



# PROGRAM PREVIEW

January 11–14, 2015 Ritz-Carlton Doha • Doha, Qatar

**Register by December 1, 2014 and save!** 

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## **MEETING INFORMATION**



Register by December 1, 2014 and SAVE!

This materials congress will focus on new materials research and development in applications of interest for Qatar and the entire Middle East and Mediterranean region. The goal of this congress is to build synergy among researchers working on different materials applications but with similar objectives of enhancing design, sustainability, and functionality of materials. The congress will also be a forum for establishing collaboration among academia, research institutions, and industry in the Middle East and Mediterranean region and the rest of the world.

Attendees are expected from government, academia, and industry and the fields of energy, sustainability, and computational materials.

### **CONGRESS ORGANIZERS**

### Lead Organizer:

• Ibrahim Karaman, Texas A&M University

### **Co-Organizers:**

- Raymundo Arroyave, Texas A&M University
- Eyad Masad, Texas A&M University at Qatar

### Additional Organizers:

- Zoubeida Ounaies, Pennsylvania State University
- Dimitris Lagoudas, Texas A&M University
- Mohammed Khaleel, Qatar Foundation
- Mariam Al-Maadeed, Qatar University
- Pradeep Sharma, University of Houston

### Local Organization Committee and Industry Liaisons:

- Eyad Masad, Texas A&M University at Qatar
- Mariam Al-Maadeed, Qatar University

- Bilal Mansoor, Texas A&M University at Qatar
- Georges Ayoub, Texas A&M University at Qatar
- Aboubakr M. Abdullah, Qatar University
- Srinath Iyengar, Texas A&M University at Qatar
- Said Mansour, Qatar Energy and Environment Research Institute, Qatar Foundation
- Abdulaziz Al Mathami, Qatar Petroleum
- Chris Devadas, Hydro Aluminum Technology Centre – Qatar
- Mabroouk Ouderni, Qatar Petrochemical Company – QAPCO
- Wakeel Ahmed Khalid Ahmed, Qatar Steel

### International Advisory Committee:

- Thomas Zacharia, Qatar Foundation, Committee Chair
- Yehia Bahei-El-Din, The British University in Egypt
- Tahir Cagin, Texas A&M University
- Hussein Zbib, Washington State University
- Imad Al-Qadi, University of Illinois at Urbana-Champaign
- Tom Scarpas, Delft University of Technology
- Zachary Grasley, Texas A&M University
- Dallas Little, Texas A&M University
- Nick Kanellopoulos, National Center for Scientific Research "Demokritos"
- Marwan Khraisheh, Qatar Energy and Environment Institute, Qatar Foundation
- **Peter Hewlett**, British Board of Agrement and University of Dundee
- Tayssir Hamieh, Lebanese University
- A.G. Mamalis, PC-NAE
- M. Enokizono, Oita University
- Tasneem Pervez, Sultan Qaboos University

### TMS would like to thank our GOLD SPONSORS

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معهد قطر لبحوث البيئة والطاقة Qatar Environment & Energy Research Institute

Member of Qatar Joundation Jeó Paualja, jógiða

*The TMS Middle East - Mediterranean Materials Congress on Energy and Infrastructure Systems* 2015

### REGISTRATION

All congress attendees, including authors, presenters, and session chairs, are required to register. To receive the discount registration rate, register at www.tms.org/MEMA2015 by December 1, 2014.

| <b>Registration Fees</b> | Discount* | Standard |
|--------------------------|-----------|----------|
| Member                   | \$475     | \$575    |
| Nonmember+               | \$575     | \$675    |
| Student**                | \$295     | \$295    |

+Includes TMS membership for 2015

\* Discount pricing through December 1, 2014

\*\*Copy of student school identification card must accompany registration form *Prices are shown in U.S. Dollars* 

### **Registration package includes:**

- One copy of the congress proceedings
- Technical sessions
- · Refreshment breaks and lunch each day
- Welcome reception on Sunday
- Poster reception on Tuesday
- Dinner event on Monday
- Banquet on Tuesday

### LOCATION, HOUSING & TRAVEL

#### **Congress Location – Ritz-Carlton Doha**

Discover the Ritz-Carlton Doha hotel and experience the breathtaking beauty of the Gulf. From the city's traditions and culture to its modern amenities and exciting attractions, this stunning luxury hotel in Qatar provides guests with convenient access to everything this unforgettable destination has to offer. For more information, visit www.ritzcarlton.com/Doha.

#### Housing

A block of rooms has been reserved at the Ritz-Carlton Doha at a special rate. Accommodations must be secured by December 10, 2014. Single occupancy is QR 950 (approximately \$260) per night and double occupancy is QR 1050 (approximately \$290) per night. The hotel rate includes breakfast and complimentary internet access in the sleeping rooms. To make your reservations visit www.tms.org/MEMA2015.

#### **Getting There**

The Ritz-Carlton Doha is located about 12 miles from the Hamad International Airport. Taxis are available at the airport.

### **NETWORKING/SOCIAL EVENTS**

Sunday, January 11 Welcome Reception 6:00 p.m. to 7:30 p.m.

Monday, January 12 A Fun Evening Out in Doha Sponsored by Texas A&M University of Qatar 7:00 p.m. to 9:00 p.m.

Buses will depart at 6:30 p.m.

Tuesday, January 13 Poster Session

3:20 p.m. to 4:30 p.m.

Banquet at Ritz-Carlton 6:00 p.m. to 8:00 p.m.

### **TECHNICAL PROGRAM**

The goal of the technical program is to leverage regional interests and expertise, particularly along three tracks:

#### **Track 1: Sustainable Infrastructure Materials**

This track will encompass materials issues and solutions pertaining to critical infrastructure and will have an overarching theme of sustainability.

### Track 2: Materials for Energy Extraction, Conversion, and Storage

In this track there will be an emphasis on materials issues for not just alternative energy sources such as energy harvesting, solar and wind power but also oil and gas, and thermal which are topics of key interest to the Mideast-Mediterranean/North Africa geographic area.

### **Track 3: Computational Materials Design**

This track will focus on computational materials design, especially as applied to energy and infrastructure systems.

The sessions will be conducted in English.

### **SPONSORSHIP OPPORTUNITIES**

Corporate sponsorship offers high visibility at the congress reception, refreshment breaks, and attendee social activities, as well as on registration amenities like reusable canvas bags, badges, and lanyards.

For more information on purchasing a corporate sponsorship, visit the Sponsorship page of the MEMA 2015 website: www.tms.org/MEMA2015.

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### MONDAY, JANUARY 12, 2014

### Plenary

| Room: Al Wosail |  |  |  |
|-----------------|--|--|--|
| 8:00 AM         | 8:00 AM Introductory Comments  |  |  |
| 8:20 AM         | Keynote<br>Modeling at Multiple Scales to Support Materials Design: David McDowell <sup>1</sup> ; 1Georgia Institute of Technology |  |  |
| 9:05 AM         | Break  |  |  |

### 1-1: Cemenetitious Materials, Composites

Room: Al Wosail 1

| 9:20 AM  | Invited<br>Computational Materials Science to Enable Sustainable Concrete Material Design: Zachary Grasley <sup>1</sup> ; Xiaodan<br>(Sonia) Li <sup>1</sup> ; <sup>1</sup> Virginia Tech  |
|----------|--|
| 10:00 AM | Vertical Scanning Interferometry: A New Method to Quantify Solute-solvent Reaction Dynamics in Cementitious Environments: Gaurav Sant <sup>1</sup> ; <sup>1</sup> University of California, Los Angeles  |
| 10:20 AM | Effect of Interface and Interphase Regions on the Elasticity of Nanocomposite Cement: <i>Ala Abu Taqa</i> <sup>1</sup> ; Ahmed Senouci <sup>1</sup> ; Rashid Abu Al-Rub <sup>2</sup> ; <sup>1</sup> Qatar University; <sup>2</sup> Masdar Institute of Science and Technology                          |
| 10:40 AM | Finite Element Simulation of the Response of No-Tension Materials: <i>Alieh Alipour</i> <sup>1</sup> ; Tom Scarpas <sup>1</sup> ; <sup>1</sup> Delft University of Technology  |
| 11:00 AM | Investigation and Modeling of the Damage Evolution in Natural Fiber Composites: Habiba Bougherara <sup>1</sup> ; Zia Mahboob <sup>1</sup> ; Fodil Meraghni <sup>2</sup> ; Laurent Peltier <sup>3</sup> ; <sup>1</sup> Ryerson University; <sup>2</sup> ENSAM - Arts et Métiers ParisTech; <sup>3</sup> |
| 11:20 AM | Lunch  |

