NSF-sponsored workshop on Materials by Design

March 17th to 19th, 2011
Loma Pelona Center, University of California, Santa Barbara

http://www.mbd.mrl.ucsb.edu/

Schedule of talks

Thursday March 17th 2011

12:30 pm to 2:30 pm	**Registration and lunch (served between 12:40 pm and 1:40 pm)**	

Session 1 (Chaired by Galen Stucky)		
2:30 pm to 2:50 pm	M. Thompson (USC)	*Opportunities and challenges in thin film organic optoelectronics.*
2:50 pm to 3:10 pm	K. S. Choi (Purdue)	*1. Shape dependent or atomic plane dependent properties.* *2. Construction of optimum semiconductor-catalyst composite structures for use in solar fuel production.*
3:10 pm to 3:30 pm	T. M. McQueen (JHU)	*1. Synthesis of new metastable, "high-quality", strongly correlated materials.* *2. Bridging the physics-chemistry language and culture gap.*
3:30 pm to 3:50 pm	L. Balents (UCSB)	*Known unknowns and unknown unknowns: How do we (theory, experiment, and growth) search for **new** physics in materials?*
3:50 pm to 4:10 pm	M. Kanatzidis (Northwestern)	*1. How do we define "materials by design"?* *2. The science of synthesis versus guided serendipity.*
4:10 pm to 4:30 pm	*Summary discussion*	
4:30 pm to 5:00 pm	**Coffee Break**	

Session 2 (Chaired by Chris Van de Walle)		
5:00 pm to 5:20 pm	K. Rabe (Rutgers)	*Materials with built-in competition: Coupled phase transitions and functional properties.*
5:20 pm to 5:40 pm	D. Mandrus (UT Knoxville)	*The indispensable role of new materials in the advance of condensed matter physics.*
5:40 pm to 6:00 pm	M. Dincă (MIT)	*Electronic properties of porous organic-inorganic hybrids.*
6:00 pm to 6:20 pm	S. Stemmer (UCSB)	*1. Novel approaches to the synthesis of highly-perfect, high-purity oxide thin films.* *2. Opportunities for novel transport phenomena in oxide heterostructures.*

6:30 pm to 8:00 pm	**Reception and dinner (served at 7:00 pm)**	
8:00 pm to 8:40 pm	A. Ramirez (UCSC)	*The NRC report*
8:40 pm to 9:40 pm	*Summary discussion*	
9:40 pm	**Transport to the Best Western**	

Friday March 18th 2011

8:20 am to 8:40 am	**Pick up at the Best Western**
8:40 am to 9:00 am	**Continental breakfast**

Session 3 (Chaired by Martin Moskovits)		
9:00 am to 9:20 am	O. Lavrentovich (Kent State)	*1. Functional liquid crystals by design. 2. Lyotropic Liquid Crystals. 3. Liquid Crystals far from equilibrium. 4. Soft and reconfigurable optical metamaterials.*
9:20 am to 9:40 am	S. Boettcher (U. Oregon)	*Inorganic materials for solar energy conversion and storage, particularly for solar water splitting.*
9:40 am to 10:00 am	D. J. Singh (ORNL)	*Interplay between materials discovery and theory.*
10:00 am to 10:20 am	J. Moore (Berkeley)	*1. Research needs for spintronic and magnetoelectric materials, including both oxides and topological insulators. 2. How to increase interaction between first-principles and phenomenological theory.*
10:20 am to 10:40 am	*Summary Discussion*	
10:40 am to 11:00 am	**Coffee Break**	

Session 4 (Chaired by Fred Wudl)		
11:00 am to 11:20 am	D. Frisbie (Minnesota)	*1. Materials challenges for realizing roll-to-roll printed electronics. 2. Understanding fundamental structure-property relationships in organic semiconductors.*
11:20 am to 11:40 am	T.-Q. Nguyen (UCSB)	*1. Intelligent materials design and synthesis. 2. Probing nanoscale properties.*
11:40 am to noon	G. Galli (Davis)	*Theory and simulations of materials for energy applications: 1. Calculations in realistic environments and comparison with experiment; 2. Can theory and simulation make a real difference?*
noon to 12:20 pm	*Summary discussion*	
12:20 to 2:00 pm	**Lunch (served 12:40 pm to 1:40 pm)**	

