

NSF/DOE Materials Genome Initiative Principal Investigators' Meeting

Poster Session I

Monday, January 11, 2016

1. **Nicholas L. Abbott**, University of Wisconsin-Madison
Chemoresponsive Liquid Crystals Based on Metal Ion-Ligand Coordination
2. **Douglas Adamson**, University of Connecticut
Polymeric Composites and Foams Based on Two Dimensional Surfactants
3. **Rakesh Agrawal**, Purdue University
Rapid Design of Earth Abundant Inorganic Materials for Future PVs
4. **John Allison**, University of Michigan
Center for Predictive Integrated Structural Materials Science (PRISMS)
5. **Raymundo Arróyave**, Texas A&M University
Accelerating the Development of Phase-Transforming Heterogeneous Materials: Application to High Temperature Shape Memory Alloys
6. **David Baker**, University of Washington
Integrating Theory, Computation and Experiment to Robustly Design Complex Protein-Based Nanomaterials
7. **Zhenan Bao**, Stanford University
High-Throughput Morphology Prediction for Organic Solar Cells
8. **Mark Bathe**, Massachusetts Institute of Technology
Computational Design Principles for Functional DNA-Based Materials
9. **Katia Bertoldi**, Harvard University
Biologically Inspired Optimized Materials and Technologies Transformed by Evolutionary Rules (BIOMATTER)
10. **Kaushik Bhattacharya**, California Institute of Technology
Designing Microstructure for Engineering Toughness
11. **Simon Billinge**, Columbia University
Novel, Data Validated, Nanostructure Determination Methods for Accelerating Materials Discovery
12. **Geoff Brennecke**, Colorado School of Mines
Computation of Undiscovered Piezoelectrics and Linked Experiments for Design
13. **Michael Brenner**, Harvard University
Self Assembly with DNA-Labeled Colloidal Particles and DNA Nanostructures
14. **Donald Brenner**, North Carolina State University
Designing of Material-Liquid-Nanoparticle Interfaces for Tribological Control
15. **William Butler**, University of Alabama
First-Principles Based Design of Spintronic Materials and Devices

16. **Marie-Carme Calderer**, University of Minnesota – Twin Cities
Materials Engineering of Chromanic and Colloidal Liquid Crystals via Mathematical Modeling and Simulation
17. **R.W. Carpick**, University of Pennsylvania
High-Throughput Discovery, Development, and Demonstration of Material Systems to Enable Low-Power NEMS-Based Computation
18. **Michael Chabinyk**, University of California – Santa Barbara
Controlling Hierarchical Nanostructures in Conjugated Polymers
19. **Ravi Chandran**, University of Utah
Computational Design, Rapid Processing, and Characterization of Multiclass Materials from Ti-B-X Platform
20. **James Chelikowsky**, University of Texas at Austin
Design and Synthesis of Novel Magnetic Materials
21. **Hai-Ping Cheng**, University of Florida
Exploring Multi-functional Molecular Electronic Materials
22. **Peter Collins**, Iowa State University
Collaboration to Accelerate the Discovery of New Alloys for Additive Manufacturing
23. **Vincent Conticello**, Emory University
Helical Protein Assemblies by Design
24. **Michael Demkowicz**, Massachusetts Institute of Technology
Designing and Synthesizing Nano-metallic Materials that Resist Flow Localization under Mechanical Deformation
25. **Chang-Beom Eom**, University of Wisconsin – Madison
Multifunctional Interfacial Materials by Design
26. **Elif Ertekin**, University of Illinois, Urbana-Champaign
Discovery and Design of Ferromagnetic Inverse-Entropy Shape Memory Alloys by Quantum Mechanical Simulation and Experiment
27. **Amar Flood**, Indiana University
Multiscale Theory for Designing Hierarchical Organic Materials Formed by Self-Assembly
28. **David Ford**, University of Massachusetts
Synthesis of Colloidal Crystals Guided by Particle-Based Theory and Simulation
29. **Seth Fraden**, Brandeis University
Programmable Chemomechanical Materials
30. **Glenn H. Fredrickson**, University of California, Santa Barbara
Computationally Driven Discovery and Engineering of Multiblock Polymer Nanostructures Using Genetic Algorithms
31. **C.M. Friend**, Harvard University
High-Throughput Computation and Machine Learning for Understanding and Designing Catalysts
32. **Laura Gagliardi**, University of Minnesota
Inorganometallic Catalyst Design Center

