for enhancing electrochemical performance of solid-state

batteries. Sulfide electrolyte coating on active material particles by the gas-phase or liquid-phase methods is effective in realizing close electrode-electrolyte contacts. The coating reduces the volume of electrolyte content in an electrode layer, and energy density of solid-state batteries is thus increased. Surface coating of electrode particles and preparation of nano-composite electrodes are useful for increasing reversible capacity of solid-state batteries and our recent approaches to form favorable interfaces will be demonstrated.

11:10 AM

(MCARE-S10-014-2016) Cubic $Li_7La_3Zr_2O_{12}$ as a Solid ElectrolyteJ. Wolfenstine^{*1}; 1. US Army Research Laboratory, USA

As a result of increased demands for higher energy and safety, there has been renewed interest in the development of an all solid-state battery with a Li metal anode and a Li-ion conducting solid electrolyte. To be used in this situation, the solid electrolyte must meet several important requirements. These include: 1) high density, 2) high ionic conductivity, 3) chemical stability against the Li anode and cathode, 4) low impedance at electrolyte/electrode interfaces and 4) good mechanical properties. Of the possible Li-ion conducting solid electrolytes cubic $Li_7La_3Zr_2O_{12}$ (LLZO) is a potential candidate. It is the purpose of this talk to review methods to obtain high density (>98%) high conductivity Li-ion conductivity ($\sim 10^{-3}$ S/cm) LLZO and report on its chemical stability with Li at room temperature and elevated temperature, interfacial impedance against Li and mechanical properties such as elastic modulus and fracture toughness. These results will be compared to other Li-ion conducting solid electrolytes such as LIPON, $Li_{0.33}La_{0.57}TiO_3$ and $Li_{1.3}Al_{0.3}Ti_{1.7}(PO_4)_3$.

11:30 AM

(MCARE-S10-015-2016) Towards all Solid State Batteries using Perovskite Solid ElectrolytesT. Bibienne^{*1}; P. Alvares¹; F. Bardé²; F. Rosciano²; M. Dollé¹; 1. University of Montreal, Canada; 2. Toyota Motor Europe, Belgium

Safety and environmental concerns are some of the main issues when considering lithium batteries technology. All Solid State Batteries (ASSB) may give a fundamental solution to solve those concerns. These solvent-free ASSB show major advantages: thermal stability, possibility of multicell assembly, possibility to use high potential electrode materials. We recently reported the approach to assemble ASSB in one step by Spark Plasma Sintering (SPS) using phosphate materials. Investigations on oxide electrolytes were considered. These electrolytes require not only being chemically stable towards electrode materials, but should also provide a good electrochemical stability over a wide potential range. Candidate materials (e.g. perovskite materials) should be relatively low cost, environmentally benign and easy to produce at an industrial scale. Several perovskite electrolytes (covering most of these requirements) were synthesized and characterized by XRD and impedance spectroscopy after sintering by SPS. Their thermal stability towards well-known electrode materials was also investigated, as well as electrodes and electrolyte interfaces using SEM and EDS. This presentation will focus on the required steps to develop ASSB using perovskite solid electrolytes.

11:50 AM

(MCARE-S10-016-2016) Thin film $Li_7La_3Zr_2O_{12}$ as electrolyte for all-solid-state batteriesS. Lobe^{*1}; H. Gehrke¹; C. Dellen¹; M. Finsterbusch¹; C. Tsai¹; S. Uhlenbruck¹; O. Guillon¹; 1. Forschungszentrum Juelich, Germany

Today's Lithium ion batteries suffer from problems related to the liquid electrolyte, like degradation or malfunction. In all-solid-state batteries, the liquid is replaced by an ion-conductive ceramic layer. Garnet-structured $Li_7La_3Zr_2O_{12}$ (LLZ) is an excellent candidate as electrolyte due to its high Li ion conductivity (up to 10^{-3} S cm^{-1}), inherent safety and electrochemical stability (up to 8V vs. Li^{+/}Li). In order to reduce the internal resistance and increase the energy density of the cells our work is focused on thin film deposition of

the LLZ. R.f. magnetron sputtering is used as deposition technique due to scalability from laboratory to industrial scale. A major challenge during LLZ deposition is the control of the Li content of the thin film, as it depends strongly on the deposition conditions used. Carefully adjusting these parameters, we were able to deposit 1 μm thin crystalline LLZ films with total Li^+ ion conductivities up to $2 \times 10^{-4} \text{ S cm}^{-1}$. The presentation will focus on the influence of different deposition parameters on film composition, morphology and ionic conductivity to obtain dense LLZ layers with high ionic conductivity. Finally, the integration of the LLZ thin film deposition process in the manufacturing of an all-solid-state thin-film battery will be shown.

S1: Functional Materials for Photoelectrochemical and Electrocatalytic Hydrogen Production

Functional Materials for Photoelectrochemical and Electrocatalytic Hydrogen Production

Room: Salons A-C

Session Chair: Sanjay Mathur, University of Cologne

1:30 PM

(MCARE-S1-001-2016) Nanoengineered Films for Renewable Energy (Invited)

Y. Yang^{*1}; 1. University of Central Florida, USA

A general solution to the energy and environmental crisis is to develop sustainable energy systems that can produce and store energy inexpensively and efficiently. It is feasible to improve the energy conversion and storage performance through tailoring the density of active sites within a defined nanostructure having a high surface area. To develop high-performance energy devices, nano-engineering has been utilized to achieve several improvements: 1) expose more edges by forming highly porous structures; 2) replace powder catalysts by thin-film catalysts to avoid activity deactivation caused by poisoning from the supporting materials; 3) enhance charge transfer and electrical conductivity in the films by phase conversion from semiconducting phase to metallic phase. By these ways, a high performance energy device is anticipated.

2:10 PM

(MCARE-S1-002-2016) Morphological, dimensional, and interfacial effects on oxide semiconductor efficiency for solar water splitting (Invited)

L. Vayssieres^{*1}; 1. Xian Jiaotong University, China

With global climate change seriously compromising our environment, security, and health, and a concomitant exponential increase in energy demand from emerging countries, a significant renewed interest in water splitting has occurred worldwide within the last decade. Large bandgap metal oxides offer a wide range of applications for renewable energy systems. Most are stable, non toxic, earth-abundant, easy to prepare on a large scale as powders, thin films, dense ceramics and ordered anisotropic arrays at various dimensional scales, i.e. nano to micro to macro-scales. They exhibit the widest range of electrical, optical, and electronic properties suitable for low cost solar water splitting and photovoltaic applications. An overview of the effects of their dimensions, morphologies, interfaces, and surface chemistry will be presented along with the latest advances in materials design which include a new strategy to combine in highly ordered arrays molecular co-catalysts and oxide semiconductors.

2:50 PM

(MCARE-S1-003-2016) The Origin of Electrochemical Activity of Cobalt Oxide Water Oxidation Catalytic Amorphous Thin Film

G. Kwon^{*1}; H. Kim²; A. Mane³; J. Emery³; A. Martinson³; P. Stair²; D. Tiede¹; 1. Argonne National Laboratory, USA; 2. Northwestern University, USA; 3. Argonne National Lab, USA

To investigate the origin of electrochemical performance as function of structural evolution of cobalt oxide water oxidation catalyst films, we utilized pair distribution function/resonant Raman/X-ray emission/inelastic X-ray scattering techniques. In this presentation, we present results on investigation of amorphous cobalt oxide film growth, domain structure, and comparison to electrochemical activity. The results show that amorphous cobalt oxide catalyst films (CoPi and CoBi) grow from nucleating small domains limiting size which depends on the nature of oxyanion present in electrolyte. Correlations between domain structures with electrocatalytic activity were investigated by comparing the catalytic activities with CoPi and CoBi films with various degrees of stacking. In addition, the electrical conductivity was directly measured using free standing cobalt oxide hollow tubes. The level of catalytic activity was found to correlate with film conductivity, number of catalytic sites, domain size, and degree of stacking. The excitation state of cobalt was lower than 0.75eV. Therefore, charge can easily travel (delocalized) at intra-domain but can't easily travel at inter-domain resulting from low conductivity which was dominated by resistance between domains. We concluded that the resistance at inter-domain limits electrochemical activity of cobalt oxide catalyst films.

3:30 PM

(MCARE-S1-004-2016) Photoelectrochemical Water Splitting via Molecular-Inorganic Hybrid System for Solar to Chemical Energy Conversion (Invited)

K. S. Joya^{*1}; 1. University of Engineering and Technology (UET), Pakistan

Application of high activity water oxidation electrocatalysts on top of semiconductor photoanodes is crucial to boost the performance of the solar to fuel conversion systems via water splitting.[1] Thin film photo-responsive semiconductor materials such as hematite ($\alpha\text{-Fe}_2\text{O}_3$), tungsten trioxide (WO_3) and bismuth vanadate (BiVO_4) on transparent conducting surfaces have been studied for light-driven water oxidation as they have moderate band gaps for visible light harvesting, and band positioning suitable for water oxidation. [1-2] Their charge transfer kinetics can be improved by nano-structuring the semiconductor materials, and charge separation and catalytic performance can be improved by synergetic interfacing with oxygen evolving cocatalysts.[3-4] Here we present functionalization of molecular electrocatalysts on top of semiconductors for better charge separation and faster hole delivery (**Figure 1**). This approach, while facilitating the light capturing abilities of the inorganic semiconductors, enhances the catalytic performance of the solar water oxidation activity even at higher driving energy.

4:10 PM

(MCARE-S1-005-2016) An insight into the influence of morphology and plasmonic silver nanoparticles on the photoelectrochemical activity of TiO_2 nanotube arrays (Invited)

D. Padiyan^{*1}; 1. Manonmaniam Sundaranar University, India

The remarkable role of annealing time on the hydrogen generation of electrochemically anodized titania films are studied. Annealing time plays a greater role in improving crystallinity, homogeneity of nanostructures, shifts the optical range from UV to visible region. To improve the photoelectrochemical activity, different approaches are used to fabricate titania nanotubes with controlled morphologies such as conical, cylindrical, stack layered and bamboo by varying the experimental parameters such as anodization potential, duration, electrolyte, pH etc. The length of the nanotube has been modified while the diameter of the nanotube has been controlled by the applied potential. Titania film also acts as a photocatalyst to

degrade the methyl orange an environmental pollutant under light irradiation and their mechanism will be presented. It has been demonstrated that the inclusion of silver nanoparticles in the titania improve their conversion efficiency due to the surface plasmon resonance properties and harvesting a large amount of the solar flux. A novel non-enzymatic electrochemical biosensor is developed using the functionalized titania and the results will be presented.

4:50 PM

(MCARE-S1-006-2016) Complex thin and ultra-thin coatings for energy applications (Invited)

G. Westin*¹; I. Uppsala University, Sweden

The development of photo- and electro-catalysts for solar fuels require robust, routes capable of producing very precise and complex multi-component, multi-functional materials at high rate and low cost. It seems that for such tough demands solution based routes are the best suited for most conceivable systems, but there is a need for further development of these processes before they can be fully exploited for industrial scale manufacture of complex tailored materials. Here is discussed two types of solution based processing routes to doped and non-doped oxide nano-particles, thin- and ultra-thin films; (i) one based on reactive alkoxides that yield pure homo and heterometallic oxides and (ii) another based on organically modified salts that yield metals and metal-in-oxide nano-composites. The oxide systems studied involve doped and non-doped transition metal oxides such as Fe₂O₃ and Co₃O₄, complex spinels such as ferrites and perovskites including ferrites, cobaltates. Further, metals such as Co and Ni and their alloys will be described, as well as metal-in ceramic nano-composites such as PtNi-Fe₂O₃. The materials deposited as thin and ultra-thin films on relevant flat and nano-structured semi-conductor substrates will be described on their contents and structures. A wide range of analytical techniques were used to describe precursors, processing and product films.

5:30 PM

(MCARE-S1-007-2016) SrTiO₃-TiO₂ Eutectic Composite - a Candidate Material for Photoelectrochemical Hydrogen Production

K. Wyszumlek*¹; J. Sar¹; K. Kolodziejak¹; P. Osewski¹; K. Orlinski¹; D. A. Pawlak²; 1. Institute of Electronic Materials Technology, Poland; 2. Centre of New Technologies, Poland

Use of highly crystalline and durable eutectic materials as the active photoanode material, has been investigated on the base of binary oxide semiconductor SrTiO₃-TiO₂ system. The transmission-spectroscopy measurements and 3D profilometry proved decreased reflectance and increased surface area of originally mirror-like electrode's surface, which resulted in increased photocurrents after extended periods of PEC analysis. SrTiO₃-TiO₂ photoanodes proved to be stable in acidic environment under irradiation. Favorable flat-band potential and high photocatalytic activity of eutectic photoanode is confirmed by electrochemical impedance spectroscopy. The preliminary results show that the conversion efficiency can be optimized 1) by improving minority charge carrier transport through reducing layer thickness and 2) by extending effective solar spectrum by introducing dopants or other semiconducting compounds. Due to various material combinations possible with eutectic composites, high crystallinity, sharp interfaces, control over phase's refinement and various ways of available engineering, these materials can result in efficient and stable PEC photoanodes. Acknowledgements: The research has been supported by a grant from Switzerland through the Swiss Contribution to the enlarged European Union with the Project PSPB 132/2010 "Hybrid semiconducting materials for solar energy conversion".

5:50 PM

(MCARE-S1-008-2016) Photocatalytic degradation of Congo red under UV-light by MoS₂/Al₂O₃ composite produced by microwave method

S. Vattikuti*¹; C. Byon¹; 1. Yeungnam University, Republic of Korea

This paper reports the synthesis of gram-scale heterostructured MoS₂/Al₂O₃ composite using a one -step facile microwave method. Cetyl trimethylammonium bromide (CTAB) was used as surfactant to prepare a series of MoS₂/Al₂O₃. The as-prepared MoS₂/Al₂O₃ composite was characterized with powder X-ray diffraction (XRD), field emission scanning electron microscopy (FESEM), high-resolution transmission electron microscopy (HRTEM), thermal gravimetric and differential thermal analysis (TG-DTA), Fourier transform infrared spectroscopy (FTIR), and X-ray photoelectron spectroscopy (XPS). The addition of CTAB influenced the growth of the large surface area heterostructured composite. The MoS₂/Al₂O₃ composite exhibit higher photocatalytic activity for the degradation of Congo red under UV light irradiation for 90 min. The photocatalytic mechanism of MoS₂/Al₂O₃ composite was elucidated and influence of CTAB on morphology was discussed.

6:10 PM

(MCARE-S1-009-2016) Photoelectrochemical Properties of TiO₂-WO₃ Self-Organized Eutectic Material

K. Kolodziejak*²; J. Sar²; K. Wyszumlek²; M. Bartsch¹; M. Niederberger¹; D. A. Pawlak²; 1. ETH, Switzerland; 2. Institute of Electronic Materials Technology, Poland

Eutectic materials are two or multiphase materials formed during cooling of a mixable melt with an eutectic composition. The possibility of considering versatile combinations of various component materials in eutectics provides a broad palette for many applications. Eutectics obtained by the self-organization mechanism also seem to be very attractive as energy-generating materials. They have potential as photoactive materials, due to their multiphase character – various available photoactive component phases and multiple band gap energies and high crystallinity. TiO₂-WO₃ eutectic is a new composite material obtained by the micro-pulling-down method. Such mixed materials made of two semiconducting phases with bandgaps enabling absorption of UV-Vis wavelengths (TiO₂ – UV light, WO₃ – visible light) may be promising for photoelectrochemical applications – especially as materials for PEC photoanodes. The growth and characterization of the eutectic microstructure from a TiO₂-WO₃ system (36 at.% TiO₂ and 64 at.% WO₃), will be presented. The preliminary photoelectrochemical results will be also discussed. Acknowledgements: The research has been supported by a grant from Switzerland through the Swiss Contribution to the enlarged European Union with the Project PSPB 132/2010 "Hybrid semiconducting materials for solar energy conversion".

S2: Spectral Conversion Materials for Energy Applications

Novel Upconversion and Downconversion Materials: Nanoparticles, Macro/Micro-sized Structures, Composites, Antenna for NIR Harvesting, Etc.

Room: Salon D

Session Chairs: Alberto Vomiero, Lulea University of Technology; Haiguang Zhao, INRS

1:40 PM

(MCARE-S2-014-2016) Rendering rare-earth photoluminescence via material design and modification: the consequences of structural and electronic alterations (Invited)

G. Liu*¹; 1. Argonne National Lab, USA

Modification of phosphor compositions is an advanced method for rendering photoluminescence; however, composition modification often deteriorates optical quality because of the resultant structural and electronic disorders. There are also specifically designed ion-host systems in which light conversion efficiency can be significantly enhanced or luminescence spectra can be tailored to meet application requirement without efficiency loss. We will discuss the basics of energetics and excited-state dynamics of rare-earth activated phosphors in which crystalline structure and ion-ligand electronic structure are purposely altered. The consequences of such alterations and their impacts on spectroscopic properties, including variations in luminescence color and intensities will be analyzed with examples of recently studies on upconversion and downshift light conversion. We will review the enhancement of Er³⁺-Yb³⁺ multiphoton upconversion achieved through fabrication of lattice clusters KYb₂F₇:Er³⁺ to contain Yb³⁺ energy migration; present a newly discovered phenomenon of isotropic rendering of Eu²⁺ photoluminescence enabled by cation nanosegregation in isostructural solid-solutions; and discuss how the mixed-valence Eu³⁺/Eu²⁺ can be stabilized and controlled in metal organic frameworks to facilitate unprecedented spectroscopic performance.

2:20 PM

(MCARE-S2-015-2016) Hetero-metallic molecular approach to Ln-doped materials; from precursor to material (Invited)

G. Westin*¹; 1. Uppsala University, Sweden

Ln-doped materials provide a wide range of cutting edge and often unique applications including; lasers, signal amplifiers, frequency up-conversion devices, light emitting diodes, fluorescent screens and lamps, and bio-markers. The special electronic properties of the 4f elements that make these applications possible are highly sensitive to the type, number and spatial placement of the neighboring atoms and phonon energy of the lattice. Further, the distance to other Ln-ions determining co-operative effects is of determining importance for the properties. In spite of this, there are few attempts to design the local structure around the Ln-ion and thereby optimise the desired properties. Different schemes for combining up-converting Ln-doped materials and a flat or structured semi-conductor can be envisaged, but most will entail a thin Ln(III) containing coating. Here we describe solution based routes using hetero-metallic alkoxide precursors to thin oxide coatings on flat and nano-structured substrates; from synthesis and design of precursors and, their structure and properties, via solution processing, to heat-treatment. Local structuring using ErAl₃(OiPr)₁₂ and ErNb₂(OiPr)₁₃ providing single, isolated Er-ions, resulting in much increased non-quenched Er doping concentration will be described as well as thin Ln-containing films on various substrates will be described.

Lanthanides, Dyes and Quantum Dots for Photovoltaic Applications

Room: Salon D

Session Chairs: Jose Marques-Hueso, Heriot-Watt University; Eva Hemmer, INRS

3:20 PM

(MCARE-S2-016-2016) Tuning nanomaterials in high-efficiency excitonic solar cells (Invited)

A. Vomiero*¹; 1. Lulea University of Technology, Sweden

The typical photoanode in dye- and quantum dot- sensitized solar cells is composed of a wide band gap semiconductor, which acts as electron transporter for the photoelectrochemical system. Anatase TiO₂ nanoparticles are one of the most used oxides and are able to deliver the highest photoconversion efficiency in this kind of solar cells, but intense research in the last years was also addressed to ZnO and other composite systems. Modulation of the composition and shape of nanostructured photoanodes is key element to tailor the physical chemical processes regulating charge dynamics and, ultimately, to boost the efficiency of the end user device, by favoring charge transport and collection, while reducing charge recombination. We investigated several systems: (i) TiO₂ nanoparticles / ZnO nanowires; (ii) Multiwall carbon nanotubes (MWCNTs) / TiO₂ nanoparticles; (iii) TiO₂ nanotubes; (iv) Hierarchically self-assembled ZnO sub-microstructures. Both dye molecules and semiconducting quantum dots were applied as light harvesters. Possible tailoring of structure and morphology of the photoanodes and of the quantum dots, and their implication in improving the functional properties of these kinds of excitonic solar cells will be discussed in detail.

4:00 PM

(MCARE-S2-017-2016) Broadband absorbing Tm²⁺ based Luminescent Solar Concentrators without self-absorption losses (Invited)

E. van der Kolk*¹; 1. Delft University of Technology, Netherlands

Electricity generating glass is a holy grail in building-integrated photovoltaics (BIPV). Luminescent Solar Concentrators (LSCs) have the potential to become a BIPV technology by trapping part of the solar spectrum with a luminescent coating that guides solar energy to solar cells at the window perimeter. Despite the large potential as PV-window, large LSCs (0.5-1 m²) reach efficiencies of only 1-3%, mainly due self-absorption losses. In this presentation we will report on cheap Thulium (Tm²⁺) doped materials like NaCl and CaI₂ that have the potential to reach a 15% LSC efficiency because they provide 65% absorption of the solar spectral range, have no losses due to self-absorption and in addition they may be developed with a uniform absorption so that windows will remain colourless. We will present absorption, luminescence excitation- and emission spectra of crystals, powders and thin-films and conclude about the luminescence mechanisms as well as about the solid solubility of Tm²⁺ in NaCl thin-films. We will also report on the combinatorial co-sputtering of Tm²⁺ and Eu²⁺ doped halide thin-films with a wide doping concentration gradient or host composition gradient and the automated xy-scanning of their luminescent properties. Finally we will present a model that accurately quantifies self-absorption losses as a function of LSC dimension and can be applied to any LSC material.

4:40 PM

(MCARE-S2-018-2016) Upconversion Quantum Yield in Lanthanide-Doped Nanoparticles: Going deeper into size, shape and host material dependencies

M. Quintanilla^{*1}; E. Hemmer²; J. Marques-Hueso³; S. Rohani²; R. Zamani⁴; V. Roddatis⁴; B. Richards⁵; F. Vetrone²; 1. CIC BiomaGUNE, Spain; 2. INRS, Canada; 3. Heriot-Watt University, United Kingdom; 4. Georg-August Universität, Germany; 5. Karlsruhe Institute of Technology, Germany

Exploiting lanthanide-based upconversion (UC) processes to enhance the efficiency of photovoltaic or photocatalytic materials is an ambitious goal whose success strongly depends on the quantum yield (QY) of UC. While QY values between 1 and 10% have been demonstrated for bulk crystals, this value can go down more than one order of magnitude in the case of nanoparticles. For this reason, applications exploiting UC try to maximize the size of the UC material as much as possible. However, certain configurations require the use of materials at smaller sizes, as is the case of solar cells that incorporate the UC materials inside the semiconductor layer or strategies that exploit the use of nanoparticles to increase the active material surface, as happens in photocatalysis. Aiming to study the reduction of UC-QY in lanthanide-doped nanoparticles and to be able to determine the material properties that affect it, in this work we have measured the QY of NaGdF₄, NaYF₄ and LiYF₄ nanoparticles. Then, for the case of NaGdF₄, we added to the study the analysis of QY variations with the size, crystal phase, and shape of the nanoparticles. The analysis of the obtained results emphasizes the importance of the distance between lanthanides within the crystal lattice as parameter to differentiate the QY in the materials considered.

Application-oriented Approaches in Spectral Conversion

Room: Salon D

Session Chairs: Eva Hemmer, INRS; Jose Marques-Hueso, Heriot-Watt University

5:00 PM

(MCARE-S2-019-2016) Exploring the use of melanin pigments for solar energy conversion (Invited)

C. Santato^{*1}; 1. Ecole Polytechnique de Montreal, Canada

Melanins are biomacromolecules responsible for the pigmentation of many plants and animals. The biological functions of melanins, also present in the inner ear and the substantia nigra of the human brain, go far beyond coloration and include photoprotection, anti-oxidant behavior, and metal chelation. Melanins are also intensively studied for their involvement in melanoma skin cancer and Parkinson's disease. Eumelanins are the most ubiquitous melanins in humans and the most studied by material scientists. Back in the 1960-70s, eumelanin in form of pressed pellets was discovered to be conductive, photoconductive, and to show threshold switching. These properties and the broadband UV-vis absorption of eumelanin were explained mostly within the amorphous semiconductor model. However, this interpretation has been challenged several times, especially considering the strong hydration dependence of the electrical properties of eumelanin. Here we report on efforts to better understand the photoconductivity properties of eumelanin and its interfaces with current collectors, e.g. based on carbon paper, to demonstrate biocompatible, sustainable electrochemical energy storage photo-devices.

S3: Ferroelectrics and Multiferroics for Energy Applications**Properties, Caloric Effects**

Room: Salon F

Session Chair: Doru Lupascu, University of Duisburg-Essen

1:40 PM

(MCARE-S3-019-2016) Giant barocaloric effects in ferrielectric ammonium sulphate (Invited)

X. Moya^{*1}; 1. University of Cambridge, United Kingdom

Giant barocaloric effects driven by hydrostatic pressure have been suggested for cooling applications, but they are only seen in a small range of magnetic materials that are relatively expensive. Here I will present pressure-dependent calorimetry data to demonstrate giant barocaloric effects in ferrielectric ammonium sulphate, which is made of cheap abundant elements.