### 2-1: Ferrocaloric Materials

Room: Al Wosail 2

| 9:20 AM  | Invited<br>The Direct Conversion of Heat to Electricity Using Multiferroic Materials: Richard James <sup>1</sup> ; <sup>1</sup> University of<br>Minnesota  |
|----------|---|
| 10:00 AM | Invited<br>Origin of Hysteresis in Multicaloric Materials: Sebastian Fähler <sup>1</sup> ; <sup>1</sup> IFW Dresden   |
| 10:40 AM | <b>Measurements of the Electrocaloric Effect in Some Relaxor Ferroelectrics</b> : <i>Mehmet Sanlialp</i> <sup>1</sup> ; Vladimir V. Shvartsman <sup>1</sup> ; Doru C. Lupascu <sup>1</sup> ; <sup>1</sup> University Duisburg-Essen   |
| 11:00 AM | <b>The Tunable Microstructure and its Influence on the Giant Magnetocaloric effect in Magnetic Shape Memory</b><br><b>Alloys:</b> <i>Nickolaus Bruno</i> <sup>1</sup> ; Yujin Huang <sup>2</sup> ; Ibrahim Karaman <sup>1</sup> ; Joseph Ross <sup>1</sup> ; Jianguo Li <sup>2</sup> ; <sup>1</sup> Texas A&M University; <sup>2</sup> Shanghai JiaoTong University   |
| 11:20 AM | Studies of Magnetic Properties of Ni-Mn-In-Co Heusler-type Glass-coated Microwires: Valentina Zhukova <sup>1</sup> ; Mihail Ipatov <sup>1</sup> ; Alexandr Aronin <sup>2</sup> ; Galina Abrosimova <sup>2</sup> ; Alexandr Kiselev <sup>2</sup> ; <i>Arcady Zhukov</i> <sup>3</sup> ; <sup>1</sup> Basque Country University; <sup>2</sup> Insitute of Solid State Physics; <sup>3</sup> Basque Country University and Ikerbasque |
| 11:40 AM | Lunch   |

### 3-1: Ab-Initio Approaches

Room: Al Wosail 3

| 9:20 AM | Invited<br>Ab Initio Thermodynamics: A Novel Route to Design Structural Materials with Superior Mechanical Properties:<br><i>Jörg Neugebauer</i> <sup>1</sup> ; Blazej Grabowski <sup>1</sup> ; Fritz Kormann <sup>1</sup> ; Tilmann Hickel <sup>1</sup> ; <sup>1</sup> Max-Planck-Institut für Eisenforschung<br>GmbH |
|---------|--|
|         |  |

10:00 AM A DFT Based Molecular Dynamics Study of Pbl<sub>3</sub>(CH<sub>3</sub>NH<sub>3</sub>): *Marcelo Carignano*<sup>1</sup>; <sup>1</sup>QEERI - Qatar Foundation

| 10:20 AM | Thermal Expansion Coefficient of Two Dimensional Materials: Cem Sevik <sup>1</sup> ; 1Anadolu University   |
|----------|--|
| 10:40 AM | Strong Stacking Between Organic and Organometallic Molecules as the Key for Material Design: <i>Snezana Zaric</i> <sup>1</sup> ; Dusan Malenov <sup>2</sup> ; Dragan Ninkovic <sup>2</sup> ; <sup>1</sup> Texas A&M University at Qatar; <sup>2</sup> Innovation Centre of the Department of Chemistry   |
| 11:00 AM | <b>Calculation of Electronic Structure and Field Induced Magnetic Collapse in Ferroic Materials</b> : Raymundo Arroyave <sup>1</sup> ; <i>P. Entel</i> <sup>2</sup> ; N. Singh <sup>3</sup> ; M. Gruner <sup>2</sup> ; A. Grünebohm <sup>2</sup> ; V. V. Sokolovskiy <sup>4</sup> ; V. D. Buchelnikov <sup>4</sup> ; <sup>1</sup> Texas A & M University; <sup>2</sup> University, Duisburg-Essen; <sup>3</sup> University of Houston; <sup>4</sup> Chelyabinsk State University |
| 11:20 AM | Lunch  |

#### 1-2: Cementitious Materials Sustainability

#### Room: Al Wosail 1

| 1:30 PM | Introductory Comments  |
|---------|--|
| 1:40 PM | Invited<br>Utilising Fine and Coarse Recycled Aggregates from Qatar in Concrete: Roderick Jones <sup>1</sup> ; Judith Halliday <sup>1</sup> ; Laszlo<br>Csetenyi <sup>1</sup> ; Li Zheng <sup>1</sup> ; Nikolaos Strompinis <sup>1</sup> ; <sup>1</sup> University of Dundee   |
| 2:20 PM | Multiwalled Carbon Nanotubes Aspect Ratio, Functionalization, Weight Fraction & Surfactant Effect on the Mechanical Properties of Cementitious Materials: <i>Mohamed Mohsen</i> <sup>1</sup> ; Rashid Abu El Rub <sup>2</sup> ; Ahmed Senouci <sup>1</sup> ; Nasser Alnuaimi <sup>1</sup> ; Khaldoon Bani Hani <sup>3</sup> ; <sup>1</sup> Qatar University; <sup>2</sup> Masdar Institute of Science and Technology; <sup>3</sup> Jordan University of Science and Technology |
| 2:40 PM | <b>Defined Polymers as Candidates for Pavement Subgrade Soil Stabilization</b> : <i>Chandramohan Ayyavu</i> <sup>1</sup> ; Srinath R. Iyengar <sup>1</sup> ; Howard J. H. M. Hanley <sup>1</sup> ; Hassan S. Bazzi <sup>1</sup> ; Dallas Little <sup>1</sup> ; <sup>1</sup> Texas A&M University at Qatar  |
| 3:00 PM | Break  |

### 2-8: Lightweight and High Performance Materials I

Room: Al Wosail 1

| 3:20 PM | Nanomaterials for "Smart" Membrane Pretreatment and RO Desalination Technologies: <i>Khaled Mahmoud</i> <sup>1</sup> ; <sup>1</sup> QEERI-Q   |
|---------|---|
| 3:40 PM | <b>3D Nanotubular Surfaces for Energy Storage and Conversion</b> : <i>Tolou Shokuhfar</i> <sup>1</sup> ; <sup>1</sup> Michigan Technological University   |
| 4:00 PM | Mechanical Properties of AI-Zr-Sc Alloys with Si and Er Micro-additions: Nhon Vo <sup>1</sup> ; Nick Barta <sup>2</sup> ; Georges Ayoub <sup>3</sup> ; Ibrahim Karaman <sup>2</sup> ; <i>David Dunand</i> <sup>1</sup> ; <sup>1</sup> Northwestern University; <sup>2</sup> Texas A&M University; <sup>3</sup> Texas A&M University at Qatar  |
| 4:20 PM | Development of High Strength and Ductile Al-xMg Alloys for Sustainable Applications: Min Zha <sup>1</sup> ; Hans Roven <sup>2</sup> ; Chris Devadas <sup>3</sup> ; <sup>1</sup> Norwegian University of Science and Technology; <sup>2</sup> Qatar University; <sup>3</sup> Hydro Aluminium QSTP Qatar  |
| 4:40 PM | Microstructural and Mechanical Characterization of Friction-Stirred Welded (FSW) TRC AZ31B Magnesium Alloy Sheets: <i>Abdelhakim Dorbane</i> <sup>1</sup> ; Georges Ayoub <sup>1</sup> ; Bilal Mansoor <sup>1</sup> ; Ramsey Hamade <sup>2</sup> ; Ghassan Kridli <sup>3</sup> ; Abdellatif Imad <sup>4</sup> ; <sup>1</sup> Texas A&M University at Qatar; <sup>2</sup> American University of Beirut; <sup>3</sup> University of Michigan-Dearborn; <sup>4</sup> Ecole Polytech'Lille |

#### 2-2: Energy Storage Materials

### Room: Al Wosail 2 1:30 PM Introductory Comments 1:40 PM Invited Nanomaterial Design Strategies for Capacitive Energy Storage Applications: Husam Alshareef<sup>1</sup>; <sup>1</sup>King Abdullah University for Science & Technology (KAUST) 2:20 PM Rechargeable Batteries: Lessons from Real Time Observation of Lithiation/Delithiation in Nanoscale Anode Materials: Reza Shahbazian-Yassar<sup>1</sup>; <sup>1</sup>Michigan Technological University

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| 2:40 PM | Electrode Materials Based on Phosphates for Lithium Ion Batteries as Efficient Energy Storage System: <i>Saadoune Ismael</i> '; Lasri Karima'; Bezza Ilham'; Ehrenberg Helmut'; Indris Sylvio'; Daniel Brandell <sup>2</sup> ; <sup>1</sup> University Cadi Ayyad Marrakech; <sup>2</sup> Uppsala University |
|---------|--|
| 3:00 PM | Break  |

### **3:20 PM** Interfacial Stresses and Degradation of Oxide Scale and Substrate Interface at High Temperatures: *Mohammed Khaleel*<sup>1</sup>; E. Stephens<sup>2</sup>; J. Stevenson<sup>2</sup>; <sup>1</sup>Qatar Foundation; <sup>2</sup>Pacific Northwest National Laboratory

**3:40 PM** Predicting Acoustic Emission and Electrochemical Impedance Spectra for Damage Stochastics in Energy Materials: Pallab Barai<sup>1</sup>; Chien-Fan Chen<sup>1</sup>; *Partha Mukherjee*<sup>1</sup>; <sup>1</sup>Texas A&M University

**4:00 PM** Novel Organic Electrodes for Organic Rechargeable Batteries: *Burak Esat*<sup>1</sup>; Sumeyye Bahceci<sup>1</sup>; Sevda Akay<sup>1</sup>; Aliyu Bawa Abdullahi<sup>1</sup>; <sup>1</sup>Fatih University

**4:20 PM** Na<sub>2</sub>Fe<sub>0.5</sub> Mn<sub>0.5</sub>P<sub>2</sub>O<sub>7</sub> as Promising Cathode Material for Rechargeable Sodium Ion Batteries (NIBs): *R. Shakoor*<sup>1</sup>; Ramazan Kahraman<sup>1</sup>; Chanseon Park<sup>2</sup>; Soo Lim<sup>2</sup>; Jang Choi<sup>2</sup>; <sup>1</sup>Qatar University; <sup>2</sup>Korea Advanced Institute of Science and Technology (KAIST)

