## 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/

Participant list, and topics.

Condensed matter experiment and crystal growth:				
Clarina de la Cruz	Oak Ridge National Laboratory	delacruzcr@ornl.gov		
1. Neutrons in the study and development of new materials. 2. New pnictide superconductors and novel multiferroic materials.				
Emilia Morosan	Rice University	emorosan@rice.edu		
1. Correlations between crystal structure and physical properties (magnetism, superconductivity). 2. Making the growth of bulk materials controllable and predictable.				
David Mandrus	University of Tennessee, Knoxville	dmandrus@utk.edu		
The indispensable role of new materials in the	The indispensable role of new materials in the advance of condensed matter physics.			
John Mitchell	Argonne National Laboratory	mitchell@anl.gov		
1. Doping in transition metal oxides: What do we mean by 'intrinsic' behavior? 2. Synthesis by design vs. materials by design				
Art Ramirez	UC Santa Cruz	apr@soe.ucsc.edu		
The NRC report.				
Theo Siegrist	Florida State University	tsiegrist@fsu.edu		
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" sampl	e? Intrinsic vs. extrinsic properties.			
Susanne Stemmer	UCSB	stemmer@mrl.ucsb.edu		
1. Novel approaches to the synthesis of highly-	perfect, high-purity oxide thin films. 2. Opportu	nities for novel transport phenomena in oxide		
heterostructures.				
	Hybrids and soft materials:			
Michael Chabinyc	UCSB	mchabinyc@engineering.ucsb.edu		
	1. Fundamental needs in ordering of polymers. 2. Electronic properties and organic/hybrid materials for energy conversion.			
Mircea Dincă	MIT	mdinca@mit.edu		
Electronic properties of porous organic-inorganic hybrids.				
Daniel Frisbie	University of Minnesota	frisbie@umn.edu		
1. New materials for printed polymer electronics. 2. A new class of gel electrolytes based on ionic liquids and block copolymers.				
Miguel Garcia-Garibay	UCLA	mgg@chem.ucla.edu		
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Robert Haddon	UC Riverside	haddon@ucr.edu		
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.				
Thuc-Quyen Nguyen	UCSB	quyen@chem.ucsb.edu		
1. Intelligent Materials Design and synthesis, and 2. Probing nanoscale properties				
Mark Thompson	University of Southern California	met@usc.edu		

		1			
Liquid crystals:					
Oleg Lavrentovich	Kent State University	olavrent@kent.edu			
	1. Functional liquid crystals by design. 2. Lyotropic Liquid Crystals. 3. Liquid Crystals far from equilibrium. 4. Soft and reconfigurable optical				
metamaterials.					
Nanomaterials:					
Shannon Boettcher	University of Oregon	swb@uoregon.edu			
Inorganic materials for solar energy conversion	Inorganic materials for solar energy conversion and storage, particularly for solar water splitting.				
Stephanie Brock	Wayne State	sbrock@chem.wayne.edu			
Prospects for achieving the kinds of compositional complexity on the nanoscale that we routinely achieve in bulk phases: ternaries and beyond.					
Kyoung-Shin Choi	Purdue	kchoi1@purdue.edu			
Shape dependent or atomic plane dependent properties: Calculations and experiments.					
Pingyun Feng	UC Riverside	pyfeng@ucr.edu			
1. Solar energy conversion using photocatalysts to produce chemical fuels (e.g. dihydrogen from water) through band-gap engineering of solid state materials. 2. Synthetic design of porous materials for energy/environment related applications such as fuel (e.g. $H_2$ , $CH_4$ ) storage, separation, and $CO_2$ sequestration.					
Song Jin	Wisconsin	jin@chem.wisc.edu			
1. Rational nanomaterial synthesis and crysta	l growth (dislocation-driven growth). 2. Strongl	y correlated materials with complex magnetic			
orderings (skyrmions and helimagnetic orderi	ng).				
Amy Prieto	Colorado State	alprieto@lamar.colostate.edu			
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.					
Sarah Tolbert	UCLA	tolbert@chem.ucla.edu			
1. Nanostructured materials for charge storage. 2. Engineering strain in nanostructured materials as a route to control over materials properties.					
Solid State Chemistry:					
Julia Chan	Louisiana State University	jchan@lsu.edu			
Crystal growth and characterization of targeted structures.					
Sossina Haile	Caltech	smhaile@caltech.edu			
From thermochemical trends to useful properties in energy conversion and storage.					
P. Shiv Halasyamani	University of Houston	psh@uh.edu			
Structure-property relationships in functional materials and crystal growth.					
Mercouri Kanatzidis	Northwestern	m-kanatzidis@northwestern.edu			
1. How do we define "materials by design"? 2. The science of synthesis versus guided serendipity.					

Susan Kauzlarich	UC Davis	smkauzlarich@ucdavis.edu		
1. Materials quality. 2. Collaboration with Physics and theory: Overcoming barriers.				
Tyrel M. McQueen	Johns Hopkins University	mcqueen@jhu.edu		
1. Synthesis of new metastable, "high-quality", strongly correlated materials. 2. Bridging the Physics-Chemistry Language and Culture Gap.				
M. A. Subramanian	Oregon State University	Mas.Subramanian@oregonstate.edu		
Exploratory synthesis in solid state chemistry: A 'scenic' route to materials by design.				
Patrick Woodward	Ohio State University	woodward@chemistry.ohio-state.edu		
Spin polarized conductors and high temperature magnets.				
Theory:				
Leon Balents	UCSB	balents@kitp.ucsb.edu		
Known unknowns and unknown unknowns: How do we (theory, experiment, and growth) search for <b>new</b> Physics in materials?				
Giulia Galli	UC Davis	gagalli@ucdavis.edu		
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?				
Craig Fennie	Cornell	fennie@cornell.edu		
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.				
Joel Moore	UC Berkeley	jemoore@berkeley.edu		
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.				
Karin Rabe	Rutgers	rabe@physics.rutgers.edu		
David Singh	Oak Ridge National Laboratory	singhdj@ornl.gov		
Interplay between materials discovery and theory.				

Also:

## **UCSB**:

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## NSF:

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