2:20 PM

(MCARE-S3-020-2016) Bulk ceramics Pb(Mg_{1/3}Nb_{2/3})O₃-PbTiO₃ as a working body for an electrocaloric cooling device (Invited)

H. Uršič^{*1}; M. Vrabelj¹; Z. Kutnjak¹; U. Plaznik²; A. Kitanovski²; B. Rozic¹; V. Bobnar¹; L. Fulanovic¹; S. Drnovsek¹; A. Bencan¹; B. Malic¹; 1. Institute Jožef Stefan, Slovenia; 2. University of Ljubljana, Slovenia

Electrocaloric (EC) effect is the change in entropy and, consequently, in temperature of a dielectric material due to the electric-field-induced changes in the polar states. The (1-x)Pb(Mg_{1/3}Nb_{2/3})O₃-xPbTiO₃ (PMN-100xPT) ceramics of selected compositions are expected to exhibit a large EC effect due to their excellent dielectric properties, such as high dielectric permittivity and polarization, and a large change of polarization with temperature. We prepared the PMN-10PT and PMN-30PT bulk ceramics with similar densities and different grain sizes by changing the sintering temperature and time and analysed their phase composition, microstructure, dielectric and EC properties. The highest measured EC temperature change for the PMN-10PT ceramic with 3.6 μm grains was 3.45 °C at 127 °C and 160 kV/cm, which is the highest reported value until now for Pb-based perovskites. The influence of the grain size on the dielectric and EC properties of PMN-10PT will be discussed in the contribution. Furthermore, we explore utilization of PMN-10PT ceramics as active elements in an EC cooling device. The experimental testing of the cooling device demonstrates the efficient regeneration and establishment of the temperature span between the hot and the cold sides of the regenerator, exceeding several times the EC temperature change of a single PMN-10PT ceramic plate. The authors thank the ARRS (L2-6768).

2:50 PM

(MCARE-S3-021-2016) Ferroelectric core-shell ceramics for energy storage and electrocaloric applications

M. Anoufa^{*1}; J. Kiat¹; 1. Labo SPMS, France

Core-shell structure in powders and ceramics of many compounds are more or less unavoidable. This situation describes the structuration of particles where the core behaves like the bulk material, whereas the shell, with typical thickness of some nm, is the part of the particle close to the surface where all kinds of defects are at play. In the case of ferroelectric compounds or related compound it can be oxygen defective surface, or unwanted defects which stands on the surface of particles, or frozen polarization with low permittivity etc. Artificial core-shell structure can also be induced on purpose by coating the surface of grains before sintering. We have used a combination of different modeling technics: effective Hamiltonien, Landau theory etc and shown that core-shell structure is not necessarily to be avoided or minimized but can be used to optimize physical properties. We have observed that optimal structuration of ceramics exists for which maximum efficiency of energy storage and electrocaloric

effect is obtained. Core-shell structure can also induced new phase transitions via the competition between particles shape anisotropy, surface tension and shear strain. Inducing a specific core-shell structure is therefore a new and easy way to tailor structural properties and to stabilize new phases that cannot exist in bulk material, just like film deposition on substrate.

Properties, Photovoltaic

Room: Salon F

Session Chair: Aiping Chen, Los Alamos National Lab

3:30 PM

(MCARE-S3-022-2016) Semiconducting Ferroelectric Photovoltaics (Invited)

J. E. Spanier^{*1}; 1. Drexel University, USA

In classic solid-state photovoltaic devices photogenerated charges are separated by the field developed at a p-n junction, a dye-sensitizer interface, a domain boundary, or due to the Dember effect. All of these photovoltaic effects have in common the following: an inhomogeneous excitation or spatially-inhomogeneous medium, and the photovoltage does not exceed the band gap. The bulk photovoltaic effect (BPVE) in non-centrosymmetric crystals is a striking physical phenomenon: photovoltage generated by the BPVE can greatly exceed the band gap, but the direct conversion of light energy to electricity is extremely low. The BPVE can be observed in crystals which belong to twenty point groups lacking a center of inversion symmetry. Cation substitution chemistries promoting cation-vacancy clusters are effective for band gap reduction without loss of ferroelectricity, enabling a completely new family of visible light-absorbing ferroelectric solid-solution semiconductors. I shall review recent progress in understanding light-matter interactions and charge carrier separation in ferroelectric perovskite oxides, particularly the BPVE. I shall discuss our recent advances in designing and producing ferroelectric oxide films, including their atomic and electronic structure, and optical, electronic and photovoltaic properties, including challenges and opportunities. Work supported by the ARO (W911NF-14-1-0500) and the NSF (DMR 1124696).

4:10 PM

(MCARE-S3-023-2016) Effect of ferroelectricity on solar light driven photocatalytic activity of BaTiO₃ -influence on the carrier separation and Stern layer formation

S. Dunn^{*1}; 1. QMUL, United Kingdom

BaTiO₃ (BTO), can exist as both a non-ferroelectric cubic phase and ferroelectric tetragonal phase at room temperature, was selected as a test catalyst in photodecolourisation of RhB under simulated solar radiation. A thermal treatment (1200°C for 10 hours) was employed to convert the phase composition of the powder catalysts from 92% cubic to 67% cubic established using XRD fitting. An increase in adsorption, as demonstrated in previous publications, that the spontaneous polarisation of ferroelectrics increases dye molecule adsorption in the Stern layer. The ferroelectric material demonstrated an enhancement of decolourisation rate, arising from the stronger adsorption and effective charge carrier separation due to the internal electric field. In addition, the photocatalytic activity was improved further by Ag deposition, where Ag act as electron traps and prohibit the recombination of electrons-holes. The results shown here give direct evidence that ferroelectrics can enhance the photocatalytic performance by comparing the same material in ferroelectric and non-ferroelectric phases. These findings provide further understanding of ferroelectric materials as catalysts and demonstrate their promising future.

4:30 PM

(MCARE-S3-024-2016) Perovskite enhanced solid state ZnO solar cells

S. Dunn^{*1}; 1. QMUL, United Kingdom

This paper will report on the design, fabrication and testing of a solid-state perovskite enhanced ZnO solar cell. The p-type perovskite material used is bismuth ferrite (BFO) which has an absorption range within the blue range of the visible light spectrum. The solid state solar cell, was sensitized with N719 dye and used a CuSCN hole conductor. A disadvantage of ZnO is its poor chemical stability in acidic and corrosive environments. As chemical solution techniques were used in depositing BFO, a buffer method using an aminosilane ((3-aminopropyltrimethoxysilane or H₂N(CH₂)₃Si(OCH₃)₃) coating was used to provide a protective coating on the ZnO nanorods before the BFO film was spin coated onto the ZnO nanorods. The photovoltaic performance of the solar cells were tested using a Keithley 2400 source meter under 100mW/cm², AM 1.5G simulated sunlight, where improvements in J_{sc} and efficiency were observed. The BFO was able to harness more electrons and also acted as a buffer from electron recombination.

S8: Self-Power Generators

Self-Powered Devices and Systems I

Room: Salon G

Session Chair: Pooi See Lee, Nanyang Technological University

1:40 PM

(MCARE-S8-010-2016) Micro-fabricated Supercapacitors for On-Chip Energy Storage (Invited)

H. N. Alshareef^{*1}; N. Kurra¹; Q. Jiang¹; 1. King Abdullah University of Science & Technology, Saudi Arabia

The talk will focus on the fabrication and characterization of micro-supercapacitors on rigid and flexible substrates. A combination of top-down lithography as well as chemical processing methods have been used to fabricate devices with excellent performance targeting integrated energy storage devices. The talk will cover several factors that were found to influence the performance of micro-supercapacitors. These include the electrode material, collector material and geometry, and the fabrication scheme used to make the devices. Metal oxide and ternary metal chalcogenide pseudocapacitive electrode materials prepared using various chemical methods will be discussed. The role of surface chemistry, nucleation layers, and chemical synthesis route in controlling the morphology of the pseudocapacitive material will be presented, along with the resultant properties from various microfabricated devices. The effect of collector material geometry, design, and scaling (2D vs 3D) will be highlighted.

2:20 PM

(MCARE-S8-011-2016) Modelling of vertical-nanowire based devices for mechanical/electrical transduction (Invited)

M. Mouis^{*1}; R. Tao¹; M. Parmar¹; G. Ardila¹; L. Montes¹; 1. IMEP-LAHC, France

Mechanical energy is one of the most widely abundant sources of energy and is thus of prime importance for future autonomous sensors which are the backbone of the internet of things. With these applications in view, our research is focused on the low-cost integration of compact sensors and nanogenerators based on mechanical-electrical transduction. Dense arrays of vertical nanowires, which can be grown by chemical bath deposition on various substrates, including flexible ones, are promising candidates. Based on electro-mechanical modelling, we will review the advantages expected from such a structure. Most of them arise from the high flexibility and enhanced piezoelectric properties that can be obtained with nanowires. However, in order to anticipate the performance

of real devices, it is necessary to account for the whole structure. Moreover, the optimum architecture can differ, depending on how the device is operated. In this paper, we will put more focus on ZnO nanowire based devices integrated at the surface of a flexible substrate, where the nanogenerator is operated in flexion. The role of device architecture will be explored, in terms of geometry or matrix material for instance, as well as the limits related to the semi-conducting nature of ZnO.

Self-Powered Devices and Systems II

Room: Salon G

Session Chairs: Mireille Mouis, CNRS, IMEP-LaHC; Miso Kim, Korea Research Institute of Standards and Science

3:30 PM

(MCARE-S8-012-2016) Towards self-powered flexible energy devices (Invited)

P. Lee^{*1}; V. Bhavanasi¹; K. Parida¹; I. Nanyang Technological University, Singapore

Piezoelectric energy harvesting has drawn great attention in recent years due to its huge potential in applications for wireless and self-powered devices. Ferroelectric polymer, poly (vinylidene fluoride - trifluoroethylene) [PVDF-TrFE], is flexible and can sustain larger strains compared to inorganic counter-parts, making it attractive for harvesting energy from the mechanical vibrations. The piezoelectric energy harvesting ability of these polymers are lower because of the lower piezo electric coefficient and Young's modulus compared to inorganic counterparts. In this talk, I will discuss our strategies employed to enhance the energy harvesting performance of PVDF-TrFE films. This includes fabrication of nanostructures that increase the piezoelectric coefficient, compressibility and Young's modulus. The poled nanostructures show 40% reduction in poling field, giving larger piezoelectric d_{33} coefficient of 44 pmV^{-1} compared to poled films. By combining the electrostatic energy harvesting with piezoelectric means, we have achieved enhanced energy harvesting performance with power output of more than $4 \mu\text{Wcm}^{-2}$. Furthermore, we have integrate the piezoelectric polymer to realize a self-powered supercapacitor. A significant 90% of the charging potential can be achieved in less than 10s demonstrating a fast charging self-powered supercapacitor.

4:10 PM

(MCARE-S8-013-2016) Mesoporous Pores as Effective Dielectrics for Enhancing Triboelectric Nanogenerator Performance (Invited)

J. Baik^{*1}; I. Ulsan National Institute of Science and Technology, Republic of Korea

Mechanical energy is one of the most ubiquitous energies in our surroundings, which can be converted into electricity at anytime and anywhere. Since the first invention of the TENG in 2012, TENGs have been proven as a cost effective, simple, and robust technique for energy harvesting. In the triboelectric process, energy conversion is achieved by a periodic physical contact between two materials that differ in the polarity of triboelectricity, which yields surface charge transfer. A key approach to improve the electrical output performance aspect is to increase the triboelectric surface charge density through material modification and surface functionalization. Here, we report highly compressible mesoporous pores as effective dielectrics for enhancing triboelectric nanogenerator performance. The nanogenerator showed very large output voltage and current of up to 130 V and 0.10 mAcm^{-2} . Au nanoparticles (NPs) were also introduced into the pores by casting a mixture of PDMS solution and DI water with Au NPs. The TENG shows the instantaneous power of 13 mW, under cycled compressive force, giving over 5-fold power enhancement, compared with the FTENG. Additionally, it was employed in applications for self-powered shape mapping sensor,

foot-step driven large-scale AMTENG, and an integrated circuit with a capacitor.

4:50 PM

(MCARE-S8-014-2016) Kinematic Designs for Sustainable and High-performance Triboelectric Nanogenerators (Invited)

D. Choi^{*1}; I. Kyung Hee University, Republic of Korea

Triboelectric nanogenerators (TENGs) have great potential to produce electrical energy by harvesting environmental mechanical energies such as wind, vibrations and even human motion. To date, many researchers have studied the working mechanism of TENGs, have shown enhancements in TENG output power, and have used TENGs in various electronic, biomedical, and sensing device applications. In some TENG systems, high power was achieved if a high input energy was captured via high contact frequencies or high contact loads. However, it is difficult to constantly supply high energy because the environmental energy depends on region, weather, population and other factors. Furthermore, obtaining high output power based on high input energy could not provide high power conversion efficiency (PCE). In this study, our goal is to improve the output energy using the same materials and the same input energy, thus providing a high PCE and long life-time for TENG systems. We adopt kinematic theories to design novel TENG systems, where gear train and cam system are applied to develop high-performance and sustainable TENG systems. We demonstrate the various effects of kinematic designs for TENG systems.

5:30 PM

(MCARE-S8-015-2016) Importance of the μ -roughness for increasing triboelectric nanogenerator performances and lifetime (Invited)

R. Hinchet^{*1}; S. Kim¹; I. SungKyunKwan University, Republic of Korea

Energy harvesting systems based on triboelectric effect are in great demand, as they can provide routes for the development of self-powered devices which are highly flexible, stretchable, mechanically durable, and can be used in a wide range of applications. Our recent research interests mainly focuses on the development of triboelectric nanogenerators (TENGs) based on micro structures such as μ -pores, μ -pyramids or μ -wires. In this talk, I will address the importance of the roughness of triboelectric thin layers used in TENGs. μ -sponge structures can increase the output performances of TENGs while making them more resistant to humidity. Similarly, μ -pyramid patterns can greatly enhance the surface and friction between triboelectric layers and thus improve TENGs' performances. But these structures are fragile and can rapidly degrade under repetitive and strong forces, leading to much lower electrical output. To address this problem, we used shape memory polymers (SMP) which solved this issue by allowing healing the TENG's μ -pattern. This can simply be done by triggering the SMP's recovery ability by heating it at 55°C . Further, I will present our recent advances and I will discuss recent research efforts that enhanced the power generation and durability of TENGs for portable and wearable devices.

S10: Batteries and Energy Storage

Batteries: Modeling and Mechanisms

Room: Salon E

Session Chairs: Naoaki Yabuuchi, Tokyo Denki University;
Anton Van der Ven, University of California, Santa Barbara

1:40 PM

(MCARE-S10-017-2016) Phase transformation mechanisms in the electrodes of Li, Na and Mg batteries (Invited)

A. Van der Ven^{*1}; M. Radin¹; D. Chang¹; 1. University of California Santa Barbara, USA

Electrode materials for Li, Na and Mg ion batteries undergo a series of phase transformations as a result of large changes in concentration during each charge and discharge cycle. The mechanisms of these phase transformations remain poorly understood but usually rely on a delicate interplay between cation diffusion, nucleation and interface migration. Phase transformations can cause path hysteresis as well as electrode particle degradation. Crystallography and symmetry play an important role in determining how a particular phase transformation can cause an undesirable electrochemical response within the electrodes. We have developed new theoretical approaches to describe and understand phase transformations in electrode materials for Li, Na and Mg ion batteries that undergo intercalation, alloying and displacement/conversion reactions. First-principles computational tools that describe processes at the mesoscale are crucial to capture the coupling between mechanics and chemistry. This is especially important in layered intercalation compounds where cation removal is often accompanied by stacking sequence changes.

2:20 PM

(MCARE-S10-018-2016) Mechano-Electro-Chemical (MEC) Coupling in Lithium Intercalation Compounds (Invited)

Y. Qi^{*1}; C. James¹; 1. Michigan State University, USA

Mechano-Electro-Chemical (MEC) Coupling in intercalation compounds can be considered in multiple ways. Large stresses caused by electrochemically induced stoichiometry changes can lead to local stress and mechanical degradation. On the other hand, MEC coupling may also provide new opportunities to characterize materials by measuring the stress/strain generated by the stoichiometry change. In this study, key material properties, such as elastic properties, fracture energy, the anisotropic chemical strain tensors were all predicted from DFT calculations for MEC coupling models. Many interesting results emerged. It is lithiation induced stiffening occurs in layered compounds but not in the spinel and olivine structures. Depends on the tendency of Li to segregate to or deplete from the fractured surface, the fracture energy of layered compound can decrease or increase with SOC, and crack instability may also occur due to phase transitions within the fracture region. Furthermore, strong correlations between oxygen and Li vacancies were found in Li-excess layered structure Li_2MnO_3 . As Li vacancies tend to form and cluster around oxygen vacancies, the oxygen vacancies hinder the diffusion of the Li ions. Thus, the nonstoichiometry strains are correlated between the two species, making the MEC coupling analysis more complex in these intercalation compounds.

3:00 PM

(MCARE-S10-019-2016) Migration Mechanism of Transition Metal Ions in $\text{LiNi}_{0.5}\text{Mn}_{1.5}\text{O}_4$

G. Xu^{*1}; K. Amine¹; Z. Chen¹; 1. Argonne National Lab, USA

Layered-layered composite cathodes for lithium ion battery have been reported to have very high energy density. However, it suffers from voltage fading during normal operation, which will not only lead to substantial loss of effective energy density of the battery, but also raise an unexpected challenge for the battery management

system. Recent intensive investigation on the structural stability of layered-layered composite cathodes has led to a speculation that the migration of transition metal ions in the oxygen framework is the fundamental cause of the voltage fade. However, the unresolved issue for this hypothesis is the selective importance of the migration of transition metal ions in layered-layered composite cathodes. Therefore, a clear understanding on the migration mechanism of transition metal ions is critical to tackle the above challenge and to shed light on potential solution for layered-layered composite cathodes. The potential migration pathway in a model material, $\text{LiNi}_{0.5}\text{Mn}_{1.5}\text{O}_4$ spinel, was investigated using *in situ* high-energy X-ray diffraction and *in situ* neutron diffraction during the solid state synthesis process. It was found that the migration of transition metal ions among octahedral sites is possible by using tetrahedral vacancies as intermediate sites. It was also suggested that the number of electrons in 3d orbitals has significant impact on their mobility in the hosting oxygen framework.

3:20 PM

(MCARE-S10-020-2016) Computational studies on diffusion of Li in oxides for rechargeable Li ion battery with infomatics (Invited)

M. Nakayama¹; R. Jalem^{*2}; 1. Nagoya Institute of Technology, Japan;
2. National Institute for Materials Science (NIMS), Japan

Olivine-type LiMXO_4 composition (main group $\text{M}^{2+}\text{-X}^{5+}$, $\text{M}^{3+}\text{-X}^{4+}$ pairs)[1] and Favorite-type LiMXO_4F composition (main group $\text{M}^{2+}\text{-X}^{6+}$, $\text{M}^{3+}\text{-X}^{5+}$ pairs)[2] were successfully investigated as a potential solid electrolyte using Li-ion jump energy (EA) consideration through a combination of first principles calculation and informatics techniques, such as partial least squares (PLS)[3] method and artificial neural network (ANN)[4] method. In olivine-type composition, About 42 descriptors extracted from structurally-relaxed unit cells of different MX pairs were used to build the PLS and/or ANN model, categorized into: structural lattice parameters, Born effective charges of cations, intra-polyhedron parameters and inter-polyhedron parameters. We found out that M ionic size and its associated octahedron distortion contributed most significantly to EA value. The results showed promising MX pairs (<0.30 eV) such as MgAs, ScGe, InGe and MgP among compositions with experimental data, and Group 13 (Al, Ga, In)-X pairs and M-Sn pairs among potential novel materials.

3:40 PM

(MCARE-S10-021-2016) Materials design guidelines for all-solid-state batteries (Invited)

Y. E. Wang^{*1}; G. Ceder²; 1. Massachusetts Institute of Technology, USA;
2. University of California, Berkeley, USA

The research field of all-solid-state batteries has recently witnessed tremendous excitement, as dramatic improvements in performance for lithium solid-state conductors have been reported. However, the ideal solid-state electrolyte has not yet been developed; many of these conductors still have other issues for a full battery such as high cost of its constituents or a lack of compatibility with electrode materials. Compared to the rapidly emerging experimental efforts, much less was understood theoretically what makes a good ionic conductor with superior conductivity and stability against electrodes. In this talk we will present our recent advances in revealing fundamental relationship between crystal structure and ionic transport in fast Li-ion conductors using first-principles modeling based on density functional theory. An underlying bcc-like anion framework is most desirable for achieving high ionic conductivity, and that indeed this anion arrangement is present in many known fast Li-ion conductors. In addition, an accurate and efficient first-principles computational methodology has been developed to evaluate thermodynamic stability of the solid-state electrolyte against battery electrodes. These findings not only provide valuable insights towards the understanding of materials behaviors in discovered conductors, but also serve as design principles for new conducting materials and all-solid-state batteries.

4:20 PM

(MCARE-S10-022-2016) How Electrode Processing Affects Li-ion Battery Performance?A. Mistry^{*1}; D. Juarez Robles¹; P. P. Mukherjee¹; I. Texas A&M University, USA

With increasing demand for high energy and power density batteries, present and next generation lithium ion batteries are invariably designed with porous electrodes, due to their high surface-to-volume ratio. Out of various practical ways of producing these electrodes, slurry based electrode preparation still remains one of the most common method employed at laboratory scale due to its simplicity, cost effectiveness and scalability. In a typical processing sequence a slurry of active particles, conductive additive, binder and suitable solvent is prepared and after sufficient mixing casted onto current collector. This layered sheet is then dried in a temperature controlled environment. Despite the long term use of this procedure, there is a lack of general understanding as to how process parameters affect final microstructure and eventual performance of the Li-ion cells. The present work is focused on understanding the evolution of casted slurry into a porous electrode microstructure. The drying process is studied subject to different drying temperatures, active particle dimensions and relative composition of solid species in the slurry. The predicted electrode structures exhibit qualitatively different variations of microstructural properties and hence affect the performance. The model predictions are qualitatively compared with in-house experiments with Li-ion electrodes and half-cell performance.

4:40 PM

(MCARE-S10-023-2016) Understanding the voltage variation of lithium-manganese rich oxides from structural perspectiveZ. Chen^{*1}; K. Amine¹; I. Argonne National Lab, USA

In the past decade, major effort has been devoted to understanding the structure and the electrochemical benefit of lithium-rich transition metal oxides for high-energy density lithium-ion batteries because of their potentially high specific capacity of up to 250 mAh g⁻¹ when the materials are electrochemically activated. However, the structural instability of the material after electrochemical activation causes a continuous decrease in its working potential, a phenomenon which we will call voltage fade, that hinders the commercial deployment of this class of high-capacity cathode materials. Here, we report our recent effort to understand the local structure of lithium-rich transition metal oxides, as well as the impact of the domain size on electrochemical performance. In situ synchrotron probes were used to characterize the structural change of materials that leads to the voltage variation of lithium-manganese rich oxides, and a voltage variation mechanism based on the migration Mn²⁺ was proposed.

5:00 PM

(MCARE-S10-024-2016) Correlations between microstructure, phase transformation, stress development and electrochemical behavior of electrode materials for Li-ion batteries (Invited)A. Mukhopadhyay^{*1}; I. Indian Institute of Technology (IIT) Bombay, India

Improvements in the performance of electrode materials mandate understandings of the influences of microstructural features, effects of structural changes and phase transformations during lithiation/delithiation on mechanical degradation, effects of 'buffer' materials and/or conducting additives on the performances. This talk aims at throwing some light on these aspects based on results obtained during investigations, including real-time monitoring of stress developments and correlations with the states of charges, pre-cycling stress states and various electrochemical phenomena, for electrode materials ranging from potential anodes to the more commonly used cathodes. Some of the interesting results will include the occurrences of plastic deformation and concomitant mechanical instability just during phase transformation in metallic anode

and ceramic cathode materials. Additionally, it will also be elucidated that graphenic carbons are more susceptible to mechanical degradation during the initial stages of lithiation and later stages of delithiation. The effectiveness of using graphene as buffer material to minimize stress developments in Si will be discussed; as also will be the effects of distribution of conducting/'reinforcing' additives with respect to electrode active crystallites (LiFePO₄) on the electrochemical behaviour.

5:40 PM

(MCARE-S10-025-2016) Insights into Voltage Variations of Lithium Transition Metal Oxides during CyclingY. Li^{*1}; Y. Liu¹; G. Xu¹; Y. Ren¹; K. Amine¹; Z. Chen¹; I. Argonne National Lab, USA

Recently, voltage fade has been noticed and identified in the lithium transition metal oxides with layered structures. Since voltage fade would be detrimental to the energy retention of the materials, it is important to understand the nature of voltage fade and resolve the voltage fade issue. Many studies have shown that the voltage fade is a nature of some lithium transition metal oxides. For example, the voltage fade for lithium and manganese rich cathode is caused by the migration of transition metals, which eventually leads the materials changing from layered structure to spinel-like structure. How to prevent and inhibit voltage fade becomes a quite important object for developing new lithium transition metal oxides. In this talk, we would like to share our recent findings about the voltage variations, including voltage fade and voltage rise, in several important lithium transition metal oxides. We would like to show the relationship between the voltage variations and the structures changing in those lithium transition metal oxides. A hypothesis and a possible solution would be provided to prevent voltage fade in lithium transition oxide materials.