33. **William Goddard**, California Institute of Technology
Multiscale Theory and Experiment in Search for and Synthesis of Novel Nanostructured Phases in BCN Systems
34. **Jeffrey Greeley**, Purdue University
Design of Multifunctional Catalytic Interfaces from First Principles
35. **Francois Gygi**, University of California, Davis
High-Performance First-Principles Molecular Dynamics for Predictive Theory and Modeling
36. **Ronald Hedden**, Texas Tech University
Combinatorial Methods to Enable Rapid Prototyping of Polymeric Pervaporation Membranes for Bio-alcohol Recovery
37. **Hendrik Heinz**, University of Colorado, Boulder
Design and Testing of Nanoalloy Catalysts in 3D Atomic Resolution
38. **Clifford Henderson**, Georgia Institute of Technology
Rapid Design and Engineering of Materials Systems for Nanomanufacturing via Directed Self-Assembly
39. **Graeme Henkelman**, University of Texas, Austin
Toolkit to Characterize and Design Bi-functional Nanoparticle Catalysts
40. **John Herbert**, The Ohio State University
Fragment-Based Quantum Chemistry for Non-Covalent Interactions and Excitation Energy Transfer
41. **Andreas Heyden**, University of South Carolina, Columbia
Design and Discovery of Multimetallic Heterogeneous Catalysts for a Future Biorefining Industry
42. **Elizabeth Holm**, Carnegie Mellon University
Mechanics of Three-dimensional Carbon Nanotube Aerogels with Tunable Junctions
43. **Kendall N. Houk**, University of California, Los Angeles
Iterative Theoretical Morphology Prediction, Synthesis, and Characterization of Novel Donor Oligomer for Accelerated OPV Materials
44. **Robert Hull**, Rensselaer Polytechnic Institute
Real Time Control of Grain Growth in Metals
45. **Michael Janik**, Pennsylvania State University
Computationally Guided Design of Multicomponent Materials for Electrocatalytic Cascade Reactions
46. **Debdeep Jena**, Cornell University
Extreme Bandgap Semiconductors
47. **Jeremiah Johnson**, Massachusetts Institute of Technology
Analysis and Optimization of Polymer Networks for Emerging Applications
48. **Peter Johnson**, Brookhaven National Laboratory
Center for Emergent Superconductivity: Designing New Correlated Electron Systems
49. **Tresa Pollock**, University of California, Santa Barbara
Accelerating the Design and Synthesis of Multicomponent, Multiphase Metallic Single Crystals
50. **Yunzhi Wang**, The Ohio State University
Accelerated Development of Next Generation Ti Alloys by ICMSE Exploitation of Non-Conventional Transformation Pathways

NSF/DOE Materials Genome Initiative Principal Investigators' Meeting

Poster Session II

Tuesday, January 12, 2016

1. **Yung Joon Jung**, Northeastern University
Engineering Strong, Highly Conductive Nanotube Fibers via Fusion
2. **Kathleen Kash**, Case Western Reserve University
Heterovalent Ternary Nitride Semiconductors and Mixed Ternary-Binary Heterostructures
3. **Chandler Becker**, NIST
The NIST Materials Resource Registry as a Platform to Improve Data Discoverability
4. **John Kieffer**, University of Michigan, Ann Arbor
Simulation-Based Predictive Design of All-Organic Phosphorescent Light-Emitting Molecular Materials
5. **Paul R. C. Kent**, Oak Ridge National Laboratory
Network for Ab Initio Many-Body Methods
6. **Stephen Klippenstein**, Argonne National Laboratory
An Ab Initio Transition-State-Theory-Based Master Equation Code for Elementary Kinetics
7. **Irena Knezevic**, University of Wisconsin, Madison
Coupling Electrons, Phonons, and Photons for Nonequilibrium Transport Simulation
8. **Sanat Kumar**, Columbia University
Modeling and Inverse Design of Anisotropic DNA-Mediated Colloidal Self-Assembly
9. **Robert Kohn**, New York University
Adaptive Fine-Scale Structure Design: From Theory to Fabrication
10. **Enrique Lavernia**, University of California, Davis
Engineering Strength and Toughness into HCP Metals Using Twin Meshes
11. **James Lewis**, West Virginia University
Designing Tunable Au-Based Bimetallic Nanocatalysts
12. **Patrick Mather**, Syracuse University
Laminated Elastomer Composites with Anisotropic Shape Memory
13. **Paul McEuen**, Cornell University
Graphene Based Origami and Kirigami Metamaterials
14. **Efstathios Meletis**, University of Texas – Arlington
Multiscale Design of Hard and High Temperature Resistant Coatings by Computation and Experiment.
15. **Thomas Miller**, California Institute of Technology
Next-Generation Nanostructured Polymer Electrolytes by Molecular Design

16. **Michael Mills**, The Ohio State University
Mechanistic and Microstructure-Based Design Approach for Rapid Prototyping of Superalloys
17. **Tim Mueller**, Johns Hopkins University
Design of Nanoscale Alloy Catalysts from First Principles
18. **Sankar Nair**, Georgia Institute of Technology
Accelerating the Discovery and Development of Nanoporous 2D Materials (N2DMs) and Membranes for Advanced Separations
19. **Jens Nørskov**, SLAC National Accelerator Laboratory, Stanford University
Predictive Theory of Transition Metal Oxide Catalysis
20. **Elsa Olivetti**, Massachusetts Institute of Technology
Data Mining and Analytics for Predictive Synthesis, Accelerating Realization of Advanced Materials
21. **Shyue Ping Ong**, University of California, San Diego
Design of Novel Sodium Superionic Conductors using Integrated High-Throughput First Principles Calculations, Data Mining and Experiments
22. **Greg Payne**, University of Maryland
Thin Film Biofabrication for Integrated Bio-electronics
23. **John P. Perdew**, Temