2013 NSF-DMR-MGI Workshop:
The Materials Genome Initiative in Ceramics, Geosciences, and Solid-State Chemistry
(NSF DMR 1115294 and NSF DMR 1216415)

Supported by the National Science Foundation through DMR Programs: SSMC and Ceramics

Glebe/Fairfax room, Holiday Inn, Arlington at Ballston. **Thursday February 21 and Friday February 22, 2013.**

Day 1: Thursday February 21, 2013

Session I [8:00 am to 10:00 am]: Nanomaterials	
Chair: KARIN RABE **Notetaker:** RAM SESHADRI	
8:00 am to 8:30 am	*Badges, welcome, and introductory remarks*
8:30 am to 8:45 am	ALEX NAVROTSKY: *Earth materials: Common ground between materials science and geology*
8:45 am to 9:00 am	LEE PENN: *Towards greener materials and nanomaterials synthesis*
9:00 am to 9:15 am	SUSAN SINNOTT: *Computational prediction of material behavior for databases and informatics*
9:15 am to 10:00 am	*Discussion*
10:00 am to 10:30 am	**Break**
Session II [10:30 am to 12:15 pm]: Clusters, hybrids, and material–molecule interactions	
Chair: ALEX NAVROTSKY **Notetaker:** LEE PENN	
10:30 am to 10:45 am	YOUNG-SHIN JUN: *Lessons from Nature: Understanding aqueous interfacial reactions of new materials*
10:45 am to 11:00 am	DANNA FREEDMAN: *Molecular synthetic methods for solid-state materials*
11:00 am to 11:15 am	CHRISTOPHER CAHILL: *Halogen-halogen and other non-covalent interactions in hybrids*
11:15 am to 12:30 pm	*Discussion*
12:30 pm to 1:30 pm	**Lunch**
Session III [1:30 pm to 3:30 pm]: High pressures and epitaxial stabilization A	
Chair: PAUL SALVADOR **Notetaker:** JAMES RONDINELLI	
1:30 pm to 1:45 pm	LANE MARTIN: *"Mining" materials for useful functionalities – a material maker's perspective*
1:45 pm to 2:00 pm	ABBY KAVNER: *Using high pressures to tune material properties*
2:00 pm to 2:15 pm	AMY WALKER: *Towards new catalytic and photocatalytic materials*
2:15 pm to 2:30 pm	KARIN RABE: *Design and discovery of novel functional materials*
2:30 pm to 3:30 pm	*Discussion*
3:30 pm to 4:00 pm	**Break**
Session IV [4:00 pm to 6:00 pm]: High pressures and epitaxial stabilization B	
Chair: ICHIRO TAKEUCHI **Notetaker:** MICHAEL SHATRUK	
4:00 pm to 4:15 pm	JAMES RONDINELLI: *Disruptive design approaches for materials discovery*
4:15 pm to 4:30 pm	NICOLE BENEDEK: *Soft mode approach to transport properties of complex oxides*
4:30 pm to 4:45 pm	PAUL SALVADOR: *Combinatorial substrate epitaxy and the epitaxial design of materials*
4:45 pm to 5:00 pm	PAT WOODWARD: *Effects of chemical, external, and epitaxial pressure on the structural and magnetic properties of complex oxides*
5:00 pm to 6:00 pm	*Discussion*
6:00 pm to 8:00 pm	Dinner at Rustico, Arlington-Ballston
8:00 pm to 10:00 pm	*Educating the next generation: A discussion*

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Day 2: Friday February 22, 2013

Session V [8:30 am to 10:00 am]: High throughput methods and data mining	
Chair: SUSAN SINNOTT **Notetaker:** PAT WOODWARD	
8:30 am to 8:45 am	ICHIRO TAKEUCHI: *Integrating high-throughput experiments, theory, and databases*
8:45 am to 9:00 am	KRISHNA RAJAN: *High throughput knowledge discovery vs. data discovery*
9:00 am to 9:15 am	GREG ROHRER: *High throughput analysis of interface complexions*
9:15 am to 10:00 am	*Discussion*
10:00 am to 10:30 am	**Break**
Session VI [10:30 am to 12:30 pm]: New Synthesis	
Chair: LEE PENN **Notetaker:** DANNA FREEDMAN	
10:30 am to 10:45 am	ERIC TOBERER: *Synthetic approaches to new thermoelectrics*
10:45 am to 11:00 am	MICHAEL SHATRUK: *Hunting for new materials: Mixing, slicing, and nanostructuring*
11:00 am to 11:15 am	EFRAIN RODRIGUEZ: *Discovering routes to metastable inorganic materials*
11:15 am to 12:30 pm	*Discussion*
12:30 pm to 1:30 pm	**Lunch**
Session VII [1:30 am to 3:30 pm]: Energy	
Chair: GREG ROHRER **Notetaker:** EFRAIN RODRIGUEZ	
1:30 pm to 1:45 pm	ANTON VAN DER VEN: *The need for kinetic theories describing meso-scale dynamics in energy storage materials*
1:45 pm to 2:00 pm	EDWIN GARCIA: *Validation, data management, and visualization challenges in the simulation of 3D battery microstructures*
2:00 pm to 2:15 pm	MICHELLE JOHANNES: *Computational input to energy materials design*
2:15 pm to 2:30 pm	RAM SESHADRI: *Datamining for thermoelectrics and lighting phosphors*
2:30 pm to 4:00 pm	*Discussion and closing remarks*