Poster Session

Room: Water's Edge Ballroom

(MCARE-S1-P001-2016) Preparation and hydrogen production characteristics of novel ZnO/carbon-based heterophotocatalystS. Hwang^{*1}; H. Seo¹; Y. Kim¹; S. Lim¹; I. DGIST, Republic of Korea

Novel ZnO/carbon-based heterophotocatalyst was prepared by growing horn-like ZnO nanocrystalline on carbon film using electrodeposition and solution casting method. Solar hydrogen production by ZnO electrodeposited onto carbon films was systematically investigated by controlling the amount of the deposited ZnO, property of carbon, and surface activation by KOH treatment in order to optimize the rate of hydrogen production. Carbon films have been prepared by polymer solution casting method using PAN solution, and subsequently annealing process. The surface of carbon film became more porous by chemically activating using KOH. And then, by electrochemical deposition, single crystalline ZnO horn was loaded on both carbon film and activated carbon film to ZnO/carbon-based heterophotocatalysts. As-prepared ZnO/CF heterophotocatalyst exhibited 64.7 % higher rate of hydrogen production on account of high adsorption ability of carbon film and fast photo-generated electron transfer to the carbon surface, compared with ZnO nanoparticle alone. Additional KOH activation on carbon film have very slightly enhanced the rate of hydrogen production, which was increased only 1.02 times as much as that by non-activated one (ZnO/CF). It could be suggested that property of substrate had a key role in hydrogen production using ZnO-based hetero photocatalysts.

(MCARE-S2-P002-2016) Tuning Microstructure and Frequency Conversion Performance of Lanthanide Nanomaterial by Impurity Doping

Y. Wang^{*1}; 1. Fujian Institute of Research on the Structure of Matter, CAS, China

In recent years, we have systematically investigated impurity doping behaviors and their impact on microstructures and frequency conversion performance of lanthanide (Ln^{3+}) nanocrystals (NCs), and lots of exciting discoveries have been explored. We evidenced that doping Ln^{3+} in alkaline-earth fluoride (MF_2) NCs allowed products with uneven size and shape to be easily converted into ultra-small nanospheres, and proposed a novel "transient electric dipole" mechanism to control nucleation and growth of NCs; we demonstrated that doping M ions into LnF_3 induced phase transition of hexagonal LnF_3 into cubic $\text{Ln}_{0.8}\text{M}_{0.2}\text{F}_{2.8}$ solid solutions, and resulted in 15 times intensified upconversion emission; we explored Ti^{4+} dopant-induced NaYF_4 phase transition from cubic to hexagonal at low temperature, and revealed the key role of Ti^{4+} ions, i.e., acting as the agglomerators for cubic NaYF_4 to accelerate its low-temperature phase transition; we found that addition of Gd^{3+} into NaYbF_4 NCs prompted phase conversion from cubic to hexagonal, reduced the size of NCs, and helped realizing tunable down- and up-conversion emissions, etc. As a conclusion, the impurity-doping strategy has a great potential in controllable syntheses and luminescent performance optimization for some nanomaterials potentially applicable in the fields such photovoltaic and photocatalysis.

(MCARE-S2-P003-2016) Spectral properties of Er^{3+} ions in Gd_2O_3 matrix

Y. Kuznetsova^{*1}; A. Zatsepin¹; 1. Ural Federal University, Russian Federation

Lanthanide ions are very well suited to use for down-conversion and up-conversion due to specialty of their energy levels structure (rich and ladder-like). In this context, Ln-doped inorganic phosphors are promising for practical important fields such as photonic, optoelectronic, sensing and photovoltaic. In this work we investigated spectral properties of Er^{3+} ions and excitation energy transfer mechanisms in host lattice Gd_2O_3 . Several excitation channels of Er^{3+} luminescence at 544 nm were observed: interband transitions, excitation by Gd^{3+} ions and intracenter excitation. Excitation of Gd^{3+} ions indicates that such ions cannot be located at regular lattice positions and may be associated with intrinsic defects of host lattice Gd_2O_3 . The mechanism of energy transfer from Gd^{3+} ions to Er^{3+} optical centers are offered and quantum efficiency of the Er^{3+} ions luminescence under intracenter excitation ($\eta_1=0,5$) and excitation by imperfect Gd^{3+} ions ($\eta_2=0,4$) are calculated. It is found that the most decay time of the Er^{3+} ions luminescence is observed under excitation by Gd^{3+} ions, however, the quantum efficiency in this case is less. It means that the major losses under indirect excitation take place at intermediate stages. So there is a reserve for minimizing these losses and the quantum efficiency of the Er^{3+} ions luminescence can be controlled by changes the defectiveness of host lattice Gd_2O_3 .

(MCARE-S2-P004-2016) Near-UV \rightarrow Red Down-Shifting $\text{Y}_2\text{O}_3:\text{Bi}^{3+},\text{Eu}^{3+}$ Nanosheets for Solar Cells

Y. Iso^{*1}; T. Matsunaga¹; Y. Kosuge¹; T. Isobe¹; 1. Keio University, Japan

$\text{Y}_2\text{O}_3:\text{Bi}^{3+},\text{Eu}^{3+}$ emits red light under near-UV excitation. $\text{Y}_2\text{O}_3:\text{Bi}^{3+},\text{Eu}^{3+}$ nanosheets are a promising candidate for transparent spectral converters for solar cells. The oxide nanosheets were produced by calcinating hydrothermally synthesized hydroxide nanosheets. An aqueous solution of $\text{Y}(\text{NO}_3)_3$ and $\text{Eu}(\text{NO}_3)_3$ was added to the ethylene glycol solution of $\text{Bi}(\text{NO}_3)_3$. After addition of triethylamine, the resulting suspension was heated in an autoclave at 160 °C for 1 h or more to obtain precursor nanosheets. After cooling, the product was centrifuged, and then dried. The resulting precursor was heated at a desired temperature to obtain $\text{Y}_2\text{O}_3:\text{Bi}^{3+},\text{Eu}^{3+}$ nanosheets. Transmission electron microscope observation confirmed that the sheet-like morphology remains

unchanged after calcination at 800 °C or less. The $\text{Y}_2\text{O}_3:\text{Bi}^{3+},\text{Eu}^{3+}$ nanosheets exhibited the red emission of Eu^{3+} at 612 nm through energy transfer from Bi^{3+} to Eu^{3+} following excitation of Bi^{3+} at ~331 nm. The change in photoluminescence (PL) intensity was measured during continuous excitation. The PL intensity decreased to more than 90% of the initial intensity soon after excitation began, and then the PL intensity recovered gradually. This result exhibits high photostability of $\text{Y}_2\text{O}_3:\text{Bi}^{3+},\text{Eu}^{3+}$ nanosheets under near-UV irradiation. The nanosheets were accumulated on an ITO-coated glass substrate by electrophoretic deposition to fabricate a down-shifting film.

(MCARE-S3-P005-2016) Phase transitions in compositionally graded ferroelectric superlattices

A. Razumnaya^{*1}; Y. Tikhonov¹; Y. Yuzyuk¹; N. Ortega²; K. Ashok²; R. Katiyar²; 1. Southern Federal University, Russian Federation; 2. University of Puerto Rico, USA

Near- and sub-Terahertz dynamics of soft and Debye-type central modes was studied by the polarized Raman spectroscopy in the series of ferroelectric $\text{BaTiO}_3/\text{Ba}_{1-x}\text{Sr}_x\text{TiO}_3$ (BT/BST-x) superlattices in the temperature range of 80-500 K where system undergoes the following sequences of phase transitions: paraelectric-tetragonal-monoclinic in BT layers and paraelectric-orthorhombic-monoclinic in BST-x layers. Due to relatively large periodicity the stress gradients exist in these BT/BST-x superlattices in the direction normal to the substrate and the phase transitions in alternating BT and BST-x layers occur at different temperatures and depend on chemical composition of the BST-x layers. It was shown that temperature evolution of the low-frequency Raman spectra can be described within the model of coexisting damped harmonic oscillator and Debye relaxator. The occurrence of the pronounced central mode can explain the recently observed relaxor-like dielectric anomalies in BT/BST-x superlattices. We demonstrate that variation of chemical composition of the BST-x layers allows to tune distortions in alternating layers and to modify the shape of the dielectric permittivity as a function of temperature.

(MCARE-S3-P006-2016) Quantitative local functional characterization at perovskite-spinel oxide interfaces in magnetoelectric composites

J. Ricote¹; I. San-Felipe¹; E. Vila¹; H. Amornin¹; W. Santa-Rosa²; M. Venet²; A. Castro¹; M. Algueró^{*1}; 1. Instituto de Ciencia de Materiales de Madrid (ICMM), CSIC, Spain; 2. Universidade Federal de São Carlos, Brazil

Magnetoelectric composites are being considered for a range of applications like the powering of low-energy devices from magnetic fields, either directional controlled ones (for the remote powering of bio-implanted devices for instance), or environmental ones (harvesting around high voltage transmission lines). Though best results have been obtained for cermets of high sensitivity piezoelectrics and giant magnetostriction alloys, ceramic composites of ferroelectric perovskite and magnetic spinel oxides might be advantageous for microsystems, for they may enable the use of standard methods for ceramic MEMS. Magnetoelectricity in these materials appears as a product property of the piezoresponses of the constituent phases. It is a thus strain-mediated and highly dependent of the characteristics of the oxide interfaces. In this communication we present a methodology based on piezoresponse force microscopy for the quantitative characterization of the local domain configuration and piezoelectric response in the ferroelectric component, devised for isolating interface effects from possible microstructural concomitant ones. Its application to a number of examples corresponding to the $\text{BiScO}_3\text{-PbTiO}_3/\text{NiFe}_2\text{O}_4$ and $(\text{K},\text{Na})\text{NbO}_3/\text{CoFe}_2\text{O}_4$ systems with different microstructural gradients is demonstrated.

(MCARE-S3-P007-2016) Poling effect on dielectric properties of lead-free $\text{Na}_{0.4}\text{K}_{0.1}\text{Bi}_{0.5}\text{TiO}_3$ relaxor ferroelectrics

V. Babu*¹; B. Bagyalakshmi¹; S. Balasubramanian¹; I. Manonmaniam Sundaranar University, India

Large recoverable energy-storage density is the desired feature in advanced pulsed capacitors. Energy-storage density of dielectric material is directly proportional to dielectric permittivity and square of operating field. Recently, large energy-storage density ($28.7\text{J}/\text{cm}^3$) was achieved in $(\text{Pb}_{0.91}\text{La}_{0.09})(\text{Zr}_{0.65}\text{Ti}_{0.35})\text{O}_3$ relaxor ferroelectrics. In the present work, electric field impact on dielectric response in lead-free $\text{Na}_{0.4}\text{K}_{0.1}\text{Bi}_{0.5}\text{TiO}_3$ relaxor ferroelectrics was studied. Rietveld refinement confirms the existence of morphotropic phase boundary. Grain size was estimated using liner intercept method from FESEM and it is $1.83\mu\text{m}$. Large piezoelectric constant ($215\text{pC}/\text{N}$) was obtained after poling at $3.3\text{kV}/\text{mm}$. Unpoled sample has strong frequency dispersion below T_d , corresponds to polar nano-domains, indicates behavior of RFE. Dielectric permittivity (ϵ_r) decreases with increase in frequency and temperature of maximum dielectric permittivity (T_m) shift towards higher temperature ($330\text{--}355^\circ\text{C}$). Reduction in dielectric diffusion (γ) from 1.81 to 1.61 and weak frequency dispersion was observed upon poling. This may be attributed to the transformation of polar nano-domains in RFE to micro-domains that results increase in dielectric constant. Improved ϵ_r upon poling may provide promising applications in energy storage devices.

(MCARE-S3-P008-2016) Electrical properties of BiFeO_3 thin films on different electrodes fabricated by Chemical Solution Deposition

P. Vilarinho*¹; I. University of Aveiro, Portugal

Bismuth ferrite (BiFeO_3 , BFO) is being hailed the most promising lead-free single-phase multiferroic candidate, due to its multiferroic nature above room temperature. However, dielectric losses, leakage current and tendency to fatigue of BFO are the main hurdles to overcome for any kind of electronic applications. Electrical properties of metal-ferroelectric-metal capacitors are also affected by the electrode. Pt is generally used due to its high electrical conductivity, good stability at high temperatures and a high Schottky barrier, which lowers the leakage currents. On the contrary, conductive metal oxide such as SrRuO_3 , IrO_2 , RuO_2 and LaNiO_3 (LNO) were found to be effective candidates to improve the fatigue behavior of PZT thin films. However, up to now, very few reports have been available on the dielectric and ferroelectric behaviour of chemical solution deposited BiFeO_3 thin films on LaNiO_3 and IrO_2 electrodes and no research focusing on the comparative study of oxide electrodes and Pt was conducted. In the present study, thin films of BiFeO_3 were prepared by CSD on $\text{Pt}/\text{TiO}_2/\text{SiO}_2/\text{Si}$, $\text{IrO}_2/\text{TiO}_2/\text{SiO}_2/\text{Si}$ and $\text{LNO}/\text{Pt}/\text{TiO}_2/\text{SiO}_2/\text{Si}$ substrates by spin-coating. The effect of IrO_2 and LNO electrodes on the growth and electrical properties of BFO thin films is investigated.

(MCARE-S3-P009-2016) The size and pressure effect on the magnetic and magnetocaloric property in HoCrO_3

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HoCrO_3 bulk powders with different grain sizes (100 - 450 nm) were synthesized via a sol-gel method by controlling the annealing temperature ($700\text{--}1300^\circ\text{C}$). The phase purity of the samples were examined by X-ray diffraction and Raman spectroscopy. The grain sizes were determined by SEM images. The magnetization data of samples with different grain sizes changes systematically with magnetic field. It is observed that the larger the grain size is, the larger the magnetic hysteresis is, which is quantitatively described by the dependence of coercive field and remnant magnetization on temperature. The magnetocaloric property show systematic dependence on the grain size. Also, by applying different pressure on the HoCrO_3 pellet, the pressure effect on the structural, magnetic and magnetocaloric property were studied.

(MCARE-S3-P010-2016) Novel lead free flexible composites for energy harvesting and sensor applications

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For a long time, the dominant piezoceramics has been based on lead zirconium titanate ($\text{Pb}(\text{Zr}_{(1-x)}\text{Ti}_x)\text{O}_3$ or PZT). In the present study, the preparation and dielectric and piezoelectric properties of potassium sodium niobate (KNN) based lead-free piezoelectric composites are investigated for sensor applications and energy harvesting. A novel double step calcination process route does lead to the formation of pure, $2\mu\text{m}$ large cubic Li-doped KNN particles. This allows the formation of long chain like structures with minimal topological defects during the dielectrophoretic structuring of KNN-epoxy composites. The structural, microstructural and piezoelectric properties are investigated and discussed in detail. The inter-particle distance between the particles within the chain is around $0.3\mu\text{m}$ which is very much lower than the similar systems. The value of the piezoelectric voltage coefficient of the structured 10 vol. % structured KNN- epoxy composites also exceeds that of all values for such functional composites reported in the literature. The double calcination strategy for KNN ceramic powder in combination with a dielectrophoretic structuring process opens a new route towards lead-free piezoelectric composites with enhanced properties for sensor and energy harvesting applications.

(MCARE-S4-P011-2016) Evaluation of precipitated $\text{Na}_3\text{Zr}_2\text{F}_{13}$ powder from the waste pickle acid

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The nuclear fuel cladding tube is made through pilgering and annealing process. In order to remove oxide film on the surface and foreign material, the pickling process proceeds. The Zirconium (Zr) is dissolved in acid solution during the pickling process and pickling waste solution in the dissolved Zr is discarded as waste. The solution precipitated by the NaF to recycle the dissolved Zr. Pickle liquors become contaminated with dissolved metals through use. As the metal concentration increases, the free acid concentration decreases and pickling efficiency drops. Additions of fresh concentrated acid are made from time to time to rejuvenate the bath but eventually it becomes spent and must be discarded. In this paper, we investigated the precipitation process of Zr^{4+} ions containing pickling acid by NaF. The characteristics of precipitated powders versus concentration of NaF were investigated and a chemical pathway for $\text{Na}_3\text{Zr}_2\text{F}_{13}$ formation is proposed.

(MCARE-S4-P012-2016) Fabrication of SiC/SiC Joints for LWR Fuel Cladding Tubes by a Diffusion Bonding Method

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SiC-based fuel cladding tubes for application into a light water reactor are being developed to enhance safety against accidents. A pressureless joining method as well as a radiation tolerant joining interface is a prerequisite for the fabrication of cladding tubes. In this study, a diffusion bonding method using metallic interlayer materials was developed for the joining of SiC ceramics. Placing a Ti foil as a main interlayer material, Si powders and/or coatings were used additionally to form the SiC/SiC joint. Joining at $1450\text{--}1510^\circ\text{C}$ under a vacuum resulted a high joining strength up to 100MPa in a torsion test. The joint interface was composed of TiSi_2 , SiC, and Si. TiSi_2 was formed by the diffusion reaction of Ti foil with Si melt. This joining mechanism was consistent when the joining was performed using a laser beam scanning. Ti foil was inserted between SiC monoliths, and Si powder was supplied during the laser beam scanning. The interlayer materials were melted instantaneously and solidified under the laser beam irradiation. A direct interlayer-forming was also performed by supplying both the Ti and Si powders simultaneously. The TiSi_2 interlayer compound was formed at the joined SiC/SiC interface. However, the reaction zone was inhomogeneous when the laser beam was applied as compared to the conventional diffusion bonding process.

(MCARE-S4-P013-2016) Alkali Fluorides and Chlorides

Characterized by TG-DSC-MS

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Fluoride and chloride mixtures or similar low melting eutectics of inorganic salts are interesting candidates as heat exchanging materials. The determination of the thermal properties, like melting point and enthalpy, thermal stability and also impurities in commercial batch material are important physical and chemical data for the technical employment. Thermal Analysis techniques like TGA and DSC are standard methods for the characterization of the thermal stability and energetic effects of materials. Evolved gas analysis techniques, like mass spectrometry, can help to identify possible evaporating gaseous products. Some of the problems are to choose the right container material for these substances. First, the sample must not react with the crucible material. Another critical point is the creeping ability of the molten salts due to wettability. In this contribution some container/sample material combinations will be discussed. Finally the melting behavior and impurities in several commercial salts detected by TG-DSC-MS will be shown.

(MCARE-S5-P014-2016) Layered double hydroxide electrode materials for today's fuel cell technology: Structural and electrochemical investigations

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Layered double hydroxides (LDHs) have been widely investigated in the past years due to their unique physicochemical properties and promising applications in chemical power sources, such as fuel cell devices. In this work we attempted to study the structural and electrochemical behavior of LDH materials modified carbon electrodes. LDH nanoparticles with Mg²⁺/Al³⁺ metal cations (at three metal ratios, 2:1, 3:1 and 4:1), with different countervailing anions (Cl⁻, NO₃⁻, CO₃²⁻) in the interlayer space and at different synthesis pH were synthesized by the co-precipitation method and tested as modified carbon electrodes (glassy carbon and carbon felt). The LDH compounds were characterized by XRD, FT-IR, SEM and TEM. The results showed that the as prepared samples were well-crystallized and hexagon layer structure. Also, we systemically investigated the electrocatalytic performance of MgAl nanoparticles in 10 mM K₄Fe(CN)₆ + 20 mM PBS (pH = 7.4). CV and EIS measurements were used in order to identify the oxidation and the reduction processes on the surface of the material. The behavior of the modified electrode prove that the electronic conductivity of the bulk material is dependent on the Mg²⁺/Al³⁺ molar ratio, the synthesis pH and the nature of the interlamellar anion and results the limiting parameter of the overall redox process.

(MCARE-S5-P015-2016) Microstructural Investigation of LSM/YSZ Composite Anode Materials for Solid Oxide Electrolysis Cells

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Solid oxide electrolysis cell (SOEC) is a promising technology for hydrogen production that will contribute to the sustainable energy of the future. An important component of this SOEC is the anode material and one of the promising anode material for such application is the Sr-doped LaMnO₃ (LSM) and Yttria-stabilized ZrO₂ (YSZ) composite material. In this study, LSM/YSZ with different weight percent compositions of LSM and YSZ were synthesized using combined solid-state reaction method and glycine-nitrate process. The obtained samples, 60LSM/40YSZ and 40LSM/60YSZ, were fully characterized for its microstructure using X-ray diffraction, TG/DTA, FTIR, SEM/EDS, and TEM/ED. TG/DTA analysis of the resulting LSM/YSZ composite revealed that the major weight loss due to the combustion of organic compounds occurred between 650°C and 850°C. EDS analysis confirmed that the actual elemental composition of the sample matched well with the theoretical computations made. Surface morphology of the sample via SEM exhibited a

well sintered and densified samples and revealed a beveled cube-like LSM morphology while the YSZ phase appeared to have a sphere-like microstructure. In addition, AC impedance measurement at intermediate temperature range (400-700°C) of the synthesized samples have been investigated.

(MCARE-S6-P016-2016) SURMOF/CNC based Designer Solids for Photonic, Optical and Energy Applications

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Here we present a particularly interesting class of surface-anchored (metal-organic frameworks and coordination network compounds) materials SURMOFs and CNCs for the fabrication e.g. of 1D (Photonic Band Gap) PBG materials, as optical sensors, low-*k* dielectric thin films, optoelectronic/electrochromic devices or as future artificial Light-Harnessing (LH) Antenna array assemblies for future PV applications.

(MCARE-S6-P017-2016) The combustion synthesis of FeTi alloy powders and the effect of additives

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In this paper, the synthesis of TiFe alloy powders from FeTiO₃+aMg mixture was investigated by a combustion method. The combustion parameters (maximum temperatures and wave propagation velocities) were evaluated using temperature-time profiles recorded in the combustion wave by thermocouples. A decrease in temperature from 1750 to 1635 °C was recorded with an increase in Mg concentration from 3 to 6 mole. X-ray diffraction analysis revealed pure-phase TiFe for Mg concentration in 4-6 mole range. FESEM studies revealed only micrometer size and shapeless alloy particles with molten morphology. The amount of oxygen in the final TiFe powder was 0.5- 2.5 wt% range upon Mg concentration. We also examined the effect of certain additives (NaCl, Mg(OH)₂, KClO₄) on the morphology and purity of FeTi alloy powders. The corresponding results were discussed in the context with the reaction mechanism. The process proposed in this study showed the possibility of being a new attractive production method for TiFe hydrogen storage alloy.

(MCARE-S6-P018-2016) Electrowinning of Al-Sc alloys in CaF₂-NaF-Na₃AlF₆-Al₂O₃-Sc₂O₃ electrolyte

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Sc metal has been used for increasing yield strength of Al alloys. Al-Sc master alloys has been very important bridgehead to the role of upstream and midstream of Al materials for aviation. So, demand of scandium has been increased in worldwide. Scandium was reduced by electrowinning process with Al liquid cathode. In this study, electrochemical investigation was performed and Al-Sc alloy was reduced by electrowinning process at 1000°C. Blank salt was CaF₂-NaF and adding Na₃AlF₆, Al₂O₃ and Sc₂O₃ in sequence. Na₃AlF₆ was added as 1, 5, 10, 15, 25wt%. Al₂O₃ and Sc₂O₃ were added as 2wt% respectively. Effects of Al₂O₃ and Sc₂O₃ addition in CaF₂-NaF-Na₃AlF₆ molten salts system were evaluated by cyclic voltammetry and chronopotentiometry. The constant current was applied -40mA, Al-Sc alloys with the scandium content of 0.16wt%.

(MCARE-S7-P019-2016) Inverted hybrid solar cells based on metal oxide nanomaterials and P3HT

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The organic-inorganic hybrid solar cells have received much attention because of ease and low cost fabrication, but devices efficiency is still low. We present hybrid solar cells based on metal oxide and P3HT. The copper oxide (CuO) and nickel oxide (NiO) are p-type semiconductor materials with band-gap energies of ~1.5 eV and ~3.5 eV, respectively. The NiO and CuO nanoparticles can be easily synthesized by a solution method, and they are easily incorporated into P3HT:PCBM polymer solar cells. The structural, optical and electrical characteristics of these materials have been investigated by FE-SEM, X-ray diffraction, UV-Vis absorption spectroscopy

and Hall Effect measurements. The hybrid solar cells based on the mixture of metal oxides and P3HT:PCBM showed enhanced power conversion efficiency as compared with the P3HT:PCBM-only devices.

(MCARE-S7-P020-2016) Perovskite Solar Cells with Nanoimprinted Mesoporous TiO₂ Thin Films

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Perovskite solar cells have recently attracted as their high energy conversion efficiency, low-cost production, simple process such as solution techniques at low temperatures, and flexibility. The increasing light harvesting is the best way to improve the energy conversion efficiency of solar cells. However, it is difficult to adapt the light harvesting materials in perovskite solar cells because the device architectures consist of thin film layers. Proper engineering of solar cell structure can improve the device performance. Here we used nanoimprint lithography technique to well-ordered nanoimprinted layer of mesoporous TiO₂ on TiO₂/FTO substrate. The nanoimprinted layer resulted in ideal scattering characteristics for optimum light trapping. Compared to the plain layer of mesoporous TiO₂, the nanoimprinted-layers device yielded 11.71% increase of power conversion efficiency.