Session 5 (Chaired by Mas Subramanian)		
2:00 pm to 2:20 pm	J. Mitchell (Argonne)	*1. Doping in transition metal oxides: What do we mean by 'intrinsic' behavior? 2. Synthesis by design vs. materials by design.*
2:20 pm to 2:40 pm	R. Haddon (Riverside)	*1. Electronic and magnetic phase transitions in crystals of spin-bearing organic molecules. 2. Chemical functionalization of graphene as a route to band gap engineering and to the realization of new electronic and magnetic graphene-based materials.*
2:40 pm to 3:00 pm	E. Morosan (Rice)	*1. Correlations between crystal structure and physical properties (magnetism, superconductivity). 2. Making the growth of bulk materials controllable and predictable.*
3:00 pm to 3:20 pm	S. Haile (Caltech)	*From thermochemical trends to useful properties in energy conversion and storage.*
3:20 pm to 3:40 pm	S. Jin (Wisconsin)	*1. Rational nanomaterial synthesis and crystal growth (dislocation-driven growth). 2. Strongly correlated materials with complex magnetic orderings (skyrmions and helimagnetic ordering).*
3:40 pm to 4:00 pm	*Summary discussion*	
4:00 pm to 4:20 pm	**Coffee Break**	

Session 6 (Chaired by Craig Hawker)		
4:20 pm to 4:40 pm	T. Siegrist (FSU/NHMFL)	*1. Connections between crystal growers and measurement: How do we learn to speak the same language? Examples from recent activities in iron arsenides. 2. What defines a "good" sample? Intrinsic vs. extrinsic properties.*
4:40 pm to 5:00 pm	S. Tolbert (UCLA)	*1. Nanostructured materials for charge storage. 2. Engineering strain in nanostructured materials as a route to control over materials properties.*
5:00 pm to 5:20 pm	P. S. Halasyamani (Houston)	*Structure-property relationships in functional materials and crystal growth.*
5:20 pm to 5:40 pm	M. García-Garibay (UCLA)	*Amphidynamic materials: Materials properties based on internal motion.*
5:40 pm to 6:00 pm	S. Brock (Wayne)	*Prospects for achieving the kinds of compositional complexity on the nanoscale that we routinely achieve in bulk phases: ternaries and beyond.*
6:00 pm to 7:00 pm	*Summary Discussion*	
7:00 pm	**Transport to Downtown Santa Barbara, no-host dinner**	

Saturday March 19th 2011

8:20 t o 8:40 am	**Pick up at the Best Western**
8:40 pm to 9:00 am	**Continental breakfast**

Session 7 (Chaired by Gui Bazan)		
9:00 am to 9:20 am	S. Kauzlarich (Davis)	*1. Materials quality. 2. Collaboration with physics and theory: Overcoming barriers.*
9:20 am to 9:40 am	J. Chan (LSU)	*Crystal growth and characterization of targeted structures.*
9:40 am to 10:00 am	A. Prieto (Colorado State)	*1. Developing synthetic methods that produce pure nanomaterials with control over impurities/dopants. 2. Exploiting low temperature routes toward making functional solids with the goal of integrating them into devices using inexpensive processing.*
10:00 am to 10:20 am	C. Fennie (Cornell)	*1. Theory-driven materials discovery, how do we best take advantage of close theory-experimental collaborations? 2. Designing properties and functionality verses designing materials: A theorist viewpoint.*
10:20 am to 10:40 am	M. Chabinyc (UCSB)	*1. Fundamental needs in ordering of polymers.* *2. Electronic properties and organic/hybrid materials for energy conversion.*
10:40 am to 11:00 am	**Coffee Break**	

Session 8 (Chaired by Ram Seshadri)		
11:00 am to 11:20 am	P. Feng (Riverside)	*Photocatalytic materials for solar energy applications.*
11:20 am to 11:40 am	P. Woodward (OSU)	*Spin polarized conductors and high temperature magnets.*
11:40 am to noon	C. de la Cruz (ORNL)	*1. Neutrons in the study and development of new materials.* *2. New pnictide superconductors and novel multiferroic materials.*
noon to 12:20 pm	*Summary discussion*	
12:20 pm onwards	**Lunch and departure**	

Also:

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