

# AGENDA

## NSF/DOE Materials Genome Initiative Principal Investigators' Meeting

**Monday, January 11, 2016**

- 8:00 – 8:30am      **\*\*\*\*\*Registration and Continental Breakfast\*\*\*\*\***
- 8:30 – 8:40am      **Welcome and Introductions from Co-chairs:**  
Meeting Chairs: **Tresa Pollock and Kristin Persson**  
UC–Santa Barbara / UC–Berkeley
- 8:40 – 9:00am      **MGI at NSF**  
**Linda Sapochak and John Schlueter**
- 9:00 – 9:20am      **MGI at DOE**  
**Linda Horton and Jim Davenport**
- 9:20 – 9:35am      **MGI at NIST**  
**Jim Warren**
- 9:35 – 9:50am      **MGI at ONR**  
**Julie Christodoulou**
- 9:50 – 10:00am      **MGI at AFRL**  
**Chuck Ward and Ali Sayir**
- 10:00 – 10:30am      **\*\*\*\*\*Break\*\*\*\*\***
- 10:30 – 10:50am      **NSF Material Innovation Platforms**  
**Sean Jones, NSF**
- 10:50 – 11:20am      **MGI and Applied Mathematics**  
**Robert V. Kohn, New York University**
- 11:20 – 11:50am      **MGI and Computer Science**  
**Jim Belak, Lawrence Livermore National Laboratory**
- 11:50 – 12:00pm      **Introduction to Breakouts**

**12:00pm      Breakout Session #1 with Working Lunch**  
*What is MGI accomplishing across Material Classes?*

- 1) Metals, Alloys, and Ceramic Materials, **Srinivasan Srivilliputhur (UNT)** and **Martin Green (NIST)**

- 2) Magnetic and Electronic Materials, **Warren Pickett (UC Davis)**, **Hai Ping Cheng (UF)**, and **Paul McEuen (Cornell)**
- 3) Molecular, Polymer, and Biomaterials, **Mike Toney (Stanford)** and **Mark Bathe (MIT)**
- 4) Materials for Catalysis & Chemical Transformations, **Jeff Greeley (Purdue)** and **Randall Snurr (Northwestern)**
- 5) Photonic and Thermoelectric Materials, **Chris Van de Walle (UCSB)** and **Irena Knezevic (Wisconsin)**

1:45 – 2:10pm	<b>Preparation of Reports</b>
2:10 – 3:00pm	<b>Presentation of Breakout Sessions (5 x 10 minutes)</b>
3:00 – 5:00pm	<b>Poster Session with Refreshments</b>
5:00pm	<b>*****Adjourn for the Day*****</b>

## Tuesday, January 12, 2016

8:00 – 8:30am	<b>*****Continental Breakfast*****</b>
8:30 – 8:50am	<b>MGI in Perspective</b> <b>Lloyd Whitman (OSTP)</b>
8:50 – 9:10am	<b>MGI in Advanced Manufacturing</b> <b>Megan Brewster (OSTP)</b>
9:10am	<b>*****Breakout for Parallel Sessions*****</b>

### **Session A: Hard Materials** Chair: **Alexis Lewis**

9:20 – 9:30am	<b>Stathis Meletis</b> , University of Texas <i>Multiscale Design of Hard and High Temperature Resistant Coatings by Computation and Experiment</i>
9:30 – 9:40am	<b>Patrick LeClair</b> , University of Alabama <i>First-principles Based Design of Spintronic Materials and Devices</i>
9:40 – 9:50am	<b>Robert Hull</b> , Rensselaer Polytechnic Institute <i>Real Time Control of Grain Growth in Metals</i>
9:50 – 10:00am	<b>Chang-Beom Eom</b> , University of Wisconsin <i>Multifunctional Interface Materials by Design</i>

10:00 – 10:10am **Maarten de Boer**, Carnegie Mellon University  
*High-Throughput Discovery, Development and Demonstration of Materials Systems to Enable Low-power NEMS-based Computation*

