



## Symposium Computational Materials Sciences, Characterization and “Critical” Materials

### Draft- Agenda

*Note: the agenda is subject to changes and additions.*

*Titles are tentative. Definitive titles will be updated as they become available.*

**Tuesday, September 15, 2015**

**Four Points by Sheraton (Ballroom)**

- 8:30 AM Greeting and Opening of the Symposium**  
*Thomas Boellinghaus, President of WMRIF (BAM)*
- Welcome Addresses**  
*Robert S. Maxwell, Material Science Division Leader*

### **Session A: Advances in Materials Informatics**

**Chairman: Robert S. Maxwell**

- 9:00 AM Daniele Passerone (EMPA)**  
**Key Note** *Computer-Aided Design of Graphene-Related Materials*
- 9:30 AM James Warren (NIST)**  
*The Materials Genome Initiative and NIST*
- 10:00 AM Xingqiu Chin (CAS-IMR)**  
*Computational Design and Simulation of Materials*
- 10:30 AM Break**
- 11:00 AM Vidvuds Ozolins (UCLA)**  
*Accurate Compressive Sensing Based Methods for First-Principles Simulations of Materials at High Temperatures*
- 11:30 AM Krishna Rajan (U Buffalo)**  
*Informatics*
- 12:00 PM Patrice Turchi (LLNL)**  
*Computational Materials Science*
- 12:30 PM Lunch Break**



## **Session B: Novel and emerging approaches**

**Chairperson: Hai-Doo Kim (KIMS)**

- 1:30 PM David Prendergast (LBL)**  
*Key Note Advanced Characterization and modeling*
- 2:00 PM S M Shivaprasad (Jawaharlal Nehru Centre for Advanced Scientific Research)**  
*Exotic properties of Nanomanifestations of Gallium Nitride*
- 2:30 PM Anssi Laukkanen (VTT)**  
*Mesoscale Modeling Assisted Materials-by-design Concepts for Novel Metallic and Composite Materials*
- 3:00 PM Igor Slowing (Ames)**  
*Structural Control of Materials at the Nano-, Meso- and Macroscales by Coupling Additive Manufacturing with Self-Assembling Methodologies*
- 3:30 PM Break**
- 4:00 PM Jen Dionne (Stanford)**  
*Inside Out: Visualizing Intercalation-Driven Phase Transformations within Individual Nanoparticles*
- 4:30 PM János Volk (MFA)**  
*Low dimensionality in materials S&T*
- 5:00 PM Dongsheng Li (PNNL)**  
*In-situ TEM*
- 5:30 PM Ann Chiaramonti Debay (NIST)**  
*Comprehensive Metrology for Advanced Laser Manufacturing*
- 7:00 PM Dinner (No Host)**  
*Speaker: A special Highlight from LLNL*



**Wednesday, September 16, 2015**

**Session C: "Critical" Materials**

**Chairperson: Erja Turunen (VTT)**

- 8:00 AM Alex King (Ames)**  
**Key Note "Critical Materials: What Can Be Done?"**
- 8:30 AM Jian Zhang (CAS-IMR)**  
*Development of Hot Corrosion Resistant Superalloys with High Temperature Capability*
- 9:00 AM Cajetan Niebedim (Ames)**  
*Magnets*
- 9:30 AM Roderick Eggert (CSM)**  
*Economic View of Critical Materials*
- 10:00 AM Coffee Break**
- 10:30 AM Steven Payne (LLNL)**  
*Phosphors and Optical Materials*
- 11:00 AM TBD**  
*TBD*
- 11:30 AM Summary, Conclusions: Priorities and Challenges**  
*Laurie Locascio and Bob Maxwell*
- 12:00-12:45 PM (No Host Lunch)**
- 12:45 PM Transport to LLNL for tours. Transportation provided by Black Tie.**  
**(Leave baggage at hotel to avoid LLNL inspection delay)**
- 1:40 PM Gate Badge Office for Bus Inspection**
- Tours of LLNL (Optional)**
- 2:00 PM Tours begin**
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|--------------------|--------------------------|
| <b>NIF Tour A</b>  | <b>2:00 PM -3:00 PM</b>  |
| <b>HEAF Tour A</b> | <b>2:00 PM -3:00 PM</b>  |
| <b>NIF Tour B</b>  | <b>3:00 PM - 4:00 PM</b> |
| <b>HEAF Tour B</b> | <b>3:00 PM - 4:00 PM</b> |
- 4:15 – 5:00 PM Transport back to Four Points by Sheraton Hotel**
- Note: Allow for travel time upon return to airport when booking return flights to: Oakland, San Francisco and San Jose**