(MCARE-S7-P021-2016) Noble Metals (Pt, Au, Ag) Doped Graphene for Photovoltaic Applications

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Metal-decorated graphene materials are highly important for photovoltaic devices. In this work, noble metal doped-graphene hybrids were prepared by a simple and scalable microwave assisted method. The thermal reductions of metal doped-graphite oxide precursors were carried out in nitrogen atmospheres and the effects of the metal components on the electrical and optical properties of the hybrid materials were studied. The solar cell application of the synthesized materials, when used as a charge transfer amplifier in inverted structure of hybrid solar cell is investigated. The metals significantly affected the light trapping due to their nano size (i.e., plasmonic effect), which is important in energy production in solar cell devices.

(MCARE-S7-P022-2016) Enhanced electron transport on active layer with TiO₂ nanotube arrays in perovskite solar cells

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The device architectures of perovskite solar cells consist of mesoporous metal oxide, perovskite structures, hole transfer materials, and top electrode. To improve the energy conversion efficiency, we studied the metal oxide, halide in perovskite, or hole transfer materials. Mesoporous TiO₂ nanoparticles (NPs) are used as the electron acceptor and scaffold in perovskite solar cells because of their transmittance, crystallinity, stability, and large band gap. Compared to 0-dimensional structures, the electron transport is much improved with 2- or 3-dimensional structures. TiO₂ nanotubes (NTs) arrays were prepared by an electrochemical method and used for make TiO₂ NPs/NTs composite films. We optimized the perovskite solar cells with using the TiO₂ NPs/NTs composite films and obtained higher energy conversion efficiency than that of device only with TiO₂ nanoparticles films.

(MCARE-S8-P023-2016) Composite flexible based on PZT/CNT/cellulose

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The piezoelectric effect has contributed to obtain materials able to capturing the mechanical wasted energy, but the vast majority of piezoelectric materials are ceramics crystal, which are rigid and in some applications there is need of flexible materials. Other materials which often is not sufficiently exploited and that can enhance

several properties are rare-earth elements. Thus, the present work aims to achieve piezoelectric properties under a flexible matrix. For this nanosized crystals Lead zirconate titanate (PZT) doped with rare-earth are functionalized in composites of cellulose attached to carbon nanotubes (CNTs). The first step should be obtained through the chemical bond between CNTs and cellulose extracted from the banana stalk. The resulting pulp is then linked to the nanotubes through esterification reaction for that nanotubes are carboxylated. The synthesis consists in a reaction between the cellulose and the carboxylated nanotubes in the presence of hydrogen as catalyst (H₂SO₄). The second step is realized the synthesis and deposition of PZT doped with rare-earth on cellulose. This was conducted by microwave hydrothermal synthesis (MHS) reaction with the cellulose is present inside the reactor with the precursors of the PZT doped. The composite electric and piezoelectric properties as function rare earth doping was monitored.

(MCARE-S8-P024-2016) Flexible composite from hydrothermal synthesis

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Lithium niobate (LiNbO₃) is an important ferroelectric material with a wide-range of applications. The use of microwave radiation to improve the hydrothermal synthesis of pure nanocrystalline LiNbO₃ was proposed to growth direct on carbon fiber substrate. Herein study reported, HNO₃-treated CF was used as the substrate for the loading of LiNbO₃. The novelty was achievement of the nanocomposite with LiNbO₃ nanoparticles grown on carbon fiber successful by hydrothermal synthesis assisted by microwave (MHS). This method offers quick, clean, cost-effective, and energy-efficient synthesis, producing a homogeneous layer of LiNbO₃ with controlled thickness. Nanoparticles prepared via MHS. The present study report a reproducible, single method to manufacture CF/LiNbO₃-MHS nanocomposites, that allow the control of the thickness of LiNbO₃ layer over CF. This synthesized nanocomposite allow opportunities in advanced applications based on electrochemical or piezoelectrics composites besides the development of flexible materials.

(MCARE-S8-P025-2016) High Power Triboelectric Nanogenerator based on nanocomposite materials

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We discuss simply fabricated BaTiO₃ / P(VDF-TrFE) nanocomposite based high performing triboelectric nanogenerator for various applications and wearable electronics. Recently, many of energy harvesting generation systems including piezoelectric, triboelectric nanogenerator, and hybridized types with electromagnetic induction might have been focused on structural design, which assumed to be important in aspect of various applications. However, it is also quite necessary to study new type of materials to explore any possibilities to overcome traditional triboelectric materials such as PTFE, Nylon, and typical metal. Here, we integrate the high dielectric material, BaTiO₃, with P(VDF-TrFE) which is apt to attract electrons due to the presence of the fluorine group. With this new type of composite as a triboelectric material, electric performance was 330 V of output voltage and 260μA of output current under gentle tapping. This work suggests that new type of nanocomposite based triboelectric nanogenerator with splendid performance under general force arisen by common human movement.

(MCARE-S8-P026-2016) Nanopatterned Yarn Based Wearable Triboelectric Nanogenerator

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There has been increasing demand for highly efficient portable energy harvesters due to the development and mass consumption

of portable electronic devices. Photovoltaic, thermoelectric, piezoelectric and triboelectric energy scavengers have become strong candidates for portable energy harvesters in future self-powered portable electronic device applications. Among these, Triboelectric energy harvesters that can convert mechanical energy into electrical energy have recently attracted attention. In this study, we report the textile based as a substrate for foldable and the wearable triboelectric nanogenerators. Nano-size patterned PDMS on the conductive woven fabric substrate by dip-coated method. For practical applications, nanopatterned yarn based nanogenerator showed the continuous driving of the liquid crystal display screen and light emitting diode successfully. Furthermore, textile based power generator showed high sensitivity acts low applying for of under 1kgf. The results presented here may create new possibilities for energy harvesting wearable devices, particularly in applications that require wearability and flexibility.

(MCARE-S8-P027-2016) Enhanced Triboelectric Nanogenerators based on the stretchable electrode

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Harvesting energy from ambient mechanical and solar energy sources is highly desirable for powering portable electronics, biomedical, and healthcare applications. Most recently, a new type of power generating device, named as triboelectric nanogenerator (TENG) based on triboelectric effects coupled with electrostatic effects have been demonstrated as powerful means of harvesting mechanical energy from living environment. Here, we demonstrate significantly improved the output performance for stretchable electrode based triboelectric nanogenerator. The fabricated TENG is based on the contact and separation between the silver nanowire (Ag NWs) conductors and the PTFE film. We report a highly conductive and stretchable conductor with Ag NWs embedded in the surface layer of poly(dimethylsiloxane) (PDMS). The physics/mechanics origin of such stable conductance is investigated. The stretchable conductors show excellent robustness under repeated mechanical loading. Different Ag NWs TENG were fabricated by variation of the applied Ag NWs concentration from 3.9 to 390 × 10³ mg/m². Higher applied Ag NWs resulted in greater roughness. As expected, the effective surface area expanded as the surface roughness increased. In general, a larger contact area produced higher triboelectricity. Output currents from TENG increased at least 3 times with Ag NWs stretchable electrode.

(MCARE-S8-P028-2016) Nano-scale Mechanisms Contributing to Lead-Free Electro-mechanical Properties

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The characterization of nano-scale mechanisms is important in controlling electro-mechanical properties in materials. Currently, lead-based materials dominate the market, but there is a need to replace these materials with lead-free alternatives possessing similar properties. Na_{1/2}Bi_{1/2}TiO₃ (NBT) is a potential alternative that shows promising electro-mechanical properties, however, the origin of such properties from nano-scale atomic interactions is poorly understood. A unique method to assess the nano-scale structures of materials is diffuse x-ray scattering, which can probe the deviations away from the average atomic structure. This study evaluated the effect of BaTiO₃ doping and application of *in-situ* electric fields to the nano-scale structure as observed by diffuse scattering. Results showed diffuse scattering features from NBT that sheds light on the nano-scale features; 1) weak satellite reflections, that have not been detected through other methods, signifies a structural modulation existing; 2) superstructure reflections show an oxygen-octahedral tilt system that is dependent on BaTiO₃ doping and application of electric fields and; 3) distinct broadening of diffuse scattering around the Bragg reflections that indicate the local environments of Na and Bi. These features will be modelled through Monte Carlo methods to elucidate the origin of the electro-mechanical properties.

(MCARE-S9-P029-2016) Enhancing thermoelectric performance of Ca(Sr)CoO ceramics through Ag-adding

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Ca_{2.95}Sr_{0.05}Co₄O₉/Ag composites were prepared by solid state reaction method. The structural and morphological properties were researched by X-ray diffraction analysis and scanning electron microscopy, respectively. By adding Ag particles, the Seebeck coefficient, S(T), and electrical resistivity, ρ(T), of composites decrease. The thermoelectric performance of Ca_{2.95}Sr_{0.05}Co₄O₉ was improved as a consequence of the significant reduction in electrical resistivity with Ag adding. The composites exhibit maximum values for the thermoelectric power factor, PF=S²/ρ, close to 14 μW/K²-cm. Thus, the behavior observed in the transport properties become these composites promising materials for use in thermoelectric devices for room-temperature applications.

(MCARE-S9-P030-2016) Thermal conductivity investigation of several half-Heusler compounds

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We have measured the thermal conductivity in a family of doped n-type half-Heusler alloys (Hf_{1-y}Zr_y)NiSn_{1-x}Sb_x (0.03 < x < 0.05; y = 0.35, 0.4). We have observed that the substitution of Sb on the Sn-site results in a beneficial reduction of the thermal conductivity. Subsequently, an investigation of ZrO₂ nano-composites added into the (Hf,Zr)NiSn samples was performed and the results show that ZrO₂ nano-composites will contribute to decrease the thermal conductivity. In this investigation we observed that the sample, Hf_{0.6}Zr_{0.4}NiSn_{0.995}Sb_{0.005} [or conversely, (Hf_{1-y}Zr_y)NiSn_{1-x}Sb_x where y = 0.4 and x = 0.005] exhibits the lowest thermal conductivity, which is nearly 3 W/m-K at 600K. The decreasing of the lattice thermal conductivity could be attributed to the increase the phonon scattering by the mass differences in Hf and Zr and the presence of the ZrO₂ nano-composite inclusions. Whereas, introducing the Sb on the Sn site will most likely be affecting the band structure and thus the electronic properties. Further measurements are in progress to determine the electronic properties at high temperatures and thus estimate the lattice thermal conductivity.

(MCARE-S10-P031-2016) Electrochemical Evaluation of Li₇La₃Zr₂O₁₂ Li-ion Conducting Solid Electrolyte

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In order to obtain a much safer and longer lasting battery, investigation of materials that can replace the flammable organic liquid electrolyte has been the trend of recent researches on Lithium and Lithium-ion batteries. And one promising candidate solid electrolyte material is the Li₇La₃Zr₂O₁₂ (LLZ). Hence, in this study, LLZ was synthesized via solid state reaction and investigated for its electrochemical performance. Full microstructural and thermal characteristics of the obtained samples were conducted using X-ray diffraction, FTIR, TG/DTA, SEM/EDS, and TEM. Results show that sintering at lower temperature (1000°C) produced tetragonal LLZ while sintering at higher temperatures (≥1150°C) produced cubic LLZ. SEM/EDS analyses revealed a dense LLZ pellet with homogeneous elemental distribution. On the other hand, AC impedance measurement revealed an ionic conductivity value of about 1.0 × 10⁻⁴ S/cm. In addition, an all-solid-state battery cell using the LLZ solid electrolyte was successfully fabricated and its electrochemical properties have been investigated.

(MCARE-S10-P032-2016) Silver based fast ion conducting glassy electrolyte: Promising material for solid state battery applications

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We present electrical nature of various silver based glasses (D% AgI-(100-D)%{M Ag₂O-F [(1-x)B₂O₃- x TeO₂]}]; synthesized by melt quenching method. D is dopant salt, M is glass modifier and F is

glass former. The glassy nature of all the samples was established by X-ray diffraction. The d.c and a.c conductivity measurements were carried out in the temperature range of 300–423K and found to increase from 10^{-4} - 10^{-1} Scm⁻¹ with increase in dopant (AgI) concentration at room temperature. The impedance was measured in the frequency range of 1kHz-3MHz and analyzed using Z-View equivalent circuit software. A.C and d.c activation energy decreased from 0.36 to 0.19 eV. The quantitative analysis of these results for all synthesized samples indicates that the electrical conductivity and transport number of silver borate glasses is enhanced with increase in dopant concentration. These observations of conductivity with dopant concentration are explained by correlating FTIR, DSC and conductivity results with conduction path model. Based on transport number and conductivity values, we conclude that these glasses are ionic conductors. Solid state batteries were fabricated with different types of cathode materials and open circuit voltages (OCV) were measured and compared. It is found that the glass with 70% dopant concentration shows enhanced ionic conduction and better OCV value.

(MCARE-S11-P033-2016) Preparation of highly porous carbon fibers from natural resources and their hydrogen storage characteristics

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Hydrogen is an advantageous energy source because it is renewable and its use would reduce the emission of pollution. The success of hydrogen economy in the future depends on our ability to discover efficient and cost-effective hydrogen storage materials. Considerable scientific efforts have been made to study carbon materials, metal-organic frameworks, metal hydrides and so on. Among the above promising materials, carbon-based materials have received continuous interest as potential hydrogen storage media due to their high surface areas, tunable texture structures and low gas-solid interactions, which provide high hydrogen uptake capacity. In this regard, highly porous carbon fibers have been successfully prepared via wet spinning and carbonization process using the cellulose derived from rice straw and paper mulberry. From the comparison of the morphological structure and specific surface area, the porous carbon fibers derived from rice straw shows a high specific surface area of 2260 m²/g. This material exhibits excellent hydrogen storage properties with a gravimetric hydrogen uptakes of 4.35 wt.% at 77K and 10 bar. In addition, it is also found that hydrogen storage capacity of porous carbon fibers could be influenced according to the source materials because the type of source materials could determine the physico-chemical properties of pristine cellulose.

(MCARE-S12-P034-2016) Surface wettability and optical properties of nanostructured ZnO/SiO₂ thin films by sol-gel method

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Thin layer of pure zinc oxide and zinc oxide includes different weight percent of silica (10%, 20%, 30% and 40%) have been prepared over the quartz glasses by sol-gel dip coating. Powders were dried 48 hours at oven in 150 C and then heat treated in 500 C for one hour. Obtained crystallite size of zinc oxide were 17, 21, 24 nm for pure ZnO, ZnO-10%wt SiO₂ and ZnO-20%wt SiO₂ thin films respectively. Wettability, optical and morphological properties of heat treated thin films was investigated at 500 C. Roughness of the surface was decreased by adding more silica according to atomic force microscope evaluation. Using more silica content also altered the Band gap energy from 3.27 eV to 3.39 eV. Hydrophilic properties of the surface was improved by addition of 20% silica to zinc oxide and low contact angle (15 degree) observed under UV light radiation accordingly.

(MCARE-S12-P035-2016) The modeling of Cold crucible induction heating for the metal 3d printing technology using Ti grade 5

Y. Kim^{*1}; D. Kim¹; J. Lee¹; 1. Chungnam National University, Republic of Korea

The metal 3D Printing Technologies, which can apply complex design, have been rapidly developed recently. Ti grade 5 is commonly used for metal 3d printing technology. In metal 3d printing technology, manufacturing of metal powder is most important process for 3d printing industry. But, manufacturing of Ti grade 5 powder is difficult because of its high melting point and reactivity with crucible materials using commercial atomization method. Fortunately, cold crucible melting process can produce Ti grade 5 powder. The skull would be generated and it protects the furnace itself by using cold crucible method. To control metal flow from the cold crucible to the orifice nozzle, we need to calculate a shape of skull and thermal behavior in cold crucible. The COMSOL multi-physics and induction heating model were used to calculate equilibrium of the skull shape. The calculation were performed at various frequency of coil, applied energy (W) and the number of coils.

Wednesday, April 20, 2016

Plenary Session III

Room: Salon E

8:30 AM

(MCARE-PL-003-2016) Next-generation Battery Chemistries: Materials Challenges and Prospects

A. Manthiram^{*1}; 1. University of Texas, Austin, USA

Development of clean, sustainable, alternative energy technologies is needed to meet the increasing demand in global energy use and to mitigate the growing environmental concerns. Renewable energy sources, such as solar and wind, will not have the anticipated impact unless we develop an efficient and economical way to store and deliver the electricity produced from the intermittent renewable sources. Rechargeable batteries are most promising option for such electrical energy storage. They are also the only viable near-term option for transportation. However, a widespread adoption of battery technologies for these large-scale applications requires optimization of several critical parameters: cost, cycle life, safety, energy density, power density, and environmental impact, all of which are directly linked to severe materials challenges. After providing a brief account of the current status of battery technologies, this presentation will focus on the development of new materials, cell chemistry, and cell configurations to overcome current problems. Specifically, the challenges and approaches of transitioning from the current insertion-compound electrodes in lithium-ion batteries to new conversion-reaction electrodes with multi-electron transfer per atom will be presented. The systems include safer antimony-based anodes, lithium-sulfur cells, sodium-sulfur cells, and hybrid lithium-air cells with a solid electrolyte.

S4: Material Challenges in Nuclear Energy

Nuclear Energy I

Room: Salons A-C

Session Chairs: Yutai Katoh, Oak Ridge National Laboratory; Qing Huang, Ningbo Institute for Materials Technology and Engineering

9:50 AM

(MCARE-S4-001-2016) High temperature oxidation behavior of cladding materials for nuclear applications (Invited)

H. J. Seifert^{*1}; 1. Karlsruhe Institute of Technology, Germany

Presently Zirconium-base alloys ("Zircalloys") are frequently-used cladding materials for applications in light water reactors (LWR). However, it became evident during the Fukushima Daiichi event that there is a need for advanced fuel-cladding systems which allow the use for extended time-periods and showing increased safety performance especially in case of accidents. Several alternate cladding materials/component systems are under worldwide investigation, such as silicon carbide matrix composites, MAX-phases (e.g. Ti_2AlC) and FeCrAl(RE) alloys, respectively. All of them show promising high-temperature chemical properties which might result in enhanced accident tolerance. The aim of our research work is to study chemical and microstructural behavior of new type of Zircalloys as well as alternate cladding materials in high-temperature and oxidizing environments. In particular, silicon carbide and silicon carbide-based composites show outstanding behavior in corrosive atmospheres. Their oxidation in dry and wet atmospheres was experimentally and theoretically studied up to 2000 °C. Also, the steam oxidation behavior of bulk Ti_2AlC was investigated in the temperature range of 1400°C-1600°C. In all cases, the development of oxide, nitride and oxinitride scales and correlated microstructures were investigated at different stages of environmental influences.

10:20 AM

(MCARE-S4-002-2016) Hydrothermal Corrosion of SiC Joints

T. Koyanagi^{*1}; Y. Katoh¹; K. Terrani¹; J. Kiggans¹; Y. Kim²; T. Hinoki³; 1. Oak Ridge National Laboratory, USA; 2. GE Global Research, USA; 3. Kyoto University, Japan

Silicon carbide fuel cladding system is attractive for accident tolerant light water reactor applications. Development of joining technology is a key issue for this application. Hydrothermal corrosion is one of the most important phenomena considered under the normal operation. This paper discusses hydrothermal corrosion behavior of 4 types of SiC joints in PWR and BWR relevant chemical conditions. The experiments were conducted in an autoclave system at GE Global Research Center. High-purity SiC bonded specimens were prepared by diffusion bonding with titanium and molybdenum inserts, slurry bonding using Ti-Si-C system, and liquid phase sintering SiC nano-powder. Most of the joints withstood the corrosion tests for 5 weeks. Corrosion rate of the bonding layers and microstructural changes of the joints will be presented. This work was sponsored by the U.S. Department of Energy, Office of Nuclear Energy, for the Fuel Cycle Research & Development program under contact DE-AC05-00OR22725 with Oak Ridge National Laboratories managed by UT-Battelle, LLC.

10:40 AM

(MCARE-S4-003-2016) Instrumented Irradiation Creep Experiment with FeCrAl Alloys and SiC (Invited)

K. Terrani^{*1}; Y. Katoh¹; Y. Yamamoto¹; L. Snead²; T. Karlsen³; 1. Oak Ridge National Laboratory, USA; 2. Massachusetts Institute of Technology, USA; 3. Halden Reactor Project, Norway

FeCrAl alloys and silicon carbide (SiC) ceramic composites are leading candidates for accident-tolerant fuel cladding for light water reactors. Dimensional stability in irradiation environment is among the key data gaps toward comprehensive understanding

of cladding behavior with these materials. In this study, irradiation creep and swelling of selected Fe-13Cr-5Al alloys and high purity, chemically vapor-deposited SiC are evaluated through a neutron irradiation experiment, instrumented for temperature and strain in a uni-axial tensile configuration, in Halden reactor. The FeCrAl specimens are tested at 350°C whereas the SiC tests are being carried out at 300°C. The initial data indicated typical power-law transient swelling for unloaded SiC and additional transient creep for loaded SiC. The FeCrAl creep strain appeared to largely vary depending on the material composition. Research sponsored by the Fuel Cycle R&D program, Office of Nuclear Energy, US Department of Energy, under contract DE-AC05-00OR22725 with UT-Battelle, LLC.

11:10 AM

(MCARE-S4-004-2016) SiC/SiC composites processing for advanced nuclear reactors

C. Sauder^{*1}; J. Braun¹; G. Loupiaz¹; D. Bossu¹; L. Briottet¹; B. Riccetti¹; 1. CEA, France

Owing to the recent progress in the fabrication of stoichiometric fibers with a good stability under neutron irradiation, SiC/SiC composites are candidate of prime interest for nuclear applications in GenIV nuclear power plant and even for Accident Tolerant Fuel (ATF) in Light Water Reactors (LWRs). In this work, some potential applications of these materials in advanced nuclear reactors will be described in details with manufacturing processes related to each application. Cladding application is a major issue for these materials, due to specific requirements, such as severe dimensional tolerances, gas tightness, and thermochemical compatibility with fuel and coolant up to very high temperature. Solutions that are developed in CEA will be presented with some promising results. Another example of a core application, dedicated to Sodium Fast Reactor (SFR), will be described. This application requires the processing of a large Hexagonal tubular structure of SiC/SiC composite. This lead to specific difficulties during processing due to the small size of SiC commercial tows. Last, it will be described how this work, dedicated to nuclear applications, could be useful for a lot of other applications (in aeronautic, nanotechnology industries ...).

11:30 AM

(MCARE-S4-005-2016) Mechanical Properties of SiC/SiC Ceramic Matrix Composite Tubes for Accident-Tolerant Fuels

G. Singh^{*1}; Y. Katoh¹; K. Terrani¹; 1. Oak Ridge National Laboratory, USA

Stability of SiC/SiC composites in nuclear reactor off-normal conditions makes it a promising candidate for the accident tolerant fuel clad system. In this work tubes made of SiC/SiC CMC with Hi-Nicalon Type S fiber, CVI SiC matrix and pyrocarbon interlayer were mechanically tested. The mechanical properties of the SiC/SiC composite tubes were determined using the axial and hoop tensile tests based on ASTM standards. This work will contribute towards expanding the limited database of the mechanical properties, particularly the statistical aspects, for this material. Research sponsored by the Fuel Cycle R&D program, Office of Nuclear Energy, US Department of Energy, under contract DE-AC05-00OR22725 with UT-Battelle, LLC.

S6: Critical Materials for Energy

Critical Materials for Energy I

Room: Salon F

Session Chairs: Wei-Sheng Chen, National Cheng Kung University;
Anja Waske, Leibniz-Institute for Solid State Materials Research

9:50 AM

(MCARE-S6-001-2016) Challenges and Opportunities in Recycling Rare Earth Materials (Invited)

R. T. Ott^{*1}; 1. Ames Laboratory (USDOE), USA

Rare Earth (RE) elements are essential to numerous advanced technologies including many green energy technologies. Despite the critical nature of REs, however, the implementation of large-scale recycling technologies has been limited. In this talk, we discuss the challenges associated with developing RE recycling processes that can be scaled-up to industrial size. Using our work on liquid metal extraction of REs from magnet scrap as a demonstration of technology, we discuss the effectiveness of this process in recovering RE metals and the suitability of these recovered RE metals for incorporation into new products (e.g., new magnet alloys). Specifically, we discuss the efficiency of different liquid metal extractants at removing the different RE elements from scrap and how effectively the metal extractants can be separated from the RE metals after processing. We present an overview of the challenges and opportunities for implementing recycling technologies along the processing chain of end-of-life material from the collection of the RE-containing scrap to the synthesis of new RE-containing products.

10:30 AM

(MCARE-S6-002-2016) Compressive creep strain of Fly ash based geopolymer concrete and effect of activator solution to fly ash ratio on it (Invited)

M. R. Islam^{*1}; 1. Louisiana Tech University, USA

This study reports the results of the study of the influence of activator solution to fly ash ratio, compressive strength on creep of geopolymer concrete prepared using Class F fly ash and sodium hydroxide and sodium silicate solution. In the case of prestressed geopolymer concrete application, there are concerns on prestress loss caused by elastic shortening and creep. Thus the values of mechanical strength ultimate creep strain and creep coefficient of GPC has to be estimated reasonably and accurately at the design stage to avoid any loss of structural capacity and premature structural failure. This paper describes the experimental setup developed following ASTM C 512 to calculate creep coefficient of geopolymer concrete in compression. The basic creep strain was determined by subtracting the shrinkage strain and instantaneous strain from the total strain. Strain results obtained from the experimental setup was plotted along with the data obtained using available prediction equation of OPC for the similar exposure condition and loaded form. Observing the test result and the graph plot best prediction equation was suggested for GPC to use the creep coefficient in GPC design equation.

11:10 AM

(MCARE-S6-003-2016) Positioning to Win Government Research, Development, and Demonstration Funding

P. Winkler^{*1}; 1. 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.

11:30 AM

(MCARE-S6-004-2016) Role of raw materials towards the decarbonisation of the European energy system and evaluation of critical materials substitution paths

C. Pavel^{*1}; D. Blagoeva¹; E. Tzimas¹; 1. European Commission, Netherlands

The European Union is highly dependent on imports of many raw materials that are crucial for a strong European industrial base. The European Commission (EC) in its analysis published in 2014 identified 20 'critical' raw materials that combine a high economic importance to the EU with a high risk associated with their supply. In our previous study, we found that several low-carbon energy technologies (i.e. wind energy, solar energy, electric vehicles and lighting) are of particular concern to potential supply risk of eight raw materials, i.e.: dysprosium, europium, gallium, neodymium, praseodymium, tellurium, terbium and yttrium. We investigate here the potential and feasibility of substitution of six rare earth elements (i.e. neodymium, praseodymium, dysprosium, europium, terbium, and yttrium) and of other three elements (i.e. indium, gallium and germanium) used in wind energy, electric vehicles, phosphors and LEDs, based on ongoing R&D activities and relevant economic & technological factors. While component substitution with reduced amount of critical raw materials or rare-earths free for fluorescent technology, alternative motors or wind turbines is available today, material substitution of critical raw materials in these technologies without component substitution and without loss of performance and/or with no additional cost is very limited.

11:50 AM

(MCARE-S6-005-2016) Corrosion behavior and surface characterization of Ta-W alloy coating layer by using MARC process

Y. Lee^{*1}; K. Kang²; K. Bae²; K. Park³; J. Lee¹; 1. Chungnam National University, Republic of Korea; 2. Korea Institute of Energy Research, Republic of Korea; 3. Korea Institute of Industrial Technology, Republic of Korea

The harsh atmosphere of the SI (Sulfur-Iodine) process used for producing hydrogen requires better corrosion resistance and mechanical properties than is possible to obtain with pure tantalum. Ta-W alloy is superior to pure tantalum but is difficult to alloy due to its high melting temperature. In this study, substrate samples were coated with Ta-W (Ta-7 W, Ta-4 W and Ta-1 W) using the multi-anode reactive alloy coating (MARC) process in molten salt (LiF-NaF-K₂TaF₇), with varying distances between cathode and anode to investigate the corrosion behavior of both coated samples and the substrate. Potentiodynamic polarization tests were employed to investigate the corrosion performance of coated samples and substrate in Sulfur-Iodine solution at 100 °C. In the case of Ta-4 W, showed highest corrosion resistance compared to Ta-7W, Ta-1W and bare substrate samples, and a corrosion rate of less than 0.011 mm/year was attained in hydriodic acid at 160 °C. The alloy coating films also contributed to significant enhancement of corrosion resistance.

S7: Emerging Materials for Next Generation Photovoltaics

Next Generation Photovoltaics I

Room: Salon D

Session Chairs: Yoon-Bong Hahn, Chonbuk National University; Hanwei Gao, Florida State University

9:50 AM

(MCARE-S7-001-2016) A Solution Processed Solid State Heterojunction Device with Zero-Dimensional Organic-Inorganic Bismuth Halide Perovskite (CH₃NH₃)₃Bi₂I₉ Sheets

S. Oez¹; J. C. Hebig²; E. Jung¹; T. Singh¹; A. Lepcha¹; S. Olthof³; J. Flohre²; Y. Gao³; R. German³; K. Meerholz³; T. Kirchartz²; S. Mathur¹; 1. Institute of Inorganic and Materials Chemistry, University of Cologne, Germany; 2. IEK-5 Photovoltaik, Forschungszentrum Jülich GmbH, Germany; 3. University of Cologne, Germany

Recently organic-inorganic hybrid perovskite solar cells have shown tremendous potential for solar energy harvesting applications. Since its discovery in 2009 by Miyasaka *et al.*, power conversion efficiencies skyrocketed beyond 20% in liquid electrolyte-free solid state devices within only 5 years of extensive research worldwide. A major drawback of the currently best performing solar cells lies in their chemical composition, namely the lead content. The toxicity of lead containing compounds remains a huge obstacle for commercialization. Although lead analogues 3D tin perovskite CH₃NH₃SnI₃ thin films were already successfully integrated into devices with moderate power conversion efficiencies (PCE~ 6%) by H. Snaith *et al.*, stability issues became even more demanding in comparison to the air and moisture sensitive lead perovskite. In an attempt to replace lead by a non-toxic metal, organic-inorganic bismuth halide perovskite sheets were prepared *via* spin-coating technique. Solid state (CH₃NH₃)₃Bi₂I₉ heterojunction devices were assembled by solution processing and their *J-V* characteristics were recorded under simulated sunlight conditions. A comprehensive investigation of the physicochemical properties of the (CH₃NH₃)₃Bi₂I₉ sheets was performed by means of SEM, XRD, UV-VIS, PDS, XPS, UPS, PL, DFT, TDDFT and Raman spectroscopy.

10:10 AM

(MCARE-S7-002-2016) Perovskite Solar Cells: Towards Stability

Q. Jiang¹; 1. Florida State University, USA

Perovskite type CH₃NH₃PbX₃ solid solar cells were reported with over 20% efficiency in only 6 years. The great improvements in efficiency achieved in the past few years indicating that this is a very promising next generation solar cell. The research now mainly are focusing on increasing efficiency, replacing lead with non-toxic tin, organic hole transport material (HTM) with cheaper inorganic HTM, and noble metal Au with cheaper materials. While, only a few studies have been performed to improve the stability of perovskite materials for this type of solar cell, which is the decomposition of perovskite materials in moist air. This is the main barrier for application of perovskite solar cells. Pseudohalides are known to have similar chemical properties and behaviors as halogens. We reported a new perovskite material for this type of solar cell with Pb(SCN)₂ as lead source was synthesized. This new material has shown more than 4 hours of stability in the accelerated experiment under air with 95% humidity, compared to less than 2 hours with CH₃NH₃PbI₃ perovskite material.

10:30 AM

(MCARE-S7-003-2016) Dielectric effects in perovskite solar cell materials

D. C. Lupascu¹; G. Lackner¹; I. Anusca¹; S. V. Vladimirov¹; N. Andreeva²; M. Fiebig³; J. Lehmann³; B. Dkhil³; P. Gemeiner³; M. Sanlialp³; 1. University of Duisburg-Essen, Germany; 2. Saint-Petersburg State Polytechnical University, Russian Federation; 3. ETH Zurich, Switzerland; 4. CentraleSupélec, France

In this contribution we want to discuss our present understanding of the potential influence of dielectric effects on the exceptional performance of the lead methylammonium hybrid perovskites as solar cell materials. We will discuss different mechanisms of formation of polarization, ferroelectricity and apparent ferroelectric effects as encountered in the different families of ferroelectrics. The latter are due to different microscopic mechanisms like electret effect or charge and ion migration. Potential influence on excitons and defect states will be discussed. A number of experimental results will be presented. The contribution is intended as a discussion ground and will not be able to experimentally prove one or the other concept of the underlying microscopic mechanisms yet.

10:50 AM

(MCARE-S7-004-2016) Mixed-Halide Perovskites: Chlorine depletion and presence of metallic lead

M. Bär¹; 1. Helmholtz-Zentrum Berlin, Germany

Recent progress in using hybrid organic-inorganic perovskites as thin-film solar cell absorber materials has demonstrated their potential as cheap, high-efficiency alternatives to silicon-wafer-based photovoltaics. In the few years since their introduction into solar cell devices, power conversion efficiencies up to 21% have been demonstrated. For solar cell applications, mixed methyl ammonium organometallic halide perovskites, CH₃NH₃XY₃ (X = Pb or Sn and Y = I, Br, and/or Cl), are predominantly used, in particular CH₃NH₃PbI₃-xCl_x. Despite significant advancements in the recent years, the fundamental properties of these materials remain poorly understood. We have used a variety of x-ray and electron spectroscopies with varying information depths to study the chemical and electronic structure of CH₃NH₃PbI₃-xCl_x with a particular focus on identifying the compositional profile of the device relevant thin-film/compact TiO₂ layer stack. By deliberately tuning the information depth, we could reveal that the near-surface region of the perovskite layer is void of chlorine. However, bulk-sensitive measurements show that chlorine is present in the proximity of the deeply buried CH₃NH₃PbI₃-xCl_x/TiO₂ interface. Furthermore, we observe "metallic" Pb in the bulk of the studied CH₃NH₃PbI₃-xCl_x perovskite samples. 1 <http://www.nrel.gov/ncpv/images/efficiency-chart.jpg>, last accessed 2015-02-03.

11:10 AM

(MCARE-S7-005-2016) Influence of GITC (guanidinium thiocyanate) on the performance of MAPbI₃ perovskite solar cells by two-step method

E. Jung¹; S. Oez¹; R. Bhattacharjee²; H. Wang²; S. Mathur¹; 1. University of Cologne, Germany; 2. Queensland University of Technology, Australia

Perovskite solar cells have emerged one of the promising next generation power sources. The most common perovskite solar cell structure is FTO/c-TiO₂/mp-TiO₂/perovskite composite layer/perovskite capping layer/spiro-OMeTAD/Au. The poor coverage and morphology control of perovskite film on top of mp-TiO₂ are the main issues of this type of perovskite solar cells. Here we demonstrated high-performance perovskite solar cell by introducing small amounts of guanidinium thiocyanate (GITC) as a morphology controller in perovskite precursor solution, which allows for improvements in the light harvesting. As a result, highly homogeneous film morphology, and the maximum short circuit current density of 22 mA/cm², consequent increasing the power conversion efficiency of 12.9% (pure MAPbI₃ perovskite solar cell: 10.4%) are

achieved. This study represents that GITC serves to make the formation of smooth film, therefore, provides efficient way to fabricate high efficiency perovskite solar cells.

11:30 AM

(MCARE-S7-006-2016) Realization of Nozzle-Jet Printing Technique for Perovskite Solar Cells

Y. Wang^{*1}; H. Yang¹; S. Seo¹; W. Rho¹; Y. Hahn¹; I. Chonbuk National University, Republic of Korea

Recently, perovskite solar cells (PSCs) have been widely investigated and considered as the most significant of the third-generation solar cells. The perovskite material is an excellent light absorber, including high absorption coefficient, long electron-hole diffusion lengths, appropriate direct bandgap, and extraordinary carrier transport. Although rapid rise of efficiency has been realized by the traditional method of spin-coating technique, it still has challenges for large-scale production, cost-effective, environmentally friendly with reduced waste of materials, and more ideal if all layers can be printed. To reach the goal, various novel deposition techniques in science community have emerged to successfully deposited perovskite materials, such as electrostatic spray deposition, blade coating, vapor deposition, slot-die coating and inkjet printing technique (IJP). In this regards, we present a novel and noncontact printing technique, named nozzle-jet printing (NJP), which is capable of achieving PSCs fabrication. With the combined optimization of printing parameters and ink compositions, BL-TiO₂, MP-TiO₂ and MAPbI₃ patterns with favorable morphology and high uniformity are realized. Compared to the conventional method spin-coating, when such printed patterns (C-TiO₂/MP-TiO₂/MAPbI₃) are embedded in PSCs, we obtain a better performance of power conversion efficiency (PCE).

S9: Direct Thermal to Electrical Energy Conversion Materials and Applications

Thermoelectric Materials I

Room: Salon G

Session Chair: Terry Tritt, Clemson University

9:50 AM

(MCARE-S9-001-2016) Thermal energy conversion via the spin Seebeck effect

S. Boona^{*1}; J. P. Heremans¹; I. Ohio State University, USA

The discovery of the spin Seebeck effect (SSE) has generated exciting new ideas for utilizing the spin degree of freedom in thermoelectric energy conversion. The SSE generally resembles the Nernst effect, in that it involves the conversion of a temperature difference into a transverse voltage, although the two effects are driven by fundamentally different processes. In the SSE, a temperature difference thermally excites a spin current in one material (e.g., a ferrimagnetic ceramic). This spin current is driven across an interface into another material (e.g., a heavy metal like Pt), where the inverse spin Hall effect converts the spin current into a transverse electric field. The end result is direct thermal-to-electric energy conversion mediated entirely by spin-dependent transport effects. This talk will provide an overview of the SSE and the mechanisms that drive it, as well as an analysis of how the spin degree of freedom may be utilized for thermoelectric energy conversion. Results will be presented relating to our recent work on thin film Pt/Y₃Fe₅O₁₂ heterostructures, which is the archetype system for studying SSE. We will also present results related to a more novel approach we have recently begun exploring for demonstrating the SSE in more practical bulk materials and devices. As we will show, the potential for utilizing SSE in thermoelectric energy conversion depends critically on materials selection and processing.

10:10 AM

(MCARE-S9-002-2016) Open-framework and other low thermal conductivity materials: Expanding our fundamental understanding in pursuit of technological applications (Invited)

G. S. Nolas^{*1}; I. University of South Florida, USA

The concept of enhanced thermoelectric performance through low thermal conductivity materials, first proposed by Glen Slack and now one of the key focus areas in the field of thermoelectrics materials research, relies on a fundamental understanding of phonon transport and structure-property relationships of complex materials and structure types. I will describe this approach with a focus on specific requirements for materials properties that may lead to efficient conversion of waste-heat to electrical energy. A fundamental understanding of bonding and what structurally relevant properties can provide desirable properties is very useful. Effective strategies for selecting thermoelectric material, specific compositions and doping for example, in order to achieve appropriate electronic structure modifications and/or effective phonon-scattering mechanisms is of interest. I will focus on recent bulk materials developments, nanostructuring in bulk materials, and briefly describe some device-related materials issues, an equally important aspect of the research effort which can also benefit from new materials research. Some of the recent research from the USF Novel Materials Laboratory will be presented while focusing on new materials-related approaches for energy-related applications.

10:50 AM

(MCARE-S9-003-2016) Recent Progress in Oxide Thermoelectric Materials: n-Type SrTiO₃-based Ceramics (Invited)

A. Dehkordi^{*1}; I. SunEdison, USA

Once believed to make poor thermoelectrics, oxide materials were shown to be promising candidates for high-temperature thermoelectric applications in recent years, from stability and cost perspectives to electronic and thermoelectric transport properties. In this talk, the current progress in oxide thermoelectric materials engineering will be reviewed. Among the n-type oxide thermoelectrics, highly doped strontium titanate-based ceramics have attracted much attention due to their intriguing electronic properties. Recent progress in understanding and improving the thermoelectric properties of strontium titanate will also be presented and discussed.

11:30 AM

(MCARE-S9-004-2016) Multinary Chalcogenides: Potential Thermoelectric Materials with Polaronic-type Conduction

K. Wei^{*1}; A. R. Khabibullin¹; T. Stedman¹; L. M. Woods¹; G. S. Nolas¹; I. University of South Florida, USA

Multinary chalcogenides form a large class of materials composed of earth-abundant and nontoxic elements that have been studied over the past decade for a variety of different applications. Very recently certain compositions have been shown to be of great interest for thermoelectric waste heat recovery, in part due to their relatively low thermal conductivities. While investigating certain compositions polaronic-type conduction was observed which may contribute to the low thermal conductivity in these chalcogenide compounds. The two-component model was employed in the study of the electrical properties, indicating strong electron-phonon coupling from polaronic conduction. The Debye model was used to further investigate the thermal properties. Our results show that due to the strong coupling between electrons and phonons in these materials polarons may hop site-to-site during transport causing absorption and emission of phonons thereby altering the lattice vibrations and shifting the phonon frequency. We will report on the transport properties of Pb₁₇(Sb_{0.75}As_{0.25})₁₆S₄₁ and Ag_{2+x}Zn_{1-x}SnSe₄ for the first time. This work also represents a new approach in exploring new material systems for energy-related applications.

S10: Batteries and Energy Storage

Li-air and Li-sulphur Batteries

Room: Salon E

Session Chairs: Valerie Pralong, CNRS ENSICAEN;

Amartya Mukhopadhyay, IIT Bombay

9:50 AM

(MCARE-S10-026-2016) Fast-ion Conductor Design for Large-Scale Energy Storage Systems (Invited)

S. Adams^{*1}; 1. National University of Singapore, Singapore

With increasing scale of energy storage systems low cost materials and processing routes become key performance indicators along with minimal operational costs, long cycle-life, and high energy density. In this situation electrochemically stable fast alkali-ion conductors (FIC) gain importance beyond solid-state-batteries as key components in large-scale metal-air, metal-sulfur, alkali-redox flow batteries etc. To enable these concepts new FICs need to be designed and realized. Ion conductivity in mixed conductors moreover controls the power performance of electrode materials. We screened a wide range of compounds for their suitability as Li^+ or Na^+ ion conductors using our bond-valence approach factoring in economic constraints. Likewise, ion mobility and power performance of cathode materials are discussed, comparing ab initio and empirical bond valence studies. Li-air batteries (LAB) stand out for their extreme energy density. Compared to the organic LABs with the highest energy densities, aqueous LABs are inherently superior in energy efficiency and power performance as long as chemical reactions of anode and catholyte are safely prevented by a high conductance membrane. Advantages and challenges of NASICON- and garnet-type ceramics as well as hybrid organic-inorganic membranes for this application will be discussed with a focus on processing, scalability, Li^+/H^+ exchange and actual performance in LABs.

10:30 AM

(MCARE-S10-027-2016) A Few Strategies for Sulfur Encapsulation in Li-S Battery (Invited)

A. J. Bhattacharyya^{*1}; 1. Indian Institute of Science, India

Battery chemistry based on lithium possesses great potential due to its high energy and power density. Lithium-ion has been the most well studied and they power several mass-scale mobile devices. The amount of energy storage in lithium-ion is however, quite low. In recent times research focus has shifted towards elemental electrodes as they tend to significantly enhance energy storage. As cathode, sulfur is very promising due to its high theoretical capacity of 1672 mAh g^{-1} (gravimetric energy density of 2500 Wh kg^{-1}), nearly an order higher compared to the known intercalation oxide cathodes (IOC) used in lithium-ion batteries. The high theoretical capacity originates from the possibility of two exchangeable lithium-ions per atom of sulfur as compared to only one Li^+ ion per formula unit of IOC. In addition to high storage, sulfur is very appealing due to its low cost, high abundance and non-toxic nature. Despite these advantages, the chemical reactions determining the mechanism and quantum of electrical energy storage in Li-S battery however, pose a formidable challenge mainly due to the various intermediate polysulfides formed during the reversible conversion of elemental sulfur to Li_2S . We will discuss various strategies for complete encapsulation of sulfur and polysulfides inside various porous hosts aimed towards lithium-sulfur batteries with very high stability at low to practical operating current densities.

11:10 AM

(MCARE-S10-028-2016) Lithium-Sulfur batteries: materials for preventing polysulfides diffusion and mechanisms at interfaces (Invited)

R. Dedryvere^{*1}; R. Chellappan¹; A. Vizintin²; V. Lapornik²; D. Foix¹; R. Dominko²; 1. University of Pau - CNRS, France; 2. National Institute of Chemistry, Slovenia

Lithium-sulfur (Li-S) batteries are one of the most promising candidates for the next generation of batteries with enhanced energy densities compared to Li-ion cells. However, these systems suffer from several limitations that still hinder their industrial development. A major problem comes from intermediate reduction products of sulfur formed upon discharge, *i.e.* polysulfides S_n^{2-} , which are soluble in the electrolyte and diffuse out from the porous carbon positive electrode. Their diffusion/migration through the electrolyte and their reduction at the surface of the metallic Li negative electrode causes active mass loss and a redox shuttle process. In this work we investigated two strategies in order to prevent this problem: (i) by including a manganese-doped zeolite in the porous carbon positive electrode in order to better retain the polysulfides within the electrode, (ii) by including a modified graphene (fluorinated reduced graphene oxide) interlayer in the separator, making it selective and blocking the diffusion/migration of polysulfides through it. Besides electrochemical characterization of the modified Li-S cells, this study was carried out by X-ray Photoelectron Spectroscopy (XPS) in order to follow the presence of polysulfides at interfaces, and understand the beneficial mechanisms taking place at both electrodes.

11:50 AM

(MCARE-S10-029-2016) Physicochemical Evolution Behavior in the Li-air Battery Electrode

A. Mistry^{*1}; D. Juarez Robles¹; P. P. Mukherjee¹; 1. Texas A&M University, USA

Lithium air batteries are proposed as a potential solution to vehicle electrification, since one of the reactants - oxygen, is not stored physically. The specific energy capacity of a Li-air battery exceeds any other available or proposed battery chemistry and is comparable to that of conventional IC engines. A typical Li-air battery design involves lithium anode and a porous carbon cathode which serves as an active surface for electrochemical reactions. The cathode is open to atmosphere and thus connected to an infinite source of oxygen. During discharge Li is being used continuously, hence anode thickness reduces and electrolyte space increases. On the other hand, precipitation in cathode decreases available pore space. Since usual electrolyte is a non-aqueous liquid, the net effect will change both pressure and electrolyte in the cell. The active cathode surface is a function of electrolyte depth and can lead to partial cathode isolation or electrolyte leakage. On the other hand, internal pressure decides the solubility of atmospheric oxygen which modifies species transport and gives an estimate of mechanical stresses. Complementary situations arise during charging process. A moving boundary problem formulation is posed at macrohomogeneous continuum scale to quantify the relative importances of these effects. The cell behavior is studied in response to different discharge rates and microstructural properties.

S4: Material Challenges in Nuclear Energy

Nuclear Energy II

Room: Salons A-C

Session Chair: Jacob Eapen, North Carolina State University

1:40 PM

(MCARE-S4-006-2016) Joining of C_f/C Composites and SiC ceramics with Ti₃SiC₂ Interlayer by Electric Field Assisted Sintering Technique (Invited)

Q. Huang^{*1}; 1. Ningbo Institute for Materials Technology and Engineering, China

Carbon fiber reinforced carbon composites (C_f/C) were joined by electric field-assisted sintering technology using a Ti₃SiC₂ (TSC) interlayer. The joint with shear strength of 26.3±1.7MPa was obtained at joining temperature of 1200°C with less than 12min in C_f/C composites. The joint morphology, interface reaction, shear fracture character along interface and shear strength properties were investigated in detail. In order to obtain a reliable joining of C_f/C composite to itself by the TSC interlayer, the current work show the crucial control of interface reaction on the shear strength and the shear fracture behavior. The optimized bonding should be achieved without the sacrifice the high strength of carbon fibers and pseudo-plasticity feature of TSC phase in the interlayer. Finally, a possible high-toughness joining structure was also proposed based on these results. Also, the electric field aided joining methodology was applied in the SiC ceramics with dimension-controlled Ti interlayer, and showed an efficient interface bonding at temperature as low as 1000°C.

2:10 PM

(MCARE-S4-007-2016) Radiation Tolerance of Pressurelessly Processed Silicon Carbide Joints (Invited)

Y. Katoh^{*1}; T. Koyanagi¹; M. Ferraris²; 1. Oak Ridge National Laboratory, USA; 2. Politecnico di Torino, Italy

Silicon carbide composite-based fuel cladding concepts are attractive options for accident-tolerant nuclear power systems due mainly to the exceptional high temperature properties, radiation stability, severe accident tolerance, and neutronics transparency of silicon carbide. For industrial manufacture of fuel rods with such ceramic claddings, it is essential to develop a technology to apply end-plugging to the cladding tubes with the minimal pressure application requirement. In this work, test articles of silicon carbide bonded together through three candidate pressureless joining methods were evaluated for tolerance against neutron irradiation. The bonding methods evaluated were transient eutectic-phase SiC joining, Si-Ti-C MAX phase joining, and calcia-alumina ceramic joining. The flat face joint samples were evaluated for mechanical integrity through torsional shear tests following the neutron irradiation in the High Flux Isotope Reactor in a temperature range 300 – 800 °C to a maximum dose of ~8 dpa. The results are discussed in relation with the observed microstructures. Research sponsored by the Fuel Cycle R&D program, Office of Nuclear Energy, US Department of Energy, under contract DE-AC05-00OR22725 with UT-Battelle, LLC.

2:40 PM

(MCARE-S4-008-2016) Properties of commercial MAX phase Ti₃SiC₂ and Ti-Al-C ceramics after moderate dose neutron irradiation

C. Ang^{*1}; C. Shih²; N. Cetiner¹; C. Silva¹; A. Campbell¹; S. Zinkle³; Y. Katoh¹; 1. Oak Ridge National Laboratory, USA; 2. General Atomics, USA; 3. University of Tennessee, USA

M_{n+1}AX_n (MAX) phase (where “A” = Si or Al) materials were neutron irradiated to 2 × 10²⁵ nm⁻² (E > 0.1 MeV) or a displacement dose of ~ 2 dpa. After (T_{irr}) irradiation at ~400°C, a 1.5% c-axis anisotropic lattice parameter swelling was observed in Ti₃SiC₂, and

a reduction in electrical and thermal diffusivity. ~33% reductions in Young’s modulus and fracture strength were recorded. Phase analysis confirmed an increase of 10-15 wt% TiC that decomposed from Ti₃SiC₂. Volumetric swelling increased with dose across all T_{irr}. Both MAX phases showed formation of microcracks after T_{irr} ~700°C, with kinking and delamination morphology found on polished surfaces that were subcritical flaws, along with recovery of physical properties to pre-irradiation values due to thermal migration associated with the Si- and Al- layer. While the response of Ti₃AlC₂-Ti₅Al₂C₃ and Ti₃SiC₂ after T_{irr} ~700°C was similar, significant differences were observed at T_{irr} ~400°C for Ti₃AlC₂-Ti₅Al₂C₃. Severe anisotropic lattice swelling was observed from XRD. While a 20% reduction in Young’s modulus was observed, the complete loss of strength was in agreement with networked microcracks from lattice swelling. Research sponsored by the Office of Fusion Energy Sciences, U.S. Department of Energy, under contract DE-AC05-00OR22725 with UT-Battelle, LLC.

3:20 PM

(MCARE-S4-009-2016) Topological Defects in Irradiated Graphite (Invited)

J. Eapen^{*1}; 1. North Carolina State University, USA

Graphite is currently pursued as a neutron moderator for the next generation, high temperature reactors. It has a lamellar structure, where the basal planes – constituted by strong, sp²-hybridized carbon atoms arranged in a hexagonal lattice – are held together through weak dispersion forces. The mechanisms of defect formation in graphite during the early stages of irradiation are still not completely resolved. We report results from a molecular dynamics investigation on early radiation damage mechanisms in graphite using AIREBO interatomic potential that has been benchmarked to several defect and thermo-mechanical properties. Using non-equilibrium radiation cascade simulations, we show that topological defects, which maintain the sp² connectivity, are generated on the basal planes in addition to three dimensional sp³ defects. We apply our results for interpreting the defect or D peak in Raman spectra of irradiated graphite.

3:50 PM

(MCARE-S4-010-2016) Study the interfacial nanostructure and chemical bonding of the multi-layered graphene-reinforced alumina ceramic nanocomposites

I. Ahmad^{*1}; 1. King Saud University, Saudi Arabia

We prepared Alumina (Al₂O₃) ceramic nanocomposites containing different multi-layered graphene (MLG) nanomaterial contents (0.25, 0.5 and 1.5 wt.%) using quick induction heating based sintering technology. The mechanical properties, microstructure, interfacial nanostructure and chemical bonding features of the resulting nanocomposites were meticulously analyzed. The thermally exfoliated MLGs showed even distributions at grain boundaries and good sticking with base Al₂O₃ ceramics which supported to attain a fracture toughness (KIC) level of 5.7 MPa.m^{1/2} against benchmark monolithic Al₂O₃ (KIC = 3.3 MPa.m^{1/2}). Further, we thoroughly examine the immediate matrix/MLG interface and extracted structural and bonding information using distinctive microscopy and combined analytical techniques. It was finally deduced that the short sintering protocol supported graphene natural planar 2D structure to maintain nanodimensionality into the matrix and formed chemically compatible interface owning firm connections with nanocomposite constituents via confined reduction chemistry, at the same time. Thus newly discovered interface allowed MLG to use its elasticity, strength and high interlayer friction in order to activate classical (pullout, crack bridging) and advanced (anchoring) toughening mechanism in nanocomposites thus exhibited higher fracture toughness.

4:10 PM

(MCARE-S4-011-2016) Strengthening of Zry-4 Fuel Cladding Tubes using Oxide Particles by Laser Beam Treatment

Y. Jung^{*1}; D. Park¹; J. Park¹; J. Park¹; H. Kim¹; Y. Koo¹; 1. Korea Atomic Energy Research Institute, Republic of Korea

Accident tolerant fuel claddings are being developed globally after the Fukushima accident with the demands for the nuclear fuel having higher safety at normal operation as well as severe accident conditions. In this study, to increase the high-temperature mechanical strength of the Zry-4, surface modification using an oxide coating and laser beam treatment was conducted. The Zry-4 plate was coated by oxides of Y_2O_3 or CeO_2 , and then laser beam treated to form a layer of mixed phases. It was observed that oxide particles were dispersed well in the Zr matrix. The thickness of the oxide-dispersed layer was varied 87–192 μm from the Y_2O_3 coating (10–30 μm). The developed layer was ~100 μm by the CeO_2 coating (20 μm). The density of oxide particles in the mixed layer was higher in the case of CeO_2 than Y_2O_3 . For the evaluation of the strengthening effect, a tensile test was performed at room temperature and elevated temperature (380°C). At room temperature, the strength of the developed samples was increased about 18% as compared to fresh Zry-4. The elongation, however, was decreased to 20–40% showing the brittle fractured surface. In contrast, the strength was increased more than 50% and reduction in elongation was less than 30% at 380°C. The investigated technology would be applicable to increase the high-temperature strength of the current Zr alloy by maintaining their bulk microstructures.

S6: Critical Materials for Energy

Critical Materials for Energy II

Room: Salon F

Session Chairs: Ryan Ott, Ames Laboratory (USDOE); Nobuhito Imanaka, Osaka University

1:40 PM

(MCARE-S6-006-2016) Ga-doped ZnO thin films from solar panel resources recycling technology (Invited)

W. Chen^{*1}; K. Chiu¹; Y. Wang¹; 1. National Cheng Kung University, Taiwan

Doped ZnO thin films have been used as front-contact transparent conducting electrodes in solar panel because its high chemical and thermal stability. The impurities doped in ZnO, such as gallium, indium, aluminum, silicon, and titanium, increase the conductivity and stability of ZnO. This study focuses on the transparent conductive zinc oxide target: Ga-doped zinc oxide (GZO). The Ga-doped ZnO film target contains gallium, indium and other rare metals. We expect to recycle gallium and indium from the GZO targets and make it effectively. The coating layer was peeled from the GZO targets. Gallium is in the structure of the GZO targets while the indium is in the coating layer. Rare metals in GZO targets were leached in different concentration of nitric acid, different solid-liquid ratio and different temperature. The liquid-liquid extraction was studied to separate gallium and indium. The rare metals were enriched from nitric acid medium by using D2EHPA and recycle gallium and indium by hydrochloric acid and sodium hydroxide as stripping reagents. The results show that 90-95% overall fraction recovery with around 95% purity of gallium was recovered. Also, it is about 95% overall fraction recovery with 99% purity of indium was recycled.

2:20 PM

(MCARE-S6-007-2016) Electro reduction characteristic of zirconia by using copper oxide as additive

B. Yoo^{*1}; K. Park²; J. Lee¹; 1. Chungnam National University, Republic of Korea; 2. Korea Institute of Industrial Technology, Republic of Korea

Not only commercial grade zirconium (containing about 4.5 percent hafnium) is used as structural material widely in the chemical processing industry because of its good corrosion resistance. But also nuclear grade zirconium becomes an irreplaceable component in the nuclear power industry due to low neutron capture cross section and good resistance to corrosion. There are a number of way to produce zirconium metal, chemical reduction and dry process such as Kroll process and electrolysis process. The dry process is known as more simple compared to chemical reduction process because it utilized the method that doesn't need toxic chemical chlorine gas and conversion step. Hence electrolysis process as a representative dry process was used in this study to reduce Zr metal from zirconia mixed with copper oxide. Although zirconia is hard to reduce by using electrolysis process because of its characteristic, mixed oxide is able to help reduction of zirconia. In this study, mixed oxide redox potential was observed by using cyclic voltammetry (CV) according to the concentration of copper oxide and the voltage change of the cell was observed by using polarization and chronopotentiometry. The microstructure and composition of reduced zirconium-copper metal was analyzed by SEM and XRD respectively.

2:40 PM

(MCARE-S6-008-2016) Extraction behaviour of rare earths with liquid Mg

T. Kim^{*1}; B. Kim¹; S. Seo¹; K. Park¹; 1. Korea Institute of Industrial Technology, Republic of Korea

Extraction behaviour of rare earths such as Nd and Dy from magnet scraps are discussed, in which it is well known that those are widely used for the permanent magnet. Even though their recycling activity is rare to find due to a couple of reason, the necessity is rapidly up-coming. It is in association with the natural mine having ununiformed concentration as well as in the environmental problem during smelting and refining process. Since the recycling process also follows the conventional chemical metallurgy process, not avoidable the problem similar to at the mining route. Recently, ReMat process, a combined terminology of recycling & Materialization, was proposed by the authors, in which the materials contained in the scrap to be recycled and the recycling agent are connected to the industrialization without any disposal. The concept is in using the lower melting point element than the scrap materials to meet a liquid – solid reaction with selectivity. at the temperature of Mg melting the Nd in the solid Nd-Fe-B scrap selectively diffused into Mg, then forming the Mg-Nd alloy. Furthermore, the intermediate product can be applied to various area. In this investigation, the diffusion behaviour of Nd and Dy to the liquid Mg was introduced with more focus on the diffusion of Dy which is differentiated depending on the existent of Nd. In addition, materials flow for REE in Korea currently updated would be briefly mentioned.

3:20 PM

(MCARE-S6-009-2016) Catalytic Combustion Type Carbon Monoxide Gas Sensor with Platinum, or Platinum-free Catalysts (Invited)

N. Imanaka^{*1}; 1. Osaka University, Japan

One of great disadvantages with conventional catalytic combustion-type CO gas sensors is that the catalysts such as Pt/ Al_2O_3 or Pd/ Al_2O_3 , requires high operating temperatures over 400 degree C for the complete oxidation of CO. Recently, we have succeeded in developing a considerably low-temperature operable sensors with the above described catalytic combustion-type, by the application of 10 wt% Pt/ $Ce_{0.68}Zr_{0.17}Sn_{0.15}O_{2.0}$ as the catalyst and they can operate at 70 degree C, which temperature is more than 300 degree C lower

compared with conventional ones. In addition, by the combination of the superior thermoelectric material of aluminum nitride (AlN) ceramics as an intermediate heat transfer layer with the Pt/Ce_{0.68}Zr_{0.17}Sn_{0.15}O_{2.0} catalyst, a novel portable catalytic combustion-type carbon monoxide gas sensor was realized, having an excellent sensing performance that drastically accelerated the sensing response to CO at the moderate operating temperature (70 degree C). It is well known that platinum is one of representative rare metals (critical metals). Therefore, Pt-free CeO₂-ZrO₂-SnO₂ solid solution based sensor is also examined by applying electronic conducting oxide instead for Pt. Details will be introduced at the presentation.

4:00 PM

(MCARE-S6-010-2016) RE-containing vs. RE-free materials for magnetocaloric refrigeration (Invited)

A. Waske*¹; B. Weise¹; M. Lee²; A. Gebert¹; 1. Leibniz-Institute for Solid State and Materials Research Dresden, Germany; 2. Korea Institute of Industrial Technology, Republic of Korea

Worldwide, more than 15% of total electric energy consumption is spent on cooling applications. Magnetocaloric cooling is a new cooling technology expected to offer significant energy savings while at the same time the use of harmful, ozone-depleting gases is eliminated. For an optimal performance the magnetocaloric effect relies on magnetic materials with a strong change of magnetization with temperature. Materials are employed close to a magnetic transition (e.g. FM to PM). As benchmark material with large magnetocaloric effect, Gadolinium comes at a too high price in order to be applied at large scales. Hence, currently the search for competitive materials in this field is dedicated to materials which minimize or eliminate the use of rare earth elements. Here, magnetic materials which undergo a structural transition that couples the magnetic phase transition are at the center of attention, as in this way, large entropy changes and hence a large magnetocaloric effect can be achieved without using rare earth elements (e.g. NiMn- / MnFeP-based alloys) or by minimizing their usage (e.g. La(Fe,Si)₁₃ and its composites). We discuss current strategies to eliminate or minimize rare earth usage in these materials and assess the potential of each candidate for an application in cooling devices. We gratefully acknowledge funding by the Korean Institute of Industrial Technology (KITECH) Incheon, Korea.

4:40 PM

(MCARE-S6-011-2016) Fabrication of Nanostructured Mixed Metal Oxide Thin Films from Single Source Precursor for Technological Applications

M. A. Ehsan*¹; A. Hakeem¹; T. Laoui¹; Z. Abdallah Yamani¹; 1. King Fahd University of Petroleum and Minerals, Saudi Arabia

Nanostructured mixed metal oxide thin films cover a wide spectrum of applications in electronics, optics, catalysis and environmental issues. Single source precursor (SSP) based chemical vapor deposition has become a well-established route to create metal oxide thin films with superior advantages of high crystallinity, spatially oriented nanostructure, excellent control over homogeneity, stoichiometry and reproducibility of the final product at relatively lower temperatures. These advantages are however, confronted by the lack of well-defined heterometallic precursors and deficiency of primary knowledge on the molecular and materials relationship. In this context, we presented the design and synthesis of well-defined heterobimetallic complexes [Cd₂Ti₄(μ-O)₆(TFA)₈(THF)₆]₂•1.5THF (1), [Zn₂Ti₄(μ-O)₆(TFA)₈(THF)₆]₂•THF (2), [Cu₄Zr₂(μ₄-O)₂(dmae)₄(OAc)₈]₂•2H₂O (3) and [Cu₄Zr₂(μ-O)₈(dmap)₄(OAc)₁₂]₂•H₂O (4) where (dmae = *N,N*-dimethylaminoethanolato, dmap = *N,N*-dimethylaminopropanolato, TFA = trifluoroacetate, OAc = acetate) and explore their potential as SSP for the formation of device grade composite thin films of CdTiO₃-TiO₂ (1), ZnTiO₃-TiO₂

(2), CuZrO₃-CuO (3) and CuO-1.5ZrO₂, respectively, via aerosol assisted chemical vapor deposition.

5:00 PM

(MCARE-S6-012-2016) Diffusion mechanism of neodymium and dysprosium contained in REE magnet to liquid Mg

Y. Kim*¹; T. Kim¹; B. Kim¹; K. Park¹; S. Seo¹; S. Nam¹; J. Lee¹; 1. Korea Institute of Industrial Technology, Republic of Korea

RE elements such as Neodymium (Nd) and Dysprosium (Dy) has become integral part of various industries due to their wide usage especially in permanent magnets. But supplies of these RE elements has been restricted by area preponderance and environmental problems. So, recycling them from permanent magnets is necessary to ensure sufficient supply. One of the possible RE recycling technology is Recycling & Materialization (ReMat) process. However, this process is focused only on the extraction of Nd and not on Dy. In this study, Liquid metal extraction (LME) process has been utilized in order to investigate the extraction behavior of Nd and Dy from UH grade magnet (65wt%Fe-19wt%Nd-6wt%Dy-6wt%Pr-3wt%Ag-1wt%Co). To study the extraction behavior of Dy, diffusion couple experiments were performed between Mg-UH grade magnets at 973K for variable holding time. The characterization of the final product was done by SEM, EDS, TEM and XRD analysis. Dy was found to have diffused out of the UH grade magnet into the liquid Mg but Dy-rich oxide phase was still remained in diffusion zone of UH grade magnet. SEM and EDS mapping results for the diffusion of Nd and Dy showed that Dy has lower tendency to diffuse into liquid Mg than Nd. Further investigation will be done in order to study the factors affecting the diffusion tendency of Dy into Mg such as affinity of each element, diffusion coefficient and oxidation.

5:20 PM

(MCARE-S6-013-2016) Charge Stage in Electret by Nanosecond Pulse Power Technology for Energy Harvesting

T. Nakayama*¹; K. Awaya¹; K. Nakata¹; H. Suematsu¹; K. Niihara¹; 1. Nagaoka Univ of Tech, Japan

Electret is a permanently charged dielectric. Therefore, it is expected to be applied to such generators, and electrostatic air purifier. To create an effective electret is a dielectric having a need to create a large charge. Method gives a charge, usually is used to polarize the sample by high-voltage direct current. Here, using the pulse discharge, as well as electronic, are expected to be effectively charged ions to ionize molecules also occur in the air. In this study, by using a semiconductor switching device to create a nano-second pulse power, by which the rubber, polymer, gave a charge to ceramics and composites of these. It was possible to control the charge as an electret type and power depending on the type of material.

S7: Emerging Materials for Next Generation Photovoltaics

Next Generation Photovoltaics II

Room: Salon D

Session Chairs: Yoon-Bong Hahn, Chonbuk National University; Hanwei Gao, Florida State University

1:40 PM

(MCARE-S7-007-2016) Textured Microstructures for DSSCs using Microsphere Lithography and Acicular Particles

I. Ayan*¹; P. A. Fuierer¹; 1. New Mexico Institute of Mining and Technology, USA

Particulate microstructures containing vertically aligned acicular particles have potential to improve device performance and give rise to new materials phenomena. In dye sensitized solar cells (DSSCs) for example, aligned nanotubes or fibers are believed to enhance

photo-electron transport, resulting in increased light-harvesting efficiency. The current study investigates a novel top-down approach to such structures with potential for scaling to large areas, where the interstitials within a monolayer of spheres accommodate the orientation of acicular particles. Potassium hexa and tetratitanates, both wide Eg semiconductors with needle morphology, are considered as candidate anode materials for DSSC. Monosized monolayers of glass microspheres, with diameter in the range of 10 - 500 μm , were fabricated by a self-assembly technique. $\text{K}_2\text{Ti}_6\text{O}_{13}$ and $\text{K}_2\text{Ti}_4\text{O}_9$ needles were synthesized by a liquid phase process. By controlling composition, temperature, time and cooling rate, needle diameter (0.5 - 20 μm) and length (10 - 500 μm) could be controlled to match microsphere and interstitial sizes. Particulate slurries were then cast over the monolayers to form the complex anode microstructures. Preliminary PV measurements on experimental DSSCs will be presented.

2:00 PM

(MCARE-S7-008-2016) Photo-enhancement of activity in spray-coated Cu_2SnSe_3 nanoparticle counter electrode for dye-sensitised solar cells

S. Dunn*¹; 1. QMUL, United Kingdom

Cu_2SnSe_3 nanoparticles are synthesised using oleylamine as both a solvent and capping agent and spray coated onto conductive glass substrates to form dye-sensitised solar cell counter electrodes. The film requires annealing at only 400 °C in nitrogen, which is a lower temperature than previous reports of nanoparticle-derived films of both Cu_2SnSe_3 and $\text{Cu}_2\text{ZnSnSe}_4$, as well as avoiding the use of Se gas in the annealing process. The composition and phase of the material is confirmed to be close-to-stoichiometric Cu_2SnSe_3 by energy-dispersive X-ray spectroscopy, X-ray diffraction and Raman analysis. Dye-sensitised solar cells using Cu_2SnSe_3 counter electrodes give a power conversion efficiency of 4.87 %, which is close to the efficiency of 5.35 % achieved when using a Pt counter electrode. Electrochemical impedance spectroscopy indicates that the performance of the Cu_2SnSe_3 electrode is enhanced under illumination, leading to a drop in the charge transfer resistance which is attributed to the higher overpotential of photoexcited carriers in Cu_2SnSe_3 . Coupled with a very high surface area resulting from the hierarchical structure of the film, this leads to effective catalytic operation of this earth-abundant counter electrode.

2:20 PM

(MCARE-S7-010-2016) Improved photovoltaic performance of inverted polymer solar cells through a sol-gel processed Al-doped ZnO anode buffer layer

T. Mahmoudi*¹; S. Seo¹; Y. Hahn¹; 1. Chonbuk National University, Republic of Korea

We have investigated the influences of aluminum dopant (0 to 2.0 mol%) on zinc oxide (ZnO) thin films regarding to electrical and optical properties for application in photovoltaic devices. Nanocrystalline Al-doped zinc oxide (n-AZO) thin film used as an electron-extraction layer can significantly enhance the performance of inverted polymer solar cells based on Poly(3-hexylthiophene-2,5-diyl) (P3HT) bulk heterojunction solar cells. AZO film with an average carrier density of $1.3 \times 10^{19} \text{ 1/cm}^3$ was prepared by a sol-gel spin-coating method, and a minimum resistivity of $2.5 \times 10^{-3} \text{ (ohm.cm)}$ was obtained for an Al-doping concentration of 1.8 at.%. When an AZO film with a 1.8 at.% Al concentration was inserted between the ITO electrode and the active layer (P3HT:ICBM), the power conversion efficiency increased from 4.7 to 5.3%.

2:40 PM

(MCARE-S7-011-2016) Defect annihilation and precipitate dissolution in N-type, Czochralski Si wafers by optical processing: enabling high efficiency solar cell fabrication

B. Sopori*¹; 1. National Renewable Energy Laboratory, USA

N-type monocrystalline silicon wafers are preferred substrates for fabrication of high efficiency solar cells because of their insensitivity to common impurities. Silicon industry has successfully developed technology for making low-cost, N-type, Czochralski silicon of long minority carrier lifetime (MCLT) needed for high efficiency cell fabrication. Unfortunately, typically only wafers from a small section of a Si ingot can yield high efficiency solar cells. Other parts of the ingot have high concentrations of oxygen and point defect, which cause degradation of the MCLT during cell fabrication by forming oxygen precipitates. We have developed a wafer treatment called Flash Annealing, which dissolves precipitate-nuclei in the wafer before cell fabrication. The wafer is heated in an optical furnace to a high temperature (about 1100 - 1250 °C) for a short period and then quenched. This causes dissolution of precipitate-nuclei below a critical size. The absence of the nuclei inhibits precipitate and swirl defect formation during lower temperature processing for cell fabrication. This paper will describe Flash Annealing process and discuss results showing greatly improved material quality and higher cell performance.

S9: Direct Thermal to Electrical Energy Conversion Materials and Applications

Thermoelectric Materials II

Room: Salon G

Session Chair: Jian He, Clemson University

1:40 PM

(MCARE-S9-005-2016) Lifting up the average thermoelectric figure of merit (Invited)

D. Wu¹; X. Liu¹; D. Feng¹; J. He*¹; 1. South University of Science and Technology of China, China

While high peak value of figure of merit is the target of most researchers in thermoelectrics, the performance of thermoelectric devices (thermoelectric generators and refrigerators) is actually dependent on the average ZT over the whole working temperature range. Here we summarize several generalized strategies which are deemed promising in lifting up the average performance of thermoelectric materials; the applicability of each strategy is also discussed. Firstly, we can seek for extremely low thermal conductivity at the expense of mildly deteriorated thermoelectric power factor, considering the different dominating scattering mechanisms of charge carriers and heat-carrying phonons. Second, functional graded materials or derivatives can be designed to pursue enhanced thermoelectric performance over an imposed temperature difference. Thirdly, one can look for possible dopants or novel mechanisms which can fulfill carrier concentration tuning with temperature so as to maximize the material's figure of merit during the whole working temperature range. These aforementioned strategies are discussed and analyzed in-depth within specific cases, and hopefully can provide some inspirations to the future researches in the field of thermoelectrics.

2:20 PM

(MCARE-S9-006-2016) Novel properties of cage-like and earth-abundant thermoelectrics via theory and simulations (Invited)

L. M. Woods*¹; 1. University of South Florida, USA

The progress in materials design for enhanced thermoelectric performance has been closely related to the fundamental science of the materials internal transport properties. It is imperative that

the transport properties and underlying scattering mechanisms are understood in terms of modelling coupled with experimental verification. In this presentation, a comprehensive review is given on recent theoretical developments of electronic structure and phonon dynamics characteristics for a variety of systems. Several materials, composed of earth-abundant constituents are investigated. First principles simulations show the importance of a maximized Coulomb interaction for decreasing the thermal conductivity in materials with lone s-pair electrons. Cage substitution coupled with particular guest atoms turns out to have unusual consequences in clathrate systems. A scattering mechanism originating from thermal fluctuations induced tunnelling is found to dominate the charge transport in highly-doped polymers. Our theoretical and computational efforts compared with experimental measurements constitute an important step towards a better understanding of transport in thermoelectric materials.

Thermoelectric Materials III

Room: Salon G

Session Chair: George Nolas, University of South Florida

3:20 PM

(MCARE-S9-007-2016) Practical Design, Development and Validation of a Thermoelectric Power Generator (Invited)

T. C. Holgate^{*1}; J. VanderVeer¹; T. E. Hammel¹; I. Teledyne Energy Systems Inc, USA

Thermoelectric generators have been used to supply remote power both terrestrially and in space for more than half a century. Research during recent decades has produced significant advancements in the efficiency of thermoelectric materials, but the practical application of these new materials is very much in the early stages of development. Beyond the characterization of these complex and advanced materials in a highly controlled research laboratory environment, successfully implementing them into a durable and reliable power source involves many challenges and constraints. Having been in the business of building radioisotope thermoelectric generators (RTGs) for space applications since the 1960's, Teledyne Energy Systems, Inc. has worked through many of these challenges to produce RTGs that powered NASA's Pioneer I & II and Viking I & II missions, and more recently, the Mars Science Laboratory Rover—*Curiosity*. An introduction into the general methods and approaches to designing, developing and validating a thermoelectric generator will be presented while giving particular attention to the material challenges involved.

4:00 PM

(MCARE-S9-008-2016) Cage substitution and guest atoms in type II Sn clathrates

A. R. Khabibullin^{*1}; G. S. Nolas¹; L. M. Woods¹; I. University of South Florida, USA

Inorganic clathrates are systems characterized with an open framework structure which can host guest atoms or molecules. The relationship between the clathrate structure and the related properties is of fundamental scientific and technological importance. The relatively high electron mobility and low thermal conductivity of these systems are particularly attractive for thermoelectric applications. The focus of our investigation are type II Sn clathrates, which have been explored to a lesser extent as compared to their Si or Ge counterparts. We present results for calculated electronic structure and phonon dynamics properties based on first principles calculations. Comparison with available experimental data is also performed. Our comprehensive investigation shows that the type of guest atoms and cage substitution via Ga atoms strongly affect the energy band structure coupled with anharmonicity effects originating from the guest atoms. Unusual effects arising from weak van der Waals interactions and negative Grüneisen parameters have also been identified. Our study expands and improves the fundamental

understanding of clathrate materials in general and it gives new perspectives for experimentalists.

4:20 PM

(MCARE-S9-009-2016) Electron and Phonon Engineering in thermoelectrics

Y. Pei^{*1}; I. Tongji University, China

Thermoelectric generators which directly convert heat into electricity have long been relegated to use in space or other niche applications, but are now actively considered for a variety of waste heat recovery systems (such as the conversion of automobile exhaust heat into electricity) to combat the global energy dilemma. Although the devices are supremely reliable and compact, the thermoelectric materials themselves are relatively inefficient requiring advancing the thermoelectric figure of merit, zT above 1.5 for widespread application. In this talk, several strategies to achieve high zT , regarding band and micro structure engineering, are proposed and demonstrated experimentally. The achieved high peak zT not only support the possibility of further development of existing materials but also guide the design of new materials. With any luck, the improvements resulting from these approaches will be large enough to promote thermoelectric devices out of niche applications into the mainstream. `<embed height="0" id="xunlei_com_thunder_helper_plugin_d462f475-c18e-46be-bd10-327458d045bd" type="application/thunder_download_plugin" width="0" />`

4:40 PM

(MCARE-S9-010-2016) Thermal Stability Measurements and Evolved Gas Analysis of Selected Thermoelectric Materials and Potential TE Standards

E. Post^{*1}; I. NETZSCH Geraetebau GmbH, Germany

Compound semiconductors of the families II-VI, III₂-VI₃, like PbTe(Se), Bi₂Te₃ etc. are excellent candidates for thermoelectric modules due to their band gaps. Also materials from the structure family of skutterudites are of increasing interest. Limitations in the application and production are often the relative low thermal stability of these compounds. During decomposition of some of these materials additionally more or less toxic gas species are evolved. The quest of TE standards is still a demanding task. Beneath of their production with reproducible electrical and thermal properties, also their thermal stability under different atmospheres is of high interest. Thermal Analysis techniques, as TGA, are excellent tools for these investigations. The thermal stability of several TE materials was measured with a STA (TG-DSC) system under different atmospheres. Further on results from a TGA coupled to a Skimmer mass spectrometer system will be presented. This simultaneous TG-DSC-MS coupling system allows also the detection of heavier gas species like Se, PbSe, PbTe etc.

5:00 PM

(MCARE-S9-011-2016) Thermal to Electric Energy Conversion: Structural Phase Transitions as a Voltage Pump

S. Tidrow^{*1}; I. Alfred University, USA

Mankind has used structural phase transitions of materials, like large bodies of water, as a source of "renewable" energy, to provide "effective" cooling in the summer through evaporative processes and to provide "effective" heating in the winter, through transformation of water to ice with ice also used as a reasonably good thermal insulator as demonstrated through the "igloo". Here, the material electrical requirements for a thermal-to-electric energy conversion device, which can be tailored to convert energy over a wide temperature range, are discussed. Temperature variation of the dielectric constant in ferroelectrics and antiferroelectrics can be used in capacitive structures to pump the potential of charge on electrodes of a capacitor from a lower energy to higher energy level. The efficiency of conversion can under appropriate conditions be extremely high, theoretically reaching 100% efficiency in

conversion. In practical terms, the energy conversion efficiency is limited by the RC time constant, which depends upon the dielectric properties of the material forming the capacitor, of the device structure as it self-discharges. The preliminary theoretic background for the energy conversion device technology is discussed along with recent efforts in material property design of ferroelectrics and anti-ferroelectrics possessing a priori specified structural phase transition temperatures.

S10: Batteries and Energy Storage

Beyond Lithium Batteries and Supercapacitors

Room: Salon E

Session Chairs: Raj Singh, Oklahoma State University; Reza Shahbazian-Yassar, University of Illinois at Chicago

1:40 PM

(MCARE-S10-030-2016) New Positive Electrode Materials for Rechargeable Li/Na Batteries (Invited)

N. Yabuuchi^{*1}; 1. Tokyo Denki University, Japan

In the past decade, lithium-enriched compounds, Li_2MeO_3 ($\text{Me} = \text{Mn}^{4+}$, Ru^{4+} etc.), have been extensively studied as high-capacity electrode materials for lithium batteries. Although the origin as the high reversible capacity has been a debatable subject for a long time, recently it has been confirmed that charge compensation is partly achieved by solid-state redox of non-metal anions, *i.e.*, oxide ions, coupled with solid-state redox of transition metals, which is the basic theory used for classical lithium/sodium insertion materials. The use of oxide ion redox is the important strategy to further increase the reversible capacity of positive electrode materials for lithium/sodium batteries because the lithium (sodium) content is potentially further enriched with a lower amount of transition metals in the framework structure. Reversible capacities as electrode materials is not limited by the absence of oxidizable transition metals as a redox center. Negatively charged oxide ions can potentially donate electrons instead of transition metals. In this study, we present new electrode materials for sodium/lithium batteries, which use anion redox for charge compensation, and from these results, the possibility for further enrichment of reversible capacity and energy density is discussed.

2:20 PM

(MCARE-S10-031-2016) NASICON $\text{Na}_3\text{V}_2(\text{PO}_4)_3$: a rich crystal chemistry (Invited)

J. Chotard^{*1}; G. Rousse²; R. David¹; O. Mentré³; F. Lalère¹; Y. Deng¹; C. Masquelier¹; 1. University de Picardie Jules Verne, France; 2. Collège de France, France; 3. UCCS, France

For more than 40 years, NASICON-type materials have been heavily investigated mainly for their properties of fast ionic conduction but also as very promising electrode materials in Li and/or Na ion batteries. In this wide family, an interesting material is the vanadium based compound $\text{Na}_3\text{V}_2(\text{PO}_4)_3$ (NVP). The crystal structure of this compound (rhombohedral unit cell, SG R-3c) was originally reported by Delmas *et al* in 1978 and was later confirmed by Gopalakrishnan *et al* in 1992. Since then, NVP has mostly always been reported to crystallize into a rhombohedral cell even though Masquelier *et al*. reported several times on the existence of a monoclinic distortion at ambient temperature with complex series of unidentified diffraction peaks. In this scope, we investigated high purity NVP sample using high resolution synchrotron and neutron powder diffraction as well as single crystal diffraction. While the high temperature γ -NVP is indeed crystallizing into a rhombohedral unit cell (R-3c), the room temperature α -NVP shows a clear monoclinic distortion together with the presence of very weak superstructure reflections. Neglected for almost 40 years, those tiny peaks have finally been successfully indexed using an incommensurate modulated structure (confirmed

by both powder and single crystal diffraction). At room temperature (α -NVP), the monoclinic distortion, induces a splitting of the Na(2) cations into two new positions.

3:00 PM

(MCARE-S10-032-2016) Can we trust half-cells in Na based batteries? (Invited)

A. Ponrouch^{*1}; 1. ICMAB - CSIC, Spain

Lithium metal anodes are widely used as counter (or also reference) electrodes in the so termed *half cell* tests, performed mostly at laboratory scale within the battery research community. These are mostly intended to assess the electrochemical performance of a given compound as either positive or negative electrode material for LIB in a simple way, avoiding the assembly of *full cells* in which electrode balancing can severely affect performance. The reliability of extrapolating such half cell testing results to potential performance in full cells relies on the stability of the Solid Electrolyte Interphase (SEI) typically formed on the surface of metal anodes (Li or Na) as a result of electrolyte degradation reactions. The reliability and representativity of half test cells in SIB research was generally taken for granted. In this context, the aim of our work was to perform a comparative study of the composition, morphology and stability of the SEI formed on lithium and sodium metal anodes with state-of-the-art electrolytes. The impact of the use of metal anodes (Li or Na) in half cell configuration on the impedance of a hard carbon negative electrode was also investigated. Our results clearly point at the existence of significant differences which cast some doubts on the representativity of half-cell tests and call to exercise care in the interpretation of their results.

3:40 PM

(MCARE-S10-033-2016) Manganese-based Layered Oxides as Cathode Materials for Na-ion Batteries (Invited)

M. Kwon¹; K. Lee^{*1}; 1. Seoul National University, Republic of Korea

According to the increasing demands for large scale energy storage systems, Li-ion batteries have been received a lot of attention because of their high energy density. However, recently, Na-ion batteries have been considered as one of the most promising alternatives to replace Li-ion batteries due to the advantage of abundant sodium resources. However, the energy density of Na-ion batteries is lower than that of Li-ion batteries, and this is the challenging issue to develop Na-ion batteries. Therefore, it is required to develop new cathode materials having high reversible capacity and redox potential to increase the energy density of Na-ion batteries. Recently, several reports have introduced Manganese-based layered oxide materials with high reversible capacity. However, their reaction and failure mechanisms were not fully understood. In this presentation, we will demonstrate the reaction and failure mechanisms of layered sodium manganese oxides through in-situ XRD analysis, and suggest a few strategies to improve electrochemical performance. Further, the role of doping in layered sodium manganese oxides for synthesis and electrochemistry will be discussed.

4:20 PM

(MCARE-S10-034-2016) Thermally and Electrochemically Driven Topotactical Transformations in Sodium Layered Oxides Na_xVO_2 (Invited)

M. Guignard^{*1}; C. Didier¹; M. R. Suchomel²; D. Carlier¹; J. Darriet¹; C. Delmas¹; 1. ICMCB-CNRS, France; 2. Argonne National Lab, USA

Phase diagrams and structural transformations in the complex Na_xVO_2 system have been studied using electrochemical (de)intercalation and in situ and operando high resolution synchrotron powder diffraction. Starting from O'3- $\text{Na}_{1/2}\text{VO}_2$ obtained by sodium electrochemical deintercalation of O3- NaVO_2 , the structural details of irreversible and reversible thermally driven transformations to P'3 and P3 type structures are presented. Subsequently, these P'3- Na_xVO_2 phases provide a platform for operando studies exploring

the Na_xVO_2 phase diagram as a function of sodium electrochemical (de)intercalation. In this system, three single phase domains have been found: a line phase $\text{P}^3\text{-Na}_{1/2}\text{VO}_2$, one solid solution for $0.53 \leq x \leq 0.55$ characterized by an incommensurate modulated structure and a second solid solution for $0.63 \leq x \leq 0.65$ with a defective structure resulting from a random stack of O^3 and P^3 layers. With further sodium intercalation ($x > 0.65$), the structure irreversibly transforms to the starting parent phase $\text{O}^3\text{-NaVO}_2$. This work reveals new details about the diverse structural prototypes found in sodium layered oxides used as electrode battery materials and the transitional pathways between them as a function of temperature and composition.

5:00 PM

(MCARE-S10-035-2016) Non-aqueous semi-solid flow battery based on Na-ion chemistry (Invited)

J. R. Morante^{*1}; 1. IREC, Catalanian Institute for Energy Research, Spain

In this contribution, we will report on the technological alternatives and performance perspectives for using sodium ion as active ion in these semi solid flow batteries. Sodium-ion batteries (SIBs) attracted increasing attention in the past few years since sodium is abundant, inexpensive, and does not alloy with aluminium which allows for cheaper current collectors and energy densities of ca. 200 Wh kg^{-1} are feasible. Moreover, sodium does offer an even larger variety of crystal chemistries than lithium. Here, we report on the first proofs of concept for a non-aqueous semi-solid flow battery (SSFB) based on Na-ion chemistry. Different used compounds like $\text{Na}_x\text{Ni}_{0.22}\text{Co}_{0.11}\text{Mn}_{0.66}\text{O}_2$ for positive electrodes or other ones like $\text{NaTi}_2(\text{PO}_4)_3$ as negative ones will be discussed. This concept opens the door for developing a new low-cost type of non-aqueous semi-solid flow batteries based on the rich chemistry of Na-ion intercalating compounds defining an exciting challenge for achieving increasing performances at low cost and overcoming the problems concerning the formation of the so-called solid electrolyte interphase on negative (SEI) and positive (CEI) electrodes.

5:20 PM

(MCARE-S10-036-2016) Recent Advances in Electrolytes for Magnesium Sulfur Batteries (Invited)

Z. Zhao-Karger^{*1}; M. Fichtner¹; 1. Karlsruhe Institute of Technology, Germany

Rechargeable magnesium (Mg) battery has been recognized as an attractive alternative for grid energy storage because Mg as anode has a high volumetric capacity of 3837 mAh cm^{-3} . Particularly promising is that the intrinsic non-dendritic growth of Mg during repetitive plating alleviates the safety concerns impeding the practical applications of a lithium and sodium metal anode in battery systems. In addition, the natural abundance of magnesium raw material makes the Mg batteries more cost-effective than lithium ion batteries. However, the development of Mg batteries are hampered by several technical obstacles, such as the absence of electrolyte which is stable in contact with the electrode materials and the quest for practical cathodes offering high accessible capacity and rate capability. Sulfur is an attractive cathode material with a high theoretical capacity, low cost and nontoxic. The combination of a magnesium anode with a sulfur cathode is one of the most promising electrochemical couples possessing a volumetric energy density of 3227 Wh l^{-1} , which is superior to a Li-S system. Recent achievement of non-nucleophilic electrolytes through one-step reaction between magnesium-bis(hexamethyldisilazide) $[(\text{HMDS})_2\text{Mg}]$ and AlCl_3 in different glymes has been successfully applied to the magnesium-sulfur (Mg-S) batteries. The performance and electrochemical conversion of Mg-S batteries will be discussed.

5:40 PM

(MCARE-S10-037-2016) Prospects for Solid State Supercapacitors Based on Calcium Copper Titanium Oxide for Energy Storage Applications (Invited)

R. N. Singh^{*1}; 1. Oklahoma State University, USA

Batteries and capacitors are extensively used for energy storage applications. Supercapacitors are particularly attractive for applications where rapid charging and discharging are needed and high storage capacity is desired. All solid-state supercapacitors based on Calcium Copper Titanium Oxide (CCTO) ceramics are attractive because of their high-dielectric constant in the range of $10^4\text{-}10^5$. However, current material system based on the CCTO suffers from leakage. To overcome this limitation, systematic approaches based on processing and selective addition of dopants/impurities are being pursued to maintain phase purity and high K values while at the same time minimizing leakage. Extensive use of complex impedance measurements, associated data analyses and modeling are done to separate contributions from grain and grain boundaries to provide a basic understanding of the overall dielectric properties and storage potential. These results along with the status of the supercapacitors based on the CCTO will be presented and discussed.

6:00 PM

(MCARE-S10-038-2016) 3D printing of graphene aerogel

C. Zhou^{*2}; D. Lin¹; 1. Kansas State University, USA; 2. University at Buffalo, USA

Graphene aerogel transfers inherent properties of graphene into macroscopic applications for composite materials, energy storage, stress sensor, thermal insulator and shock damping. However, fabrication of graphene aerogel with tailored macrostructures utilizing scalable and controllable methods remains a significant challenge. Here we report rapid three-dimensional printing technique, which is developed for printing graphene aerogel architectures. Moreover, this 3D printing technique also enables aligning microstructure of printed graphene aerogel along printing direction. Based on our knowledge, we firstly demonstrate 3D printed graphene aerogel truss architecture with overhang features. The 3D printed graphene aerogels are ultra-light densities (from 0.5 to 10 mg cm^{-3}), significant electrical conductivity ($\sim 15.4 \text{ S m}^{-1}$), and high compressibility, and they are much stiffer than their counterparts, such as bulk GA with comparable density. Adapting this novel methodology realizes the design and fabrication of complex 3D graphene aerogels architectures on myriad applications.

Thursday, April 21, 2016

Plenary Session IV

Room: Salon E

8:30 AM

(MCARE-PL-004-2016) Patenting Materials for Alternative & Renewable Energy: Challenges and Opportunities

C. Paradies^{*1}; 1. Paradies Law, USA

The number and diversity of patent filings on materials useful for alternative and renewable energy technologies is growing, worldwide, as are the number and diversity of patents on technologies using such new materials to save energy, generate new or more efficient sources of energy and store energy generated by renewable energy sources. Advances in materials useful for alternative and renewable energy production and storage, in particular, have the potential to cause disruption in the global energy marketplace, which presents both challenges and opportunities. The cost of introducing these new materials into energy generation and storage solutions and delays in implementation of major changes in infrastructure and energy distribution required to use alternatives and renewables could limit return on investment from new material research and

development. Nevertheless, investments in developing new materials for energy savings, generation and storage must be made to meet international goals for reduction of greenhouse gas emissions. The author addresses the challenges and opportunities in the patenting of materials for alternative and renewable energy and offers practical solutions.

S5: Materials Challenges in Fuel Cells

Materials Challenges in Fuel Cells

Room: Salon D

Session Chair: Olivier Guillon, Forschungszentrum Juelich

9:50 AM

(MCARE-S5-001-2016) Processing and Properties of Hierarchical Porous and Multi-layered Ceramics for Energy Applications – Experiments and Simulations (Invited)

R. K. Bordia^{*1}; C. Martin²; 1. Clemson University, USA; 2. Université de Grenoble - Alpes, France

Porous ceramics have many applications in energy conversion technologies. Most of these applications demand optimization of a multitude of properties many of which have conflicting requirements on the microstructure. Materials with designed anisotropic and hierarchical microstructures have the potential to optimally address the requirements. Results will be presented on the processing approaches to make these designed microstructures. With the developed processing protocols, it will be shown that it is possible to independently control several relevant microstructural parameters. The quantification of the 3D microstructure at different length scales and meso-scale simulations to simulate the mechanical and transport properties and their comparison with experimental results will be presented. Specifically, with respect to the mechanical properties, using both simulations and experimental results, the role of heterogeneities and anisotropy has been investigated. The advantages of these types of microstructures, in comparison to homogeneous and isotropic porous microstructures will be highlighted.

10:30 AM

(MCARE-S5-002-2016) Particle Atomic Layer Deposition for Synthesis of Fuel Cell Catalytic Material

W. W. McNeary^{*1}; A. M. Lubers¹; A. W. Weimer¹; M. E. Maguire¹; D. Ludlow²; A. Drake¹; M. Faust³; M. Seipenbusch³; 1. University of Colorado, Boulder, USA; 2. Ludlow Electrochemical Hardware, USA; 3. Karlsruhe Institute of Technology, Germany

Fluidized bed Atomic Layer Deposition (ALD) was carried out to deposit platinum nanoparticles on functionalized and unmodified carbon black. Organometallic ligands were removed via combustion and hydrogenation chemistries. The synthesized materials were evaluated as oxygen reduction reaction (ORR) catalysts in both rotating disk electrode half-cell and proton exchange membrane fuel cell experiments and compared to commercial catalyst. The Pt ALD catalyst on unmodified carbon using hydrogen as a second precursor had similar nanoparticle characteristics and fuel cell performance to the commercial catalyst. The catalysts deposited on functionalized carbon performed well in electrochemical hydrogen pumping tests (on par with commercial), but were not effective in the fuel cell due to reduced hydrophobicity within the catalyst layer. Additional work has been done to increase the durability of commercial Pt/C catalysts using ALD thin films of metal/metal oxide materials. Preliminary results suggest that ALD coatings stabilize the Pt nanoparticles and aid in sintering prevention, which manifests as increased retention of electrochemical surface area (ECSA) over voltage cycling.

10:50 AM

(MCARE-S5-003-2016) Post-test analysis of a rechargeable oxide battery (ROB)

C. M. Berger¹; O. Tokariev¹; N. H. Menzler¹; M. Bram¹; O. Guillon^{*1}; 1. Forschungszentrum Jülich GmbH, Germany

Solid oxide cells (SOC) have made large advances in their performance owing to the development of new materials, microstructural optimisations, and better manufacturing routes. Using their ability to be used in reverse mode as electrolysis cells, their combination with a storage material leads to so-called rechargeable oxide batteries (ROB). An ROB comprises a SOC and a reversible storage for oxygen ions. Whereas the SOC converts power and steam into hydrogen or vice versa, the iron oxide base storage is reduced by H₂ or oxidised by H₂O to store or to release energy. As the SOC is already far-advanced as compared to the storage material, the focus of the development is on the latter. Porous storage components were manufactured by tape casting or extrusion, sintered, exposed to simulated conditions of an ROB, and finally working ROB were assembled. The ROB were operated at 800°C for 200 charge-discharge cycles at 150 mA/cm² and 1 V/cell. After the test, the battery was dismantled and post-test analysed. The storage components were examined using SEM and XRD for microstructure and materials interaction characterisation. Depending on the chemical composition and microstructure the formation of relatively thick layers of FeO were detected close to the surface of the initially porous storage body. These detrimental effects were suppressed by the increase of porosity as well as the use of CaO instead of ZrO₂ as a scaffold.

11:10 AM

(MCARE-S5-004-2016) Proton-Conducting Ceramic Electrolyte Fuel Cell for the Conversion of Natural Gas to Electricity and Liquid Fuels

B. Balachandran^{*1}; T. H. Lee¹; S. E. Dorris¹; 1. Argonne National Laboratory, USA

We are developing a fuel cell technology that operates on excess natural gas being produced at a natural gas well-pad to generate electrical power and ethylene, which, when integrated with a chemical process, produces a liquid fuel or higher value chemical that is more readily transported to market. One of the keys to this technology is the development of a novel proton-conducting fuel cell that is capable of operating efficiently at 500-700°C. We have fabricated a solid oxide fuel cell (SOFC) using a BaCe_{0.8}Y_{0.2}O_x (BCY) proton conductor as the electrolyte. A dense BCY film (≈10-μm thick) was deposited on a porous Ni/BCY cermet (i.e., ceramic/metal composite) substrate by a dip-coating process. The Ni/BCY cermet substrate was used as the anode, and platinum paste served as the cathode. The current-voltage characteristics of the BCY-based SOFC were measured in the temperature range 500-700°C. The open-circuit voltage was close to the theoretical value at lower temperatures (<600°C) and was about 85% of the theoretical value at 800°C. The peak power density of the fuel cell was ≈120 and ≈600 mW/cm² at 500 and 700°C, respectively. Our efforts to develop SOFCs based on proton conductors will be summarized in this talk. Work supported in part by the U.S. Department of Energy, Advanced Research Projects Agency – Energy (ARPA-E) under Contract DE-AC02-06CH11357

S6: Critical Materials for Energy

Critical Materials for Energy III

Room: Salon F

Session Chairs: Bum Sung Kim, KITECH; Michitaka Ohtaki, Kyushu University

9:50 AM

(MCARE-S6-014-2016) ZnO-based Oxide Thermoelectric Materials with Microstructure Control for Selective Phonon Scattering (Invited)

M. Ohtaki^{*1}; 1. Kyushu University, Japan

ZnO is one of the most promising n-type oxide thermoelectric materials for waste heat recovery. Nevertheless, the light constituting elements and strong interatomic bonding in ZnO lead to a high sound velocity of acoustic phonons carrying heat. Accordingly, the thermal conductivity, κ , of ZnO is very high compared with other non-oxide thermoelectric materials, limiting the thermoelectric performance of the oxide. Recently, we have successfully reduced the κ value of ZnO by co-doping of Al and Ga. The thermoelectric performance of the oxide was markedly improved by the co-doping, reaching $ZT = 0.47$ at 1000 K and $ZT = 0.65$ at 1275 K for $Zn_{0.96}Al_{0.02}Ga_{0.02}O$. This is the highest ZT values so far reported on bulk n-type oxides. In this paper, microstructure control of ZnO-based oxides will be reported. Upon the binary doping of ZnO with Al and Ga, the amount of a Ga-related impurity phase is revealed to show an excellent quantitative agreement with the decrease in the thermal diffusivity. The bulk nanocomposite structure spontaneously formed in the bulk oxide found to be crucial to achieve a considerable reduction in the thermal conductivity with keeping high electrical conductivity, leading to a remarkable improvement in the ZT value of the ZnO-based oxide. The selective phonon scattering will be discussed in terms of the mean free path and microstructure in the oxides.

10:30 AM

(MCARE-S6-015-2016) Two-step process for recycling used ZrF4-containing pickling (Invited)

J. Lee^{*1}; B. Yoo¹; Y. Lee¹; S. Han¹; D. Park¹; H. Nersisyan¹; I. Chungnam National University, Republic of Korea

A two-step process was developed to purify a ZrF₄-containing pickling solution for reuse in subsequent pickling operations and to transform the zirconium compound extracted from the pickling solution into a CuZr alloy. The first step, the precipitation of ZrF₄ and purification of the pickling solution, was accomplished using NaF and AlF₃ additives. Under optimized precipitation conditions, Na₅Zr₂F₁₃ salt was obtained as a solid, and the residual concentrations of Zr⁴⁺ and Na⁺ ions in the purified pickling solution were less than 100 and 500 ppm, respectively. In the second step, the Na₅Zr₂F₁₃ salt was converted into a CuZr alloy using a molten salt electro-winning process followed by vacuum distillation.

11:10 AM

(MCARE-S6-016-2016) Effect of Flow Dynamics for the Synthesis of Cadmium Selenide Quantum Dots in a Microreactor

B. Kim^{*1}; D. Jenog¹; J. Park¹; T. Kim¹; T. Seong²; 1. Korea Institute of Industrial Technology, Republic of Korea; 2. Korea University, Republic of Korea

Colloidal semiconductor nanocrystals, or quantum dots (QDs), are applicable in optoelectronic devices, photovoltaic devices. QDs are usually produced in small batches using laboratory-scale reactors. However, with larger reactor sizes, temperature control and homogeneous mixing is harder to accomplish. Synthesis of QDs using a microreactor is a promising technique, and can be easily scaled-up. Microreactor is possible to control in-situ process parameters such as temperature, reaction time related flow rates each precursors. In

the current study, CdSe QDs were synthesized using an indigenously designed microreactor with octylamine as the solvent. The effect of octylamine flow rate on the structure, morphology, and optical properties of the CdSe QDs synthesized has been investigated. The flow rate of octylamine was varied from 0.005 to 0.030 ml/min, and the optical properties of the synthesized particles were analyzed by UV-vis and PL. We determined that, by controlling octylamine flow rate, the particle size of the quantum dots could be controlled. The flow rates of octylamine affected on luminescence wavelengths and intensities, because nucleation and growth mechanism of QD have a relationship with the quantity of octylamine. This method will help to determine the optimal octylamine flow conditions for synthesizing nanoparticles for use in a diverse range of applications.

11:30 AM

(MCARE-S6-017-2016) Production of Potassium Manganese Oxide Nanowires with the Inclusion of Bird Feathers in the Central Membrane

M. S. Solangi^{*1}; 1. United Energy Pakistan Limited, Pakistan

Oil is one of the basic and essential commodities required by humans in their daily life. Oil as in one case is a marvel simultaneously, also acts as, a menace if misused or if any technological mishap takes place. In the latter it readily affects our environment causing ample damage to our ecological system. In this study, it is proposed to reduce this menace, keeping in mind all the technological mishap's which result in the spillage of oil, there is a need to develop a material which can absorb oil readily from an oil and water mixture. Hence a similar material can be created if we use, (Potassium Manganese Oxide) interwoven mesh of nanowires as the central membrane, the pores of which will be mounted with bird feathers and finally this material will be covered with a water repellent coating of silicon which will refrain it from absorbing water. Here we present a self-assembly method for constructing thermally stable, free-standing nanowire membranes that exhibit controlled wetting behavior. This material if manufactured successfully will be able to absorb oil about 25-30 times of its own weight. Which can be used to revive our eco-system and millions of liters of oil can be regained from sea water and further it will also help us to eliminate other hydrophobic impurities from water.

11:50 AM

(MCARE-S6-018-2016) Enhanced thermoelectric properties of p-type BiSbTe based alloys through the dispersion of nano inclusions

B. Madavali¹; C. Lee¹; H. Kim²; J. Koo¹; S. Hong^{*1}; 1. Kongju National University, Republic of Korea; 2. Aems Lab, Iowa State University, USA

Thermoelectric (TE) power generation is increasingly drawing attention as a viable technology to make significant contributions towards recovering waste heat and increasing energy efficiency of heat engines. TE devices are the semiconductor systems that can either directly convert thermal energy into electricity for power generation, or perform cooling or heating with electric power. Recently, embedded nanoparticles in the matrix can significantly increase thermoelectric figure of merit by the reduction of thermal lattice thermal conductivity through the scattering of phonons at numerous grain boundaries and newly formed interfaces. In this research, we have fabricated p-type BiSbTe based nanocomposite thermoelectric alloys by MA then subsequently consolidated by SPS at 673K. The microstructure and crystal structure of the nanocomposites have been characterized by the scanning electron microscopy and X-ray Diffraction respectively. Vickers hardness values are increased due to the formation of fine microstructure and high relative density. The nanocomposite bulk samples shows the lower thermal conductivity values due to scattering of phonons and carriers at interfaces and numerous grain boundaries. The maximum figure of merit, ZT is achieved for nanostructured bulk samples owing to the reduction of thermal conductivity and improvement of Seebeck coefficient values.

S9: Direct Thermal to Electrical Energy Conversion Materials and Applications

Thermoelectric Materials IV

Room: Salon G

Session Chair: Arash Dehkordi, SunEdison

9:50 AM

(MCARE-S9-012-2016) Design and optimization of high performance p-type half-Heusler thermoelectric materials with $zT > 1$ (Invited)

T. Zhu^{*1}; 1. Zhejiang University, China

Half-Heusler (HH) compounds are important high temperature thermoelectric (TE) materials having attracted considerable attention in the recent years. In this talk, we show that a new p-type HH solid solutions with a high band degeneracy, Ti doped $\text{FeV}_{0.6}\text{Nb}_{0.4}\text{Sb}$, can achieve a high zT of 0.8. The enhanced phonon scattering by alloying leads to a reduced lattice thermal conductivity. Further investigation shows that increasing Nb content in the $\text{Fe}(\text{V}_{1-y}\text{Nb}_y)$ Sb solid solutions can achieve lower valence band effective mass and consequently higher carrier mobility. In addition, increasing Nb content in $\text{Fe}(\text{V}_{1-y}\text{Nb}_y)_{1-x}\text{Ti}_x\text{Sb}$ will prevent the degradation of the TE performance at high temperatures due to the larger band gap for FeNbSb . We obtain a high zT of 1.1 at 1100K for $\text{FeNb}_{1-x}\text{Ti}_x\text{Sb}$ without V substitution. More recently, we found that Hf doped FeNbSb exhibits a record high zT of 1.5 at 1200K due to simultaneously optimized electrical power factors and reduced lattice thermal conductivity. In view of abundantly available elements, good stability and high zT , FeNbSb alloys can be great promising for high temperature power generation.

10:30 AM

(MCARE-S9-013-2016) On the Role of NaBH_4 toward Enhancing Thermoelectric Performance of Bi_2Te_3 and SiGe (Invited)

J. He^{*1}; T. M. Tritt¹; 1. Clemson University, USA

In this presentation we will compare the role of NaBH_4 toward enhancing the thermoelectric performance of Bi_2Te_3 and SiGe . As a strong surfactant widely used in nanomaterial synthesis, NaBH_4 was found to play an interesting role in Bi_2Te_3 and SiGe , two important class of thermoelectric materials. In pulverized Bi_2Te_3 hydrothermally treated by NaBH_4 and followed by hot pressing, a nm-thin layer formed on the grain boundary of Bi_2Te_3 and led to favorable changes in the carrier concentration, carrier mobility, compatibility factor and mechanical properties. The effect was more pronounced in finer grained materials, suggesting this is a grain boundary effect. In SiGe , however, NaBH_4 was decomposed into Na, B, H_2 , and boron-rich sodium in the spark plasma sintering process. The Na and B doped the SiGe crystal lattice, leading to favorable changes in the carrier concentration and the power factor. In the mean time, the boron-rich sodium formed as nanoparticles helped suppress the lattice thermal conductivity. As a result, a state-of-the-art ZT was obtained for SiGe . It is thus highly desired to extend the study to other alkali metal boron hydrides and other thermoelectric materials.

11:10 AM

(MCARE-S9-014-2016) Probing the role of La Fillers and Sb vacancies in CoSb_3 Skutterudites

X. Zeng^{*1}; C. Hu²; J. He¹; J. Huang³; B. Sumpter³; H. Zhao¹; T. M. Tritt¹; 1. Clemson University, USA; 2. University of Minnesota-Twin cities, USA; 3. Oak Ridge National Lab, USA

A combination of a doping, nanocomposites and-filling (rattlers) approach has proven to be quite effective in enhancing the thermoelectric (TE) performance of CoSb_3 based skutterudites. Therefore we used La as the single control to study the interplay between La filler atoms, a Lanthanum antimonide secondary

phase, and Sb vacancies in CoSb_3 by means of DFT calculations, along with synthesis, elemental characterization and TE property measurements. The DFT calculations was able to reveal the variation of conduction type with increasing La content and provided insight on the impact of La fillers and Sb vacancies on the electron band structure. Experimentally, we prepared and characterized $\text{La}_y\text{Co}_4\text{Sb}_{12-8}$ ($y = 0.1, 0.2, 0.4, \text{ and } 0.6$) samples. The results of combined theoretical and experimental studies have shown La is a filler not rattler, and Sb vacancy due to the formation of (La, Sb) secondary phase also acts as donor. As a result, without the rattler effect often observed in other filled CoSb_3 skutterudites, a ZT value of ~ 0.4 is attained at 700 K in $\text{La}_{0.6}\text{Co}_4\text{Sb}_{12}$. These results led us to proposed a synergistic “doping, nanocomposites-and filling approach” in order to further improve the thermoelectric performance of CoSb_3 based skutterudites.

11:30 AM

(MCARE-S9-015-2016) Characterization, Mechanical and Thermal Properties of Thermoelectric Materials and Nanocomposites

K. Lilova^{*1}; 1. Setaram Inc., USA

The thermoelectric materials and nanocomposites applications require a thorough study of their mechanical and thermal properties. The Thermomechanical analysis was used to determine the optimal sintering temperature and choose the appropriate technique (CS or SPS) for n-type bulk and nano $\text{Ca}_{0.9}\text{Yb}_{0.1}\text{MnO}_{3-\delta}$ powders. The ThermoGravimetric Analysis is used for quantitative characterization of the impurities, decomposition, corrosion. The Differential Scanning Calorimetry provides important data about the heat capacity, melting behavior, phase transitions, polymorphism, thermokinetics. TGA was used to study the thermal stability (decomposition and oxidation) of BiCuSeO based materials simulating real application conditions. The thermal stability and the activation energies of another type of compounds with thermoelectric properties - $\text{K}_2\text{Bi}_8\text{Se}_{13}$ -based nanocomposites, was determined by DSC. The high temperature heat capacity data of p-type $\text{Yb}_{14}\text{MnSb}_{11}$ was used to calculate the thermal conductivity, revealing an extremely low lattice thermal conductivity in this case. The thermal conductivity of organometallic coordination polymers (NC-CuTCNQ), thin films of NrA-CuTCN , and p-type composite ternary tellurides for scalable thermoelectric generator devices was also measured directly applying Modified Transient Plane Source (MTPS) technique.

11:50 AM

(MCARE-S9-016-2016) Development and performance of thermoelectric materials and modules (Invited)

R. Funahashi^{*1}; T. Barbier¹; 1. National Institute of Advanced Industrial Science & Technology, Japan

Thermoelectric properties for $(\text{BaCoO}_{3-y})_n\text{B}_3\text{Co}_8\text{O}_{11}$ have been investigated at 373-973 K in air. All samples show a p-type character. Electrical resistivity, ρ of BaCoO_{3-y} ($n=\infty$) decreases monotonically with increasing temperature. On the other hand, a transition in the electrical conduction is observed in the $\text{BaCo}_9\text{O}_{11}$ ($n=0$), $\text{Ba}_2\text{Co}_9\text{O}_{14}$ ($n=1$), and $\text{Ba}_3\text{Co}_{10}\text{O}_{17}$ ($n=2$) around 500 K. Thermal conductivity looks to be decreased by the corner shared CoO_6 structure. The values of dimension-less figure of merit, ZT increase with increasing temperature and reach about 0.03 at 973 K for the $n=1$ sample. The substitution at the Ba site by Na is the most effective to enhance the S values at temperatures lower than 573 K. The values of power factor ($=S^2/\rho$) for the samples substituted by Na and Sr are reach 0.1 mW/m.K^2 at 773 K. Thermoelectric modules consisting of the oxides and the silicides have been fabricated. In the case of the oxide modules, thermoelectric generation units were produced and tested in incinerators and industrial furnaces. Thermoelectric efficiency is about 5 %. On the other hand, the output power of the silicide module reaches 9.4 W at the heat source temperature of 873 K in air. The durability at the heat-source temperature of 773 K is

improved by optimization of Ag paste to form junctions. This work was supported by Thermal Management Materials and Technology research Association (TherMAT), Japan.

S10: Batteries and Energy Storage

Battery Processing

Room: Salons A-C

Session Chairs: Aninda Bhattacharyya, Indian Institute of Science; Kristina Lilova, Setaram Inc.

9:50 AM

(MCARE-S10-040-2016) Low-Cost Lithium-Ion Electrode Processing and Manufacturing Science (Invited)

D. L. Wood^{*1}; J. Li¹; D. Mohanty¹; Z. Du¹; L. David¹; Y. Sheng¹; S. An²; C. Daniel¹; 1. Oak Ridge National Laboratory, USA; 2. University of Tennessee, USA

Lithium-ion battery pack costs have dropped significantly over the past few years from about \$500-600/kWh down to \$275-325/kWh due to economies of scale, improvements in electrode and cell quality control, and more efficient production methods. However, much more development on electrode processing cost reduction, coating deposition quality control, and cell assembly methods needs to occur in order to meet the DOE ultimate pack cost of \$125/kWh for battery electric vehicles (BEVs). In addition, cell energy densities still need to be increased from 150-180 Wh/kg to 350 Wh/kg to provide sufficient BEV driving range. This presentation will cover several of the major research activities that are contributing to cost reduction and energy density improvements in lithium-ion cells: All-aqueous electrode dispersion processing for lithium-ion pouch cells. Tailored thick electrode architectures for reduced cost and increased cell energy density. In-line non-destructive evaluation of electrodes and analysis of coating defects on cell performance. High-voltage cathode and high-capacity anode materials for increasing cell energy density. Reducing cell wetting and formation time and optimizing pouch cell electrolyte content.

10:30 AM

(MCARE-S10-041-2016) New challenges to future electrochemical power devices for automotive application (Invited)

Y. Tabuchi^{*1}; 1. Nissan Motor Co., Japan

Li-ion Battery and Polymer electrolyte membrane fuel cell (PEMFC) are regarded as promising alternative power source for zero emission vehicle. Regarding Li-ion battery, not only higher energy density with lower cost but also higher power density are required for various kinds of vehicle system because Li-ion battery is one of common power devices. In order to meet these vehicle requirements, better performance and robustness under severe environment are necessary in electrochemical power device for automotive application. However, complex electrochemical and mass transport phenomena caused road blocks such as significant increase in overpotential and degradation. With this background, state of Li-ion concentration should be managed such as Li-ion concentration in electrolyte, active material, and interface between them. In addition, heat transport also affects these states in both applications. For this purpose, the phenomena in different length scale should be investigated from macro-scale phenomena in cell level to μm scale phenomena inside porous electrode and nm order phenomena at the surface of catalyst. In this presentation, the fundamental research for this purpose will be presented, especially, focusing on multi-scale and multi-physics diagnostic and numerical modeling in Li-ion battery application.

11:10 AM

(MCARE-S10-042-2016) Pre-lithiation of Freestanding Flexible Si Nanoparticles-Carbon Nanotubes Composite Anodes for Lithium Ion Batteries By Stabilized Lithium Metal Powder

K. Yao^{*1}; J. P. Zheng¹; R. Liang¹; 1. Florida State University, USA

Freestanding flexible light-weight silicon nanoparticles-carbon nanotubes (SiNPs-CNTs) composite paper anodes for lithium ion batteries (LIBs) have been prepared by ultrasonication and pressure filtration without adoption of conductive additive, binder or current collector. Electrochemical testing has shown that the SiNPs-CNTs composite electrode material achieves first cycle specific discharge and charge capacities of 2298 and 1492 mAh/g, respectively. To address the first cycle irreversibility, stabilized lithium metal powder (SLMP) has been utilized to pre-lithiate the composite anodes, leading to a reduction of first cycle irreversible capacity loss from 806 to 28 mAh/g and an increase of first cycle coulombic efficiency from 65% to 98%. The relationship between different SLMP loading and the cell performance has been established to optimize the construction of Si-based cells. Use of the SiNPs-CNTs anodes incorporating SLMP as the source of lithium opens the door to a broad range of non-lithium-providing cathode materials and enables the creation of future high capacity and high energy LIBs.

11:30 AM

(MCARE-S10-043-2016) Influence of morphology of $\text{Li}_4\text{Ti}_5\text{O}_{12}$ anode on lithium storage performance

S. N. Reddy^{*1}; V. Ramar¹; C. Wang¹; R. Desapogu¹; P. Balaya¹; 1. National University of Singapore, Singapore

$\text{Li}_4\text{Ti}_5\text{O}_{12}$ (LTO) is considered to be one of the most promising non carbon-based Li-ion battery anodes, as it can deliver high reversible capacity at fast charge and discharge-rate, impressive cycle life, and excellent safety at extreme operating conditions. For achieving such a high performance anode it is mandatory to improve synthesis conditions of active materials and optimize their porous electrode microstructure. Herein, we compare the electrochemical performance of LTO anode prepared by two different approaches especially with different drying conditions which affected the morphology significantly and hence their storage performances. The synthesized LTO - based cells tested against lithium metal exhibit charge capacities in the range 140-160 mAh/g depending on the morphologies. This study demonstrates that the microstructure of LIB electrodes significantly influences key performance metrics such as rate capability and cyclability. Some preliminary results of 18650 Li-ion cells fabricated by our pilot line using LTO anode of different morphologies will also be presented.

11:50 AM

(MCARE-S10-044-2016) Thermal behavior, Thermal Runaway, Kinetic, and Surface Properties of Bulk and Nano Battery and Battery Elements Studied by Thermal Analysis and Calorimetry

K. Lilova^{*1}; L. Brown¹; 1. Setaram Inc., USA

Among the most important characteristics of the batteries are the thermal stability of their constituents, their energetics and kinetics of charge/discharge cycling, safety performance, etc. The thermal stability, heat capacity, and the heat generated during charge/discharge of different lithium batteries were determined using a Calvet type calorimeter large enough to fit the test batteries. The properties of solid and liquid electrolytes, battery elements (e.g. iron oxide nanowires), and additives (4-isopropyl phenyl diphenyl phosphate) were investigated to predict their behaviour in real conditions. Thermogravimetric analysis was the preferred method to characterize carbon nanocomposites for lithium-ion battery anodes and lithium manganese vanadates. The Mg-doped $\text{LiNi}_0.80\text{Co}_0.15\text{Al}_0.05\text{O}_2$ cathode material is more stable during cycling than the undoped one. In order to determine whether the improved performance is due to thermodynamic or kinetics factors, the enthalpies of formation

were measured using high temperature oxide melt solution calorimetry. Using nanosized materials in the lithium batteries adds the surface properties as a highly contributing factor to their most important characteristics. The experimental determination of the surface energy of LiCo₂ and its implication for electrodes will be shown as an example.

Advanced Characterization

Room: Salon E

Session Chairs: Siegbert Schmid, University of Sydney; V. Yartys, Institute for Energy Technology

9:50 AM

(MCARE-S10-045-2016) Real-Time Observations of Electrochemical Reactions in Rechargeable Energy Storage Systems (Invited)

R. Shahbazian-Yassar^{*1}; 1. University of Illinois at Chicago, USA

Electrodes in rechargeable batteries undergo complex electrochemically-driven phase transformations upon driving Li ions into their structure. Such phase transitions in turn affect the reversibility and stability of the battery. This presentation gives an overview of the PI's research program on in-situ transmission electron microscopy (TEM) of battery materials. In-situ TEM has been shown to be a very powerful technique in shedding light to some of the mysteries in electrochemical performance of new materials. Various anode materials including SnO₂, MnO₂, ZnSb were subjected to lithiation process and the transport of Li ions was visualized within their atomic structure. For SnO₂ nanowires, it was observed that the Li ion transport results in local strain development preferably along (200) or (020) plans and [001] crystallographic directions. The lithiation behavior in the presence of twin boundary defects was completely different compared to pristine state with no twin boundary defect. We investigated the microstructural changes and phase evolution of the Zn-Sb intermetallic nanowires using in-situ TEM. Zn-Sb alloys also exhibit a new cubic alloying phase Li₂ZnSb that form by intermixing of the ABAB atomic ordering in hexagonal LiZnSb due to Li inclusion in their lattices.

10:10 AM

(MCARE-S10-046-2016) Comparative Analysis of *Ex-situ* and *Operando* X-ray Diffraction Experiments for Lithium Insertion Materials (Invited)

S. Schmid^{*1}; 1. The University of Sydney, Australia

A comparative study of *ex-situ* and *operando* X-ray diffraction experiments using the fast lithium ion conductor Li_{0.18}Sr_{0.66}Ti_{0.5}Nb_{0.5}O₃ will be presented. *Ex-situ* analysis of synchrotron X-ray diffraction data suggests that a single phase material exists for all discharges to as low as 0.422 V. For samples with high lithium content, it is possible to determine the lithium position from the X-ray data. However, *operando* X-ray diffraction reveals a kinetically driven two phase region on cycling below 1 V. Monitoring the change in unit cell dimension during electrochemical cycling showed a reduction in the rate of unit cell expansion part way through the first discharge and during the second discharge, caused by a drop in lithium diffusion into the bulk material for higher lithium contents. A more significant change is a jump in the unit cell expansion once the lithium content exceeds one lithium ion per vacant site, caused by damping of octahedral rotations. This provides a link between lithium content and octahedral rotations. Using *operando* diffraction may enable to determine the strength of octahedral rotations in defect perovskites and indicate correlations with the large variance of ionic conductivities in these materials.

10:50 AM

(MCARE-S10-047-2016) Structure and Electronic Structure of Battery Materials at Atomic Scale (Invited)

L. Gu^{*1}; 1. Institute of Physics, Chinese Academy of Sciences, China

Performance optimization of lithium-ion batteries necessitates information about structural evolution of electrode materials at an atomic scale. The annular-bright-field (ABF) imaging in aberration-corrected scanning transmission electron microscopy (STEM) allows simultaneous imaging of light and heavy elements, providing an unprecedented opportunity to probe the nearly equilibrated local structure of electrode materials after electrochemical cycling at atomic resolution. In this report, we will present our recent efforts on revealing the atomic-scale structure of selected electrode materials with different charge and/or discharge state, e.g., the lattice distortion, phase interface structure, transition metal migration, surface reconstruction with (partial) intercalation and de-intercalation, to extend the current understanding of electrochemical reaction mechanism with the ABF and high-angle annular dark-field (HAADF) STEM imaging. Future prospect on the relationship between atomic-level structure evolution and microscopic reaction mechanisms of electrode materials for rechargeable batteries is envisaged.

11:30 AM

(MCARE-S10-048-2016) Evolution of Surface and Subsurface Phases on High-Voltage Aging of LiNi_{0.8}Co_{0.15}Al_{0.05}O₂ Cathode Materials-A STEM/EELS Study

P. Mukherjee^{*1}; S. Sallis²; L. Piper²; N. Pereira¹; G. G. Amatucci¹;

F. Cosandey¹; 1. Rutgers University, USA; 2. Binghamton University, USA

Ni-rich complex oxide LiNi_{0.8}Co_{0.15}Al_{0.05}O₂(NCA) with its large discharge capacity, has emerged as the most important battery cathode material with potential to be used in automobile and power grids. To achieve near full capacity of NCA high cell voltage needs to be applied. At high voltages capacity fade and impedance increase limit the usability of NCA. These detrimental phenomena are attributed to the formation of surface and subsurface phases over pristine NCA. These phases possess different crystal symmetry (Cubic), composition, and valence state of transition metal (TM) than the pristine NCA (Rhombohedral). Although, the existence of surface phases different from the pristine NCA has been determined in cycled materials, critical parameters, such as, the exact composition, valence states of TM, and the interfacial behavior of surface electrolyte are not known. In this talk, we will present a quantitative analysis of the aforementioned parameters using atomic-resolution scanning transmission electron microscopy (STEM) and electron energy loss spectroscopy (EELS). The results will be compared with the x-ray absorption spectroscopy (XAS). The funding for this work is provided by NECESS, an Energy Frontier Research Center funded by the U.S. Department of Energy, Office of Science, Office of Basic Energy Sciences under Award Number DE-SC0001294.

11:50 AM

(MCARE-S10-049-2016) *In Operando* neutron diffraction study of lithium-ion and metal hydride batteries

V. A. Yartys^{*1}; 1. Institute for Energy Technology, Norway

In situ neutron powder diffraction was employed to investigate phase-structural evolution in the advanced (La,Nd,Mg)Ni₃ anodes of the metal hydride battery and of the electrodes in a commercial LIB, as related to their electrochemical performance. The time resolution of the NPD data was 3-5 min. Location and redistribution of light elements, H/D and lithium, were studied *in operando* at a C(D)/12 rate. A contrast in neutron scattering between Ni/Co/Mn allowed monitoring a complex electrochemical performance of a three-phase mixture of oxides (LiCoO₂, NMC and LiMn₂O₄), acting as cathode material. The reaction pathway observed for the graphite anode included a continuous phase transformation

LiC₁₂→LiC₁₈ at the end of discharge. For the advanced MH battery anodes, Nd-substituted La_{2-x}Nd_xMgNi₉ intermetallics were in focus as offering a superior performance at high discharge currents. The mechanism of structural evolution in LaNdMgNi₉ was compared for using deuterium gas and for the electrochemical charge-discharge of the anode.

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