**Session B: Soft Materials**  
Chair: **Mark Pederson**

9:20 – 9:40am **Ilja Siepmann**, University of Minnesota  
*Nanoporous Materials Genome: Methods and Software to Optimize Gas Storage, Separation, and Catalysis*

9:40 – 9:50am **Randy Snurr**, Northwestern University  
*Simulation-Driven Design of Highly Efficient MOF/Nanoparticle Hybrid Catalyst Materials*

9:50 – 10:00am **Lian Yu**, University of Wisconsin  
*Engineering Organic Glasses*

10:00 – 10:10am **Mohammad Islam**, Carnegie Mellon University  
*Mechanics of Three-Dimensional Carbon Nanotube Aerogels with Tunable Junctions*

10:10 – 10:40am \*\*\*\*\***Refreshment Break and Poster Setup**\*\*\*\*\*

**Session C: Hard Materials**  
Chair: **Matthias Graf**

10:40 – 11:00am **Kristin Persson**, University of California – Berkeley  
*Materials Project*

11:00 – 11:20am **John Perdew**, Temple University  
*SCAN Meta-GGA: An Accurate, Efficient, and Soundly Based Density Functional for MGI?*

11:20 – 11:30am **Kristjan Haule**, Rutgers University  
*Enhanced Functionalities in 5d Transition-Metal Compounds from Large Spin Orbit Coupling*

11:30 – 11:40am **Lian Li**, University of Wisconsin – Milwaukee  
*Emergent Functionalities at the Epitaxial Interfaces of Correlated and Spin-Orbit Materials*

11:40 – 11:50am **Alex Zunger**, University of Colorado  
*Theory-Guided Experiments in Search of Designed Topological Insulators and Band-Inverted Insulators*

**Session D: Soft Materials**  
Chair: **David LaVan**

10:40 – 10:50am **Darrin Pochan**, University of Delaware  
*Materials with Predetermined Nanostructures via the Computational Design and Solution Assembly of Peptides*

- 10:50 – 11:00am **Todd Yeates**, University of California – Los Angeles  
*Integrating Theory, Computation, and Experiment to Robustly Design Complex Protein-Based Nanomaterials*
- 11:00 – 11:10am **Kris Delaney**, University of California – Santa Barbara  
*Computationally Driven Discovery and Engineering of Multi-block Polymer Nanostructures using Genetic Algorithms*
- 11:10 – 11:20am **H. Jerry Qi**, Georgia Institute of Technology  
*Laminated Elastomer Composites with Anisotropic Shape Memory*
- 11:20 – 11:30am **Ronald Hedden**, Texas Tech University  
*Combinatorial Methods to Enable Rapid Prototyping of Polymeric Pervaporation Membranes for Biofuels*
- 11:30 – 11:40am **Brad Olsen**, Massachusetts Institute of Technology  
*Analysis and Optimization of Polymer Networks for Engineering Applications*
- 11:40 – 11:50am **Hamish Fraser**, The Ohio State University  
*Design Knowledge Base of Low-Modulus Titanium Alloys for Biomedical Applications*
- 11:50 – 12:00pm **Introduction to Breakouts**
- 12:00pm **Breakout Session #2 with Working Lunch**  
*Accelerating Materials Research*
- 1) Data Repositories, **Carrie Campbell (NIST)** and **Stefano Curtarolo (Duke)**
  - 2) Mathematics, Software and Cyberinfrastructure, **Elsa Olivetti (MIT)** and **John Allison (Michigan)**
  - 3) Advanced Manufacturing, **Peter Collins (Iowa State)** and **Cliff Henderson (Georgia Tech)**
  - 4) Transitioning Fundamental Science to Technology and Applications, **Volker Sorger (GWU)** and **Bill Tumas (NREL)**
  - 5) Equipping and Educating the Next Generation, **Kathlene Kash (Case Western)**, and **Richard LeSar (Iowa State)**
- 1:45 – 2:10pm **Preparation of Reports**
- 2:10 – 3:00pm **Presentation of Breakout Sessions (5 x 10 minutes)**
- 3:00 – 5:00pm **Poster Session with Refreshments**
- 5:00pm **\*\*\*\*\*Adjourn\*\*\*\*\***