**4:40 PM** Nanomaterial-based Ultracapacitor for Power Integrated Circuits: Daniel Choi<sup>1</sup>; Waqas Gill<sup>1</sup>; Maarten Geest<sup>1</sup>; <sup>1</sup>Masdar Institute of Science and Technology

### **3-2: Energy Materials Simulation**

Room: Al Wosail 3

| 1:30 PM | Introductory Comments  |
|---------|--|
| 1:40 PM | Invited<br>Application of Phase-field Method to Modeling Microstructure Evolution in Li-ion Batteries: Long Qing Chen <sup>1</sup> ;<br><sup>1</sup> Penn State University   |
| 2:20 PM | Modeling of Thermal Behavior and Efficiency of Photovoltaic Panels: Said Ahzi <sup>1</sup> ; <sup>1</sup> University of Strasbourg/Qatar Foundation  |
| 2:40 PM | A Biomimetic-computational Approach to Optimizing the Quantum Efficiency of Photovoltaics: Andreas Holzenburg <sup>1</sup> ; Lisa Perez <sup>1</sup> ; <sup>1</sup> Texas A&M University   |
| 3:00 PM | Break  |
| 3:20 PM | Using Nonlinear Electret Effects to Design Piezolectricity and Magnetoelectricity in Soft Materials: Pradeep Sharma <sup>1</sup> ; <sup>1</sup> University of Houston  |
| 3:40 PM | Stability, Mechanical, Dielectric and Piezoelectric Properties of {AxA'(1-x)}{ByB'(1-y)}O <sub>3</sub> Ceramics: <i>Berna Akgenc</i> <sup>1</sup> ; Çetin Tasseven <sup>2</sup> ; Tahir Cagin <sup>3</sup> ; <sup>1</sup> Kirklareli University; <sup>2</sup> Yildiz Technical University; <sup>3</sup> Texas A&M University   |
| 4:00 PM | Martensitic Transformation of Ni <sub>2</sub> FeGa Magnetic Shape Memory Alloy Studied by Density Functional Theory:<br>Sevgi Özdemir Kart <sup>1</sup> ; Cengiz Soykan <sup>1</sup> ; Cem Sevik <sup>2</sup> ; Tahir Çagin <sup>3</sup> ; <sup>1</sup> Pamukkale University; <sup>2</sup> Anadolu University; <sup>3</sup> Texas A&M University   |
| 4:20 PM | <b>Revealing the Role of Organic Ligands in Hybrid Halid Perovskites for Phovoltaics Applications</b> : Carlo Motta <sup>1</sup> ;<br><i>Fadwa El-Mellouhi</i> <sup>2</sup> ; Fahhad Alharbi <sup>2</sup> ; Nouar Tabet <sup>2</sup> ; Kais Sabre <sup>2</sup> ; Stefano Sanvito <sup>1</sup> ; <sup>1</sup> Trinity College Dublin and CRANN;<br><sup>2</sup> QEERI   |
| 4:40 PM | <b>Tailoring Thermal Conductivity of Ge/Si Core-Shell Nanowires</b> : <i>Sevil Sarikurt</i> <sup>1</sup> ; Cem Sevik <sup>2</sup> ; Alper Kinaci <sup>3</sup> ; Justin Haskins <sup>4</sup> ; Tahir Cagin <sup>5</sup> ; <sup>1</sup> Dokuz Eylul University; <sup>2</sup> Anadolu University; <sup>3</sup> Argonne National Laboratory; <sup>4</sup> NASA Ames Research Center; <sup>5</sup> Texas A&M University |

### TUESDAY, JANUARY 13, 2014

### Plenary

| 8:00 AM | Introductory Comments  |
|---------|--|
| 8:10 AM | Keynote<br>Materials Research for the Energy Industry Collaboration Opportunities between Energy Industry and<br>Academia: <i>Rustom Mody</i> <sup>1</sup> ; <sup>1</sup> Baker Hughes |
| 8:55 AM | Break  |
|         |  |

### 1-3: Multi-scale Characterization and Simulations of Infrastructure Materials

#### Room: Al Wosail 1

| 9:10 AM  | Invited<br>Quantifying Material, Environmental, and System Variables Influencing the Structural Performance of<br>Reinforced Concrete Structures Affected by Alkali Silica Reactions: David Trejo <sup>1</sup> ; Joseph Bracci <sup>2</sup> ; Paolo Gardoni <sup>3</sup> ;<br><sup>1</sup> Oregon State University; <sup>2</sup> Texas A&M University; <sup>3</sup> University of Illinois at Urbana-Champaign |
|--|--|
| 9:50 AM  | Invited<br>Monitoring Concrete Infrastructure Condition Using Acoustic Sensing and Imaging: John Popovics <sup>1</sup> ; <sup>1</sup> University<br>of Illinois  |
| 10:30 AM   | Multiscale Design of Palm Natural Fiber Based Composite: Yehia Bahei-El-Din <sup>1</sup> ; Taher Wahba <sup>1</sup> ; Tarek Hatem <sup>1</sup> ;<br><sup>1</sup> British University in Egypt   |
| 10:50 AM   | Mechanical Properties of Concrete Containing Qatar's Municipal Wastes: <i>Nesibe Gozde Ozerkan</i> <sup>1</sup> ; Deniz Tokgoz <sup>1</sup> ; Joseph Antony <sup>2</sup> ; <sup>1</sup> Qatar University; <sup>2</sup> University of Leeds   |
| 11:10 AM   | Stochastic Framework for the Modeling and Propagation of Linear Viscoelastic Material Properties of Asphalt Mixtures in Pavement Structures: Loujaine Mehrez'; Eyad Masad <sup>1</sup> ; <sup>1</sup> Texax A&M University at Qatar  |
| 11:30 AM   | Lunch  |
| 2-3: Nano-Engineered Materials for Energy Conversion |  |
| Room: Al Wosail 2                                    |  |
| 9:10 AM  | Invited<br>Challenges and Opportunities for Nano Engineered Materials: Pulickel Ajayan <sup>1</sup> ; 1Rice University   |
| 9:50 AM  | Towards Engineering Efficient Thermoelectrics: Large-scale Synthesis of Nanowires and their Assembly into Stable Welded Nanowire Networks: <i>Sreeram Vaddiraju</i> <sup>1</sup> ; <sup>1</sup> Texas A&M University   |
| 10:10 AM   | <b>Design of New Electroactive Materials Based on Nanoparticle-modified Polymers</b> : <i>Zoubeida Ounaies</i> <sup>1</sup> ; Nirmal Shankar Sigamani <sup>1</sup> ; <sup>1</sup> The Pennsylvania State University  |
|  |  |

- **10:30 AM** Active Nanocomposite Materials for Photo-mechanical Actuation: *Igor Krupa*<sup>1</sup>; Klaudia Czanikova<sup>2</sup>; Maria Omastova<sup>2</sup>; <sup>1</sup>Qatar University; <sup>2</sup>Polymer Institute SAV
- **10:50 AM** Inherent Nonlinear Non-conservative Behavior of Resonant Piezoelectric Energy Harvesters: A Dynamical Systems Approach: Stephen Leadenham<sup>1</sup>; *Alper Erturk*<sup>1</sup>; <sup>1</sup>Georgia Institute of Technology
- **11:10 AM** A Multiscale-Based Model for Composite Materials with Embedded PZT Filaments for Energy Harvesting: Yehia Bahei-El-Din<sup>1</sup>; Ahmed El-Etriby<sup>1</sup>; Mohamed Abdel-Meguid<sup>1</sup>; Khalid Shalan<sup>1</sup>; Tarek Hatem<sup>1</sup>; <sup>1</sup>British University in Egypt
- 11:30 AM Lunch

### 3-3: Modeling Materials Across the Scales

| 9:10 AM  | Invited<br>Computational Modeling of Deformation Mechanisms in Mg and Mg Alloys: <i>W Curtin</i> <sup>1</sup> ; M. Ghazisaedi <sup>2</sup> ; A. Luque <sup>3</sup> ;<br>Z. Wu <sup>3</sup> ; <sup>1</sup> EPFL; <sup>2</sup> Ohio State University; <sup>3</sup> Ecole Polytechnique Federale de Lausanne                       |
|----------|---|
| 9:50 AM  | Multiscale Modeling and Design of Advanced Interface Materials for High Energy Environments: <i>Hussien Zbib</i> <sup>1</sup> ; <sup>1</sup> Washignton State University  |
| 10:10 AM | <b>Periodic Homogenization of SMA Composites under Isothermal Conditions</b> : <i>George Chatzigeorgiou</i> <sup>1</sup> ; Yves Chemisky <sup>1</sup> ; Fodil Meraghni <sup>1</sup> ; <sup>1</sup> Arts et Metiers ParisTech  |
| 10:30 AM | Modeling the Deformation Mechanisms in Magnesium Single Crystals: Multiscale Dislocation Dynamics Analyses: Wassim Jaber <sup>1</sup> ; Mutasem Shehadeh <sup>1</sup> ; <sup>1</sup> American University of Beirut  |
| 10:50 AM | Analysis of Solid State Bonding in the Extrusion Process of Magnesium Alloys -Numerical Prediction and Experimental Verification: <i>Nabeel Alharthi</i> <sup>1</sup> ; Wojciech Misiolek <sup>2</sup> ; Anthony Ventura <sup>2</sup> ; <sup>1</sup> Lehigh University and King Saud University; <sup>2</sup> Lehigh University |

**11:10 AM** Multiscale Modeling of Discontinuous Precipitation in U-Nb: *Thien Duong*<sup>1</sup>; Alexander Landa<sup>2</sup>; Robert Hackenberg<sup>3</sup>; Patrice Turchi<sup>2</sup>; Raymundo Arroyave<sup>1</sup>; <sup>1</sup>Texas A&M University; <sup>2</sup>Lawrence Livermore National Laboratory; <sup>3</sup>Los Alamos National Laboratory

### 11:30 AM Lunch

### 1-4: Environmental Degradation

Room: Al Wosail 1

| 1:30 PM | Introductory Comments  |
|---------|--|
| 1:40 PM | Invited<br>Corrosion Challenges for the Oil and Gas Industry in the State of Qatar: <i>Roy Johnsen</i> <sup>1</sup> ; <sup>1</sup> Norwegian University<br>of Science and Technology   |
| 2:20 PM | Effect of Electroless Co-P and Co-Ni-P Coatings on Cavitation Erosion-corrosion Resistance: <i>Shemy Mohamed Ahmed Gaber Gaber</i> <sup>1</sup> ; Mohammed Aboraia <sup>2</sup> ; Mohammed Doheim <sup>2</sup> ; Salem Karrab. A <sup>3</sup> ; <sup>1</sup> Majmaah University; <sup>2</sup> Assiut University.; <sup>3</sup> Misurata University |
| 2:40 PM | Prevention of Chloride Stress Corrosion Cracking (CSCC) using Thermally Sprayed Coating (TSC): Rehan Ahmed <sup>1</sup> ; <sup>1</sup> Petronas Carigali   |
| 3:00 PM | New Self-Healing Coatings Technique for Corrosion Protection: <i>Eman Fayyad</i> <sup>1</sup> ; Mariam Al-Maadeed <sup>1</sup> ; <sup>1</sup> Qatar University   |

### 2-4: Ferroelectric Materials in Energy Conversion

Room: Al Wosail 2

| 1:30 PM | Introductory Comments   |
|---------|---|
| 1:40 PM | Invited<br>Insights into the Nature and Dynamics of Point Defects in Ferroelectric Materials: <i>Clive Randall</i> <sup>1</sup> ; <sup>1</sup> Penn State<br>University   |
| 2:20 PM | Flexoelectricity and Nanoscale Energy Harvesting: Pradeep Sharma1; 1University of Houston   |
| 2:40 PM | Investigation of Electrical and Piezoelectricity of New Nanocomposites Based on Nanofibrillated Cellulose<br>and Copolymers Containing Fluorinated and Nitrile Derivatives with Controlled Structure: Kaddami Hamid <sup>1</sup> ;<br>Kadimi Amal <sup>1</sup> ; Ounaies Zoubeida <sup>1</sup> ; Raihane Mustapha <sup>1</sup> ; <sup>1</sup> Cadi Ayyad University |
| 3:00 PM | Novel Polymeric Materials for Mechanical Energy Harvesting: <i>Miroslav Mrlík</i> <sup>1</sup> ; Mariam Al Maadeed <sup>1</sup> ; <sup>1</sup> Qatar University   |

### 3-4: Alloy and Microstructure Design

| 1:30 PM | Introductory Comments  |
|---------|--|
| 1:40 PM | Invited<br>Discovery of Sustainable Magnesium Alloys: Pedro Rivera-Diaz-del-Castillo <sup>1</sup> ; <sup>1</sup> University of Cambrdige   |
| 2:20 PM | Alloy Design Strategies through Computational Thermodynamics and Kinetics Approaches: <i>Raymundo Arroyave</i> <sup>1</sup> ; Shengyen Li <sup>2</sup> ; Ruixian Zhu <sup>2</sup> ; Ibrahim Karaman; <sup>1</sup> Texas A&M University |
| 2:40 PM | Microstructure Design and Homogenization using Correlation Functions: Hamid Garmestani <sup>1</sup> ; <sup>1</sup> Georgia Institute of Technology   |
| 3:00 PM | Development of Tailored Residual Stress States Through Microstructurally Informed Modeling: Dimitris Lagoudas <sup>1</sup> ; Brian Lester <sup>1</sup> ; <sup>1</sup> Texas A&M University   |

### **Poster Session**

Room: Foyer • 3:20 PM – 4:30 PM

A Durability Analysis of Super-Quiet Pavement Structures: Santosh Srirangam<sup>1</sup>; Kumar Anupam<sup>1</sup>; Tom Scarpas<sup>1</sup>; Cor Kasbergen<sup>1</sup>; Peter The<sup>2</sup>; <sup>1</sup>Delft University of Technology; <sup>2</sup>Directie Techniek en Technisch Management/Afdeling Wegen en Geotechniek, Rijkswaterstaat ,Dienstonderdeel Grote Projecten en Onderhoud (GPO)

A New Test for Asphalt Binder Ductility and Intermediate Temperature: *Alaedddin Mohseni*<sup>1</sup>; Haleh Azari<sup>2</sup>; <sup>1</sup>Pavement Systems; <sup>2</sup>AASHTO

**A New Test Method for Asphalt Mixture Fatigue Characterization**: *Alaedddin Mohseni*<sup>1</sup>; Haleh Azari<sup>2</sup>; <sup>1</sup>Pavement Systems; <sup>2</sup>AASHTO

Active Composite Materials Undergoing Damage: A Homogenization Approach: George Chatzigeorgiou<sup>1</sup>; *Fodil Meraghni*<sup>1</sup>; Yves Chemisky<sup>1</sup>; Hassene Ben Atitallah<sup>2</sup>; Zoubeida Ounaies<sup>2</sup>; <sup>1</sup>Arts et Metiers ParisTech; <sup>2</sup>Pennsylvania State University

Alignment of Nanofibrillated Cellulose (NFC) in Silicone Oil by an Electrical Field: Impact on Effective Electrical Properties: *Kaddami Hamid*'; Kadimi Amal<sup>1</sup>; Raihane Mustapha<sup>1</sup>; Ounaies Zoubeida<sup>2</sup>; <sup>1</sup>Cadi Ayyad University; <sup>2</sup>The Pennsylvania State University

Boron Removal from Seawater Using B-Cyclodextrin Modified Magnetic Nanoparticles Fixed on Cellulose Nanocrystals: *Deema Almasri*<sup>1</sup>; Tarik Rhadfi<sup>1</sup>; Khaled Mahmoud<sup>1</sup>; <sup>1</sup>QEERI

Computational Assessment of the Performance of Lead Halide Perovskite Solar Cells using Inorganic Layers as Hole Transport Materials: *Mohammad Hossain*<sup>1</sup>; Fahhad Alharbi<sup>1</sup>; Nouar Tabet<sup>1</sup>; <sup>1</sup>QEERI

Control of Grain Refinement of A356 Aluminum Alloy by Computer Aided Cooling Curve Analysis: Ahmad Sharifi'; Najmeddin Arab<sup>1</sup>; <sup>1</sup>Islamic Azad University

**Controlled Growth of (1-D) ZnO Nanorod Supported Platinum Nanoparticle as Catalyst Materials**: *Sarim Dastgir*<sup>1</sup>; Reem Al-Alawi<sup>2</sup>; Joydeep Dutta<sup>2</sup>; <sup>1</sup>Qatar Environment and Energy Research Institute; <sup>2</sup>Sultan Qaboos University

Coupled Turbulent Flow and Solidification Modeling in a Brass Slab Continuous Caster: Mandana Adeli<sup>1</sup>; M. Reza Aboutalebi<sup>1</sup>; <sup>1</sup>Iran University of Science & Technology

**Crystal Plasticity Simulations Using Discrete Fourier Transforms**: *Hamad Alharbi*<sup>1</sup>; Suray Kalidindi<sup>2</sup>; <sup>1</sup>King Saud University; <sup>2</sup>Georgia Institute of Technology

Damage Mechanisms of AZ31B Twin Roll Cast (TRC) at Different Strain Rates and Temperatures: Ana Rodriguez<sup>1</sup>; Georges Ayoub<sup>2</sup>; Amine Benzerga<sup>1</sup>; <sup>1</sup>Texas A&M University; <sup>2</sup>Texas A&M University at Qatar

Density Functional Theory Based Theoretical Calculations for Investigation of Highly Active Visible Light Driven TiO Based Photocatalyst Photoelectrochemical Applications: *Matiullah Khan*<sup>1</sup>; Wenbin Cao<sup>2</sup>; Bilal Mansoor<sup>1</sup>; <sup>1</sup>Texas A&M University at Qatar; <sup>2</sup>University of Science and Technology Beijing

Design of Advanced Materials with Tailor-Made Properties Using Molecular Simulation: Ionic Liquids for the Chemical Process Industries: *Ioannis Economou*<sup>1</sup>; Eleni Androulaki<sup>2</sup>; Niki Vergadou<sup>2</sup>; <sup>1</sup>Texas A&M University at Qatar; <sup>2</sup>National Center for Scientific Research "Demokritos"

Development of a Redox Model for SOFC Anodes: Bora Timurkutluk<sup>1</sup>; Mahmut Mat<sup>2</sup>; <sup>1</sup>Nigde University; <sup>2</sup>Meliksah University

**Different Approaches to Fabricate Doped-Graphene Composite Films and their Application as a Photovoltaic Transparent Electrode:** *Adnan Ali*'; Khaled Mahmoud'; Marwan Khraisheh<sup>1</sup>; <sup>1</sup>Qatar Environment and Energy Research Institute

Direct Observation of Effects of Foam Density, Gating Design and Pouring Temperature on Mold Filling Process in Lost Foam Casting of A356 Alloy: *Ahmad Sharifi*'; Mehdi Mansouri Hasan Abadi'; Roholla Ashiri'; <sup>1</sup>Islamic Azad University

Discrete Element Simulation of Asphalt Mixtures Fracture: Enad Mahmoud<sup>1</sup>; Shadi Saadeh<sup>2</sup>; <sup>1</sup>UTPA; <sup>2</sup>CSLB

Effect of RE Elements on the Sorption Properties of Nanocrystalline Zr-Co Getters Prepared by Mechanical Alloying: *Ali Heidary Moghadam*<sup>1</sup>; Valiollah Dashtizad<sup>2</sup>; Ali Kaflou<sup>2</sup>; Hossein Yoozbashizadeh<sup>3</sup>; <sup>1</sup>Department of Materials Science and Engineering, Dezful Branch, Islamic Azad University, Dezful, Iran; <sup>2</sup>Department of Advanced Materials and Renewable Energy, Iranian Research Organization for Science and Technology, Tehran, Iran; <sup>3</sup>Department of Materials Science and Engineering, Sharif University of Technology, Tehran, Iran

Efficient Route for Functionalization of Graphene Nanosheets with Catechol for Preparation of Performance Supercapacitor Electrodes: *Efat Jokar*<sup>1</sup>; Azam Iraji Zad<sup>1</sup>; Saeed Shahrokhian<sup>1</sup>; <sup>1</sup>Sharif University of Technology

**Electrowinning of Aluminium Using a Depolarized Gas Anode**: *Geir Martin Haarberg*<sup>1</sup>; <sup>1</sup>Norwegian University of Science and Technology and Qatar University

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Evaluation of Asphalt Mixes Workability and Compactability Using Laboratory and Accelerated Field Testing: *Samer Dessouky*<sup>1</sup>; Manuel Diaz<sup>1</sup>; <sup>1</sup>University of Texas-San Antonio

Thermo-Mechanical Description of AISI4140 Steel at Elevated Temperatures: Farid Abed<sup>1</sup>; <sup>1</sup>American University of Sharjah

**Fabrication of Bulk Nanocomposites by Mechanical Allying and Shock Compaction**: *Nikoloz Chikhradze*<sup>1</sup>; Guram Abashidze<sup>1</sup>; Mikheil Chikhradze<sup>1</sup>; Akaki Gigineishvili<sup>1</sup>; George Oniashvili<sup>1</sup>; <sup>1</sup>Mining Institute/Georgian Technical University

Finite Element Analysis in Static and Dynamic Behaviors of Dental Prosthesis: *Djebbar Noureddine*<sup>1</sup>; <sup>1</sup>Université Djillali Liabes de Sidi Bel Abbes

Fluid Flow and Heat Transfer Modeling to NOx Characterization in Electric Arc Furnace (EAF): *Ali Ershadi*<sup>1</sup>; <sup>1</sup>Department of Mechanic Engineering, Dezful Branch, Islamic Azad University, Dezful, Iran

Fracture Topography of Forged and Direct Quenched Ti/Nb/V HSLA Steels: Sikaddour Yacine<sup>1</sup>; Lebaili Soltane<sup>1</sup>; <sup>1</sup>USTHB

**Graphene /TiO, Composite Electrodes Toward Oxygen Reduction Reaction**: *Halema Al-Kandari*<sup>1</sup>; Aboubakr Abdullah<sup>2</sup>; Ahmad Mohamed<sup>3</sup>; Shekhah Al-Kandari<sup>3</sup>; <sup>1</sup>PAAET (Public Authority of Applied Education and Tranining); <sup>2</sup>Qatar University; <sup>3</sup>Kuwait University

High Haze Nano-Textured Aluminum doped Zinc Oxide with Plasmonic Silver Nanoparticles for Enhanced Optical Absorption and Photocurrent of a-Si:H Thin Film: Hisham Nasser<sup>1</sup>; Engin Ozkol<sup>1</sup>; Alpan Bek<sup>1</sup>; *Rasit Turan*<sup>1</sup>; <sup>1</sup>Middle East Technical University (METU)/ The Center for Solar Energy Research and Application (GUNAM)

Hydrogen Embrittlement in Pd: Binding Energetics and Structure at Grain Boundaries: Tahir Cagin<sup>1</sup>; <sup>1</sup>Texas A&M University

Improved Q-factor Cavities with Variation of Deposited Nanomaterials' Densities: Ishac Kandas<sup>1</sup>; *Nader Shehata*<sup>1</sup>; Yong Xu<sup>2</sup>; <sup>1</sup>Alexandria University; <sup>2</sup>Virginia Tech

Influence of Joining Time on Microstructure and Mechanical Properties of TLP-joined IN-738LC to GTD-111: *Mahdi* Asgharzadeh Ghadi<sup>1</sup>; Mohammad Amin Amjadi<sup>1</sup>; Mohammad Saeed Shahriari<sup>1</sup>; Meysam Khakian<sup>1</sup>; <sup>1</sup>Mapna/Mavadkaran

Mass Production and Large-scale Assembly of Degradation-resistant Nanowires: *Venkata Vasiraju*<sup>1</sup>; Yongmin Kang<sup>1</sup>; Sreeram Vaddiraju<sup>1</sup>; <sup>1</sup>Texas A&M University

Mechanical Response and Evolution of Damage of Al 6061-T6 Under Different Strain Rates and Temperatures: *Abdelhakim Dorbane*<sup>1</sup>; Georges Ayoub<sup>1</sup>; Bilal Mansoor<sup>1</sup>; Ramsey Hamade<sup>2</sup>; Ghassan Kridli<sup>3</sup>; Abdellatif Imad<sup>4</sup>; <sup>1</sup>Texas A&M University at Qatar; <sup>2</sup>American University of Beirut; <sup>3</sup>University of Michigan-Dearborn; <sup>4</sup>Ecole Polytech'Lille

Methane Production from Carbon Dioxide and Increasing Energy Investment -EROI in Shale Oil: Osama Akoubeh

**Modeling of Carbon Dioxide Absorption Process by Solvent MEA & MEDA**: *Forough Kazemzadeh*<sup>1</sup>; Mohammad Heidary Moghadam<sup>2</sup>; <sup>1</sup>Chemical Engineering, Dezful Branch, Islamic Azad University, Dezful, Iran; <sup>2</sup>Electrical Engineering, Dezful Branch, Islamic Azad University, Dezful, Iran; <sup>2</sup>Electrical Engineering, Dezful Branch, Islamic Azad University, Dezful, Iran; <sup>2</sup>Electrical Engineering, Dezful Branch, Islamic Azad University, Dezful, Iran; <sup>2</sup>Electrical Engineering, Dezful Branch, Islamic Azad University, Dezful, Iran; <sup>2</sup>Electrical Engineering, Dezful Branch, Islamic Azad University, Dezful, Iran; <sup>2</sup>Electrical Engineering, Dezful Branch, Islamic Azad University, Dezful, Iran; <sup>2</sup>Electrical Engineering, Dezful Branch, Islamic Azad University, Dezful, Iran; <sup>2</sup>Electrical Engineering, Dezful Branch, Islamic Azad University, Dezful, Iran; <sup>2</sup>Electrical Engineering, Dezful Branch, Islamic Azad University, Dezful, Iran; <sup>3</sup>Electrical Engineering, Dezful Branch, Islamic Azad University, Dezful, Iran; <sup>4</sup>Electrical Engineering, Dezful Branch, Islamic Azad University, Dezful, Iran; <sup>4</sup>Electrical Engineering, Dezful Branch, Islamic Azad University, Dezful, Iran; <sup>4</sup>Electrical Engineering, Dezful Branch, Islamic Azad University, Dezful, Iran; <sup>4</sup>Electrical Engineering, Dezful Branch, Islamic Azad University, Dezful, Iran; <sup>4</sup>Electrical Engineering, Dezful Branch, Islamic Azad University, Dezful, Iran; <sup>4</sup>Electrical Engineering, Dezful Branch, Islamic Azad University, Dezful, Iran; <sup>4</sup>Electrical Engineering, Dezful Branch, Islamic Azad University, Dezful, Iran; <sup>4</sup>Electrical Engineering, Dezful Branch, Islamic Azad University, Dezful, Iran; <sup>4</sup>Electrical Engineering, Dezful Branch, Islamic Azad University, Dezful, Iran; <sup>4</sup>Electrical Engineering, Dezful Branch, Islamic Azad University, Dezful, Iran; <sup>4</sup>Electrical Engineering, Dezful Branch, Islamic Azad University, Dezful Branch, Islamic Azad Univer

**Molecular Dynamics Study on Physical Properties of Cu Nanoparticles**: *Hasan Kart*<sup>1</sup>; Hüseyin Yildirim<sup>2</sup>; Sevgi Ozdemir Kart<sup>1</sup>; Tahir Cagin<sup>3</sup>; <sup>1</sup>Pamukkale University; <sup>2</sup>Karabuk University; <sup>3</sup> Texas A&M University

Multicomponent Pyrophosphate as a Promising Cathode Material for Rechargeable Lithium Ion Batteries (LIBs): *R. Shakoor*<sup>1</sup>; Ramazan Kahraman<sup>1</sup>; Chanseon Park<sup>2</sup>; Soo Lim<sup>2</sup>; Jang Choi<sup>2</sup>; <sup>1</sup>Qatar University; <sup>2</sup>Korea Advanced Institute of Science and Technology (KAIST)

Non-destructive Assessment of Concrete Mixtures at Cryogenic Temperatures: Towards Primary LNG Containment: *Reginald Kogbara*<sup>1</sup>; Srinath Iyengar<sup>1</sup>; Zachary Grasley<sup>2</sup>; Eyad Masad<sup>1</sup>; Dan Zollinger<sup>2</sup>; <sup>1</sup>Texas A&M University at Qatar; <sup>2</sup>Texas A&M University

Numerical Optimization of Lead Free Perovskite Solar Cell: *Mohammad Hossain*<sup>1</sup>; Ounsi Daif<sup>1</sup>; Nowshad Amin<sup>2</sup>; Fahhad Alharbi<sup>1</sup>; Nouar Tabet<sup>1</sup>; <sup>1</sup>QEERI; <sup>2</sup>National University of Malaysia

On the Effects of Plastic Anisotropy on the Ductile Fracture of Mg Alloys: Amine Benzerga<sup>1</sup>; *S. Basu*<sup>1</sup>; E. Dogan<sup>1</sup>; I. Karaman<sup>1</sup>; <sup>1</sup>Texas A&M University

**Optimization of Soft Magnetic Properties in Nanocrystalline Glass-coated Microwires**: Valentina Zhukova<sup>1</sup>; Ahmed Talaat<sup>2</sup>; Juan Blanco<sup>2</sup>; Mihail Ipatov<sup>2</sup>; Juan del Val<sup>2</sup>; *Arcady Zhukov*<sup>3</sup>; <sup>1</sup>Basque Country University, UPV/EHU ; <sup>2</sup>Basque Country University, UPV/EHU; <sup>3</sup>Basque Country University and Ikerbasque

**Organic Molecule-Functionalized Zn**<sub>3</sub>**P**<sub>2</sub> Nanowires for Photochemical H<sub>2</sub> Production: DFT and Experimental Analyses: G. Ramos-Sanchez<sup>1</sup>; M. Albornoz<sup>1</sup>; Y-H. Yu<sup>2</sup>; Z. Cheng<sup>1</sup>; V. Vasiraju<sup>3</sup>; S. Vaddiraju<sup>1</sup>; *Fadwa El-Mellouhi*<sup>4</sup>; P. B. Balbuena<sup>1</sup>; <sup>1</sup>Artie McFerrin Department of Chemical Engineering; <sup>2</sup>Department of Materials Science & Engineering, Texas A&M University; <sup>3</sup>Department of Materials Science & Engineering, Texas A&M University; <sup>4</sup>QEERI

Phenomenological Model for Phase Transformation Characteristics of Textured Shape Memory Alloys: *D. Chatziathanasiou*<sup>1</sup>; Y. Chemisky<sup>1</sup>; F. Meraghni<sup>1</sup>; E. Patoor<sup>1</sup>; <sup>1</sup>Arts et Métiers ParisTech

**Predictive Modeling For Sustainable Energy Solutions**: *Chaker El Amrani*<sup>1</sup>; Othmane Bouhali<sup>2</sup>; <sup>1</sup>Abdelmalek Essaadi University, Tangier; <sup>2</sup>Texas A&M University at Qatar

Principles of Improvement the Energy Efficiency in Pyrometallurgy of Copper: Utilization the Secondary Heat Energy of Intermediate Products: *Milorad Cirkovic*<sup>1</sup>; Mile Bugarin<sup>1</sup>; Vlastimir Trujic<sup>1</sup>; Zeljko Kamberovic<sup>1</sup>; <sup>1</sup>Mining and Metallurgy Institute Bor, Serbia

Process Optimization of Seed Assisted Growth of Vertically Aligned ZnO Nanorods via Facile Solution Synthesis: *Muhammad Aftab Akram*<sup>1</sup>; <sup>1</sup>National Uiversity of Sciences and Technology Pakistan

Pulsed Electrodeposition of Nano-Crystalline Ni with Uniform Co-Deposition of Micron Sized Diamond Particles on Annealed Copper Substrate: Prashant Kumar<sup>1</sup>; <sup>1</sup>Indian Institute of Technology Banaras Hindu University Varanasi

RAETEX Sustainable Pavement Technology: Michelle Ward1; Shayan Barmand1; 1RAETEX Industries

**Rejuvenation of Long-Term Exposed Nimonic 90 Made Turbine Blades**: *Mohammad Saeed Shahriary*<sup>1</sup>; Mohammad Cheraghzadeh<sup>1</sup>; Ali Khanjani<sup>1</sup>; <sup>1</sup>Mavadkaran Engineering Company

Simulation of Solidification, Relaxation and Long-Term Behavior of a Borosilicate Glass: *Nicolas Barth*<sup>1</sup>; Daniel George<sup>2</sup>; Said Ahzi<sup>1</sup>; Yves Rémond<sup>2</sup>; Mohammad Ahmed Khaleel<sup>3</sup>; Frédéric Bouyer<sup>4</sup>; <sup>1</sup>University of Strasbourg/Qatar Foundation; <sup>2</sup>University of Strasbourg–CNRS; <sup>3</sup>Qatar Foundation; <sup>4</sup>CEA (French Alternative Energies and Atomic Energy Commission)

Storage and Release of Thermal Energy of Phase Change Materials Based on Linear Low Density Polyethylene, Paraffin Wax and Expanded Graphite Applicable in Building Industry: *Patrik Sobolciak*<sup>1</sup>; Mustapha Karkri<sup>2</sup>; Igor Krupa<sup>3</sup>; Mariam Al. Maadeed<sup>3</sup>; <sup>1</sup>Qatar University; <sup>2</sup>Université Paris-Est; <sup>3</sup>Qatar University

Structural Alloy AA6082 – Joining by Friction Stir Welding: Zhiui Zhang<sup>1</sup>; Christophe Herbelot<sup>1</sup>; Abdellatif Imad<sup>1</sup>; *Rajashekhara Shabadi*<sup>1</sup>; <sup>1</sup>University of Science and Technology of Lille

Surfactant Less Microwave Synthesis of Hierarchical Nanostructures of Titania and Their Application: Sofia Javed'; <sup>1</sup>National University of Sciences and Technology Pakistan

Synthesis and Evaluation of Heterogeneous Nano-catalyst : Cr, O, Loaded in to MCM-41: Ali Salemi Golezani; 'KIAU

The Effect of Using a Titanium Interlayer in Explosively Welded Cu/AI Plates: *Majid Etminanbakhsh*<sup>1</sup>; Mandana Adeli<sup>2</sup>; <sup>1</sup>Iran Research Center; <sup>2</sup>Iran University of Science & Technology

Thermal Analysis of Solar Panels: *Nicolas Barth*<sup>1</sup>; Joao Pedro de Magalhaes Correia<sup>2</sup>; Said Ahzi<sup>1</sup>; Mohammad Ahmed Khaleel<sup>3</sup>; <sup>1</sup>Qatar Foundation/University of Strasbourg; <sup>2</sup>University of Strasbourg; <sup>3</sup>Qatar Foundation

Thermo-mechanical Fatigue and Fracture of NiTiHf High Temperature Shape Memory Alloys: *Ceylan Hayrettin*<sup>1</sup>; Omer Karakoc<sup>1</sup>; Ibrahim Karaman<sup>1</sup>; <sup>1</sup>Texas A&M University

Toughness Improvement of Ferritic Mn Steels for Low Temperature Application: II-Cheol Yi<sup>1</sup>; Yunik Kwon<sup>1</sup>; Yumi Ha<sup>1</sup>; Hakcheol Lee<sup>2</sup>; Nack J. Kim<sup>1</sup>; <sup>1</sup>POSTECH; <sup>2</sup>POSCO

Transport through Quantum Dots: Hamidreza Vanaie1; 1Islamic Azad University

Trends in (Poly)olefination Catalyst Development for Energy and Environment Application: Sarim Dastgir<sup>1</sup>; <sup>1</sup>Qatar Environment and Energy Research Institute

Warm Mix Asphalt: Microstructural, Chemical and Thermal Analyses: *Ilaria Menapace*<sup>1</sup>; Eyad Masad<sup>1</sup>; Dallas Little<sup>2</sup>; Emad Kassem<sup>2</sup>; Amit Bhasin<sup>3</sup>; <sup>1</sup>Texas A&M University at Qatar; <sup>2</sup>Texas A&M University; <sup>3</sup>The University of Texas at Austin

### WEDNESDAY, JANUARY 14, 2014

Introductory Commonte

Plenary

Room: Al Wosail

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|-----------|--|
| 8:10 AM   | Keynote<br>Achievable Innovation in a Sustainable Infrastructure: Dallas Little <sup>1</sup> ; <sup>1</sup> Texas A&M University |
| 8:55 AM   | Break  |

### 1-5: Asphaltic Materials

Room: Al Wosail 1

| 9:10 AM  | <b>DEM Simulation of the Asphalt Concrete Flow Number Test</b> : <i>Thomas Papagiannakis</i> <sup>1</sup> ; Habatamu Zelelew; <sup>1</sup> University of Texas San Antonio  |
|----------|---|
| 9:30 AM  | Assessment of the Benefits of Implementing Warm Mix Asphalt (WMA) for Roadways in Qatar: Yara Hamdar <sup>1</sup> ;<br><i>Ghassan Chehab</i> <sup>2</sup> ; Issam Srour <sup>3</sup> ; <sup>1</sup> Graduate Research Assistant, Corresponding Author; <sup>2</sup> Associate Professor,<br>Department of Civil and Environmental Engineering; <sup>3</sup> Assistant Professor, Engineering Management Program |
| 9:50 AM  | <b>Effect of Warm Mix Asphalt on Aging of Asphalt Binders</b> : <i>Ala Abbas</i> <sup>1</sup> ; Munir Nazzal <sup>2</sup> ; Savas Kaya <sup>2</sup> ; Sunday Akinbowale <sup>1</sup> ; Bijay Subedi <sup>1</sup> ; Lana Abu Qtaish <sup>2</sup> ; <sup>1</sup> The University of Akron; <sup>2</sup> Ohio University  |
| 10:10 AM | Investigation of Long- and Short-term Moisture Damage Characteristics of Warm Asphalt Mixtures Containing Reclaimed Asphalt: <i>Aikaterini Varveri</i> <sup>1</sup> ; Stavros Avgerinopoulos <sup>2</sup> ; Athanasios (Tom) Scarpas <sup>1</sup> ; <sup>1</sup> Delft University of Technology; <sup>2</sup> De Montfort University  |
| 10:30 AM | Improving Asphalt Mixtures Performance by Mitigating Oxidation Using Anti-Oxidants Additives: Samer Dessouky <sup>1</sup> ; Manuel Diaz <sup>1</sup> ; <sup>1</sup> University of Texas-San Antonio   |
| 10:50 AM | An Innovative Concept for Testing Rutting Susceptibility of Asphalt Mixture: <i>Alaedddin Mohseni</i> <sup>1</sup> ; Haleh Azari <sup>2</sup> ; <sup>1</sup> Pavement Systems; <sup>2</sup> AASHTO  |
| 11:10 AM | <b>Evaluation of Performance Characteristics of Warm Mix Asphalt in Qatar</b> : <i>Emad Kassem</i> <sup>1</sup> ; Lorena Garcia Cucalon <sup>2</sup> ; Eyad Masad <sup>3</sup> ; Dallas Little <sup>2</sup> ; <sup>1</sup> Texas A&M Transportation Institute; <sup>2</sup> Texas A&M University; <sup>3</sup> Texas A&M University-Qatar   |
| 11:30 AM | Lunch   |

### 2-5: Shape Memory Alloys in Energy Conversion

### Room: Al Wosail 2

| 9:10 AM         | <b>On the Fracture Response of Shape Memory Alloy Actuators</b> : <i>Dimitris Lagoudas</i> <sup>1</sup> ; Theocharis Baxevanis <sup>1</sup> ; <sup>1</sup> Texas A&M University   |
|-----------------|---|
| 9:30 AM         | High-temperature Shape Memory Alloys for Actuation and Damping Applications – Functional Properties and Degradation Behavior: <i>Thomas Niendorf</i> <sup>1</sup> ; Philipp Krooss <sup>2</sup> ; Hans Maier <sup>3</sup> ; <sup>1</sup> TU Bergakademie Freiberg; <sup>2</sup> University of Paderborn; <sup>3</sup> Leibniz Universität Hannover  |
| 9: <b>50 AM</b> | Thermal Stability of Ni-rich Ni-Ti-Hf and Ni-Ti-Zr High Temperature Shape Memory Alloys Containing H-phase<br>Precipitates: Aquilina Perez-Sierra <sup>1</sup> ; Alper Evirgen <sup>2</sup> ; <i>Jaume Pons</i> <sup>1</sup> ; Ruben Santamarta <sup>1</sup> ; Ibrahim Karaman <sup>2</sup> ; Ronald Noebe <sup>3</sup> ; <sup>1</sup> University of the Balearic Islands; <sup>2</sup> Texas A&M University; <sup>3</sup> NASA Glenn Research Center |
| 10:10 AM        | Large Strains and Nondissipative Character of Superelastic Behavior of Ni-Fe-Ga(Co) Single Crystal: Volodymyr Chernenko <sup>1</sup> ; Victor Lvov <sup>2</sup> ; Elena Villa <sup>3</sup> ; Jose Manuel Barandiaran <sup>4</sup> ; <sup>1</sup> BCMaterials,UPV(EHU) & Ikerbasque; <sup>2</sup> Institute of Magnetism; <sup>3</sup> IENI-CNR; <sup>4</sup> BCMaterials & UPV(EHU)   |
| 10:30 AM        | <b>Development of SMA Actuated Morphing Airfoil for Wind Turbine Blade Load Alleviation</b> : Anargyros Karakalas <sup>1</sup> ; Theodore Machairas <sup>1</sup> ; Alexandros Solomou <sup>1</sup> ; Vasilis Riziotis <sup>2</sup> ; <b>Dimitris Saravanos</b> <sup>1</sup> ; <sup>1</sup> University of Patras; <sup>2</sup> National Technical University of Athens   |
| 10:50 AM        | Identification of Model Parameter for the Simulation of SMA Structures using Full Field Measurements: <i>Yves Chemisky</i> <sup>1</sup> ; F. Meraghni <sup>1</sup> ; N. Bourgeois <sup>2</sup> ; S. Cornell <sup>3</sup> ; R. Echchorfi <sup>1</sup> ; E. Patoor <sup>1</sup> ; <sup>1</sup> Arts et Metiers ParisTech; <sup>2</sup> Université de Lorraine; <sup>3</sup> Texas A&M University  |
| 11:10 AM        | Comparison of the Work Output Values of Gradually Changing Porosity Samples and the Samples with Single Percent Porosity Level: Halil Tugrul <sup>1</sup> ; Sule Cakmak <sup>1</sup> ; Benat Kockar <sup>1</sup> ; <sup>1</sup> Hacettepe University  |
| 11:30 AM        | Lunch   |

### 2-7: Materials Issues in Energy Conversion

| 9:10 AM | Synthesis, Characterization and Environmental Impact Assessment of Graphene: Mariam AIAIi AIMa'adeed <sup>1</sup> ; Noorunnisa Khanam Patan <sup>1</sup> ; Maryam AI-Aji <sup>1</sup> ; Roda F. AI-Thani <sup>1</sup> ; <sup>1</sup> Qatar University          |
|---------|--|
| 9:30 AM | Numerical Modeling of Cathode Contact Material Densification in SOFCs: <i>Mohammed Khaleel</i> <sup>1</sup> ; Brian Koeppel <sup>2</sup> ; Elizabeth Stephens <sup>2</sup> ; <sup>1</sup> Qatar Foundation; <sup>2</sup> Pacific Northwest National Laboratory |

| 9:50 AM      | Thin Film Coated Interconnectors Used in Solid Oxide Fuel Cells (SOFC) Via RF Magnetron Sputtering Method:<br><i>Fatma Aydin</i> <sup>1</sup> ; Ali Özmetin <sup>2</sup> ; Mahmut Mat <sup>2</sup> ; <sup>1</sup> University of Nigde; <sup>2</sup> University of Meliksah   |
|--------------|--|
| 10:10 AM     | <b>Perovskites Of Type LaBO</b> , <b>Prepared by the Microwave-assisted Method for Oxygen Production</b> : Shimaa Ali <sup>1</sup> ; Nada Atta <sup>1</sup> ; Yasser Abd Al-Rahman <sup>1</sup> ; <b>Ahmed Galal</b> <sup>1</sup> ; <sup>1</sup> Cairo University, Faculty of Science  |
| 10:30 AM     | Nitrogen-Doped Carbon Nanofiber – Supported Nickel Oxide Composite for Methanol Oxidation: <i>Aboubakr Abdullah</i> <sup>1</sup> ; Abdullah Al-Enizi <sup>2</sup> ; Ahmed El-Zatahry <sup>2</sup> ; Salem Al-Deyab <sup>2</sup> ; <sup>1</sup> Qatar University; <sup>2</sup> King Saud University   |
| 10:50 AM     | Aluminum and Tin Doping Effect of ZnO Thin Films on the Photovoltaic Parameters of Culn1-xGaxS,/B-In2-<br>xAlxS,/ZnO Solar Cells: <i>Najoua Kamoun</i> <sup>1</sup> ; Mejda Ajili <sup>1</sup> ; <sup>1</sup> Faculty of Science TUNIS/ Physics Condensed Matter<br>Laboratory   |
| 11:10 AM     | Ammonia Borane (AB) as a Portable Source & Storage Material for Hydrogen: Muhammad Sohail <sup>1</sup> ; 1QEERI  |
| 11:30 AM     | Lunch  |
| 2-9: Lightwe | ight and High Performance Materials II   |
| Room: AI Wo  | osail 1  |
| 1:30 PM      | Introductory Comments  |
| 1:40 PM      | Sustainable Novel Technology for Producing New Generations of Structural Al-alloys and Al Containing Bi-<br>metals: Hans Roven <sup>1</sup> ; Kristian Skorpen <sup>2</sup> ; Oddvin Reiso <sup>3</sup> ; Chris Devadas <sup>4</sup> ; <sup>1</sup> Qatar University; <sup>2</sup> Norwegian University of<br>Science and Technology; <sup>3</sup> Hydro ASA; <sup>4</sup> Hydro Aluminium QSTP Qatar  |
| 2:00 PM      | <b>Modification of Aluminium Surfaces with Metal Oxides</b> : <i>Rajashekhara Shabadi</i> <sup>1</sup> ; Vishweshvara Gudla <sup>2</sup> ; Flemming Jensen <sup>3</sup> ; Rajan Ambat <sup>2</sup> ; Aude Simar <sup>4</sup> ; <sup>1</sup> University of Science and Technology of Lille; <sup>2</sup> Department of Mechanical Engineering, Technical University of Denmark; <sup>3</sup> Bang & Olufsen Operations A/S; <sup>4</sup> Université Catholique de Louvain |
| 2:20 PM      | Parametric Study for Crash Safety Improvement of a Car Bonnet Made from a Hybrid Aluminum and Natural Fiber Composite Structure: Sofiene Helaili'; Moez Chafra <sup>1</sup> ; Yvon Chevalier <sup>2</sup> ; <sup>1</sup> LASMAP; <sup>2</sup> SUPMECA  |
| 2:40 PM      | Adhesion Improvement Between Polyethylene and Aluminum Using Eco-friendly Plasma Treatment: Anton <b>Popelka</b> <sup>1</sup> ; Igor Krupa <sup>1</sup> ; Igor Novák <sup>2</sup> ; Mabrouk Ouederni <sup>3</sup> ; Fatima Abdulaqder <sup>1</sup> ; Shrooq Al-Yazedi <sup>1</sup> ; Taghreed Al-Gunaid <sup>1</sup> ; Thuraya Al-Senani <sup>1</sup> ; <sup>1</sup> Qatar University; <sup>2</sup> Slovak Academy of Sciences; <sup>3</sup> QAPCO                       |
| 3:00 PM      | The Effect of Tool Geometry on Material Mixing During Friction Stir Welding (FSW) of Magnesium AZ31B Welds:<br>Zeina El-Chlouk <sup>1</sup> ; Haig Achdjian <sup>1</sup> ; George Ayoub <sup>2</sup> ; Ramsey Hamade <sup>1</sup> ; <sup>1</sup> American University of Beirut; <sup>2</sup> Texas A&M University at Qatar   |
| 3:20 PM      | <b>Microstructural Design of Mg Alloys for Lightweight Structural Applications</b> : <i>Ebubekir Dogan</i> <sup>1</sup> ; Matthew Vaughan <sup>1</sup> ; Ibrahim Karaman <sup>1</sup> ; Gwénaëlle Proust <sup>2</sup> ; Georges Ayoub <sup>3</sup> ; Amine Benzerga <sup>1</sup> ; <sup>1</sup> Texas A&M University; <sup>2</sup> School of Civil Engineering, The University of Sydney; <sup>3</sup> Texas A&M University at Qatar                                     |
| 3:40 PM      | <b>Correlation of Magnetic Properties and Plastic Deformation Distribution in Steel Welds:</b> <i>Athanasios Mamalis</i> <sup>1</sup> ; Evangelos Hristoforou <sup>2</sup> ; <sup>1</sup> PC-MAE; <sup>2</sup> National TU of Athens   |
| 4:00 PM      | Role of Multiscale Characterization to Examine the Mechanical Properties for Promoting New Material Developments: Application to Ni-base Superalloys: Bilal Mansoor1; <i>Mustapha Jouiad</i> 1; 1Masdar Institute of Technology  |

### 2-6: Photovoltaics and Solar-Thermal Energy Conversion

| 1:30 PM | Introductory Comments  |
|---------|--|
| 1:40 PM | <b>Sponge-like Silicon Nanostructures for Third Generation Photovoltaic Solar Cells</b> : <i>Rasit Turan</i> <sup>1</sup> ; Serim Ilday <sup>1</sup> ; Emel Ozen <sup>2</sup> ; Sinan Gundogdu <sup>2</sup> ; Atilla Aydinli <sup>2</sup> ; <sup>1</sup> Middle East Technical University; <sup>2</sup> Bilkent University |
| 2:00 PM | <b>Mono-crystalline Bulk Silicon Based High-Efficiency Flexible Solar Cell</b> : <i>Rabab R. Bahabry</i> <sup>1</sup> ; Jhonathan P. Rojas <sup>1</sup> ; Aftab Hussain <sup>1</sup> ; Muhammad M. Hussain <sup>1</sup> ; <sup>1</sup> Integrated Nanotechnology Lab, King Abdullah University of Science and Technology   |
| 2:20 PM | Hole Mobility and Stresses in PECVD a-Si Thin Films: Nouar Tabet <sup>1</sup> ; 1QEERI   |
| 2:40 PM | Sonochemical Synthesis of Cu <sub>2</sub> ZnSnS <sub>4</sub> and Cu <sub>2</sub> ZnSnSe <sub>4</sub> Nanocrystals for Absorber Layer Application in Thin Film Solar Cells: <i>Mohammad Islam</i> <sup>1</sup> ; Syed Shah <sup>2</sup> ; <sup>1</sup> King Saud University; <sup>2</sup> University of Delaware            |

| Electrochemical Deposition of High Purity Silicon from Molten Salts: Geir Martin Haarbergi:   | <sup>1</sup> Norwegian                             |
|---|--|
| <b>3:20 PM</b> Electrochemical Deposition of High Purity Silicon from Molten Salts: <i>Geir Martin Haarberg</i> <sup>1</sup> ; University of Science and Technology, and Qatar University   | Norwegian  |
| 3:40 PM Cationic (V,Y)-codopedTiO, with EnhancedVisible Light Induced Photocatalytic Activity for Photoelec<br>Applications: <i>Matiullah Khan</i> <sup>1</sup> ; Wenbin Cao <sup>2</sup> ; Bilal Mansoor <sup>1</sup> ; <sup>1</sup> Texas A & M University at Qatar; <sup>2</sup> Universi<br>and Technology Beijing  | trochemical<br>ty of Science                       |
| <b>4:00 PM</b> Enhancement of the Kinetics of Heat Storage by Means of Cellular Metals: <i>Olaf Andersen</i> <sup>1</sup> ; Je <sup>1</sup> Fraunhofer-Gesellschaft; <sup>2</sup> Fraunhofer IFAM Dresden   | ens Meinert2;                                      |
| <b>4:20 PM Economic Technical Solutions for Enhancing the Efficiency of Thermal Solar Water Heating</b> : <i>Iman E</i><br>Nagwa Khattab <sup>2</sup> ; Ahmed Abdel- Rehim <sup>3</sup> ; Sayed Akl <sup>3</sup> ; <sup>1</sup> Cairo University; <sup>2</sup> National Research Centre; <sup>3</sup> Briti<br>in Egypt | <b>l Mahallawi</b> <sup>ı</sup> ;<br>sh University |

### 3-5: Computational Approaches towards Mechanical Damage, Environmental Degradation

| Room: Al Wosail 3 |   |
|-------------------|---|
| 1:30 PM           | Introductory Comments   |
| 1:40 PM           | Invited<br>Predicting Ductile Fracture Toughness: Alan Needleman <sup>1</sup> ; <sup>1</sup> Texas A&M University   |
| 2:20 PM           | Investigation of Damage and Fracture in Two Magnesium Alloys: Amine Benzerga <sup>1</sup> ; B. Kondori <sup>1</sup> ; <sup>1</sup> Texas A&M University   |
| 2:40 PM           | <b>Micromechanical Fatigue Visco-damage Model for Short Glass Fiber Reinforced Polyamide-66</b> : Nicolas Despringre <sup>1</sup> ; Yves Chemisky <sup>1</sup> ; Gilles Robert <sup>2</sup> ; <i>Meraghni Fodil</i> <sup>1</sup> ; <sup>1</sup> ENSAM - Arts et Métiers ParisTech; <sup>2</sup> Solvay Engineering Plastics   |
| 3:00 PM           | Break   |
| 3:20 PM           | Crystal Plasticity and Fracture Simulations Using a New 2.5D Dislocation Dynamics Method: <i>Shyam Keralavarma</i> <sup>1</sup> ; William Curtin <sup>2</sup> ; <sup>1</sup> Indian Institute of Technology Madras; <sup>2</sup> Ecole Polytechnique Federale de Lausanne   |
| 3:40 PM           | Multiparadigm Modeling of Material Safety and Sustainability: Stress Corrosion Cracking: <i>Tahir Cagin</i> <sup>1</sup> ; Hieu Pham <sup>1</sup> ; Amine Benzerga <sup>1</sup> ; <sup>1</sup> Texas A&M University   |
| 4:00 PM           | <b>Understanding Dusting Corrosion in Iron from Kinetic Monte Carlo Simulations</b> : Oscar Antonio <sup>1</sup> ; <i>Fadwa El-Mellouhi</i> <sup>2</sup> ; Othmane Bouhali <sup>3</sup> ; Charlotte Becquart <sup>4</sup> ; Normand Mousseau <sup>1</sup> ; <sup>1</sup> Universite de Montreal; <sup>2</sup> QEERI; <sup>3</sup> Texas A&M University at Qatar; <sup>4</sup> École Nationale Supérieure de Chimie de Lille |
| 4:20 PM           | Analysis of Thermo-Mechanical Rigidity of Continuously Cast Steel Slabs: Mostafa El-Bealy <sup>1</sup> ; <sup>1</sup> Ain Shams University, (CC)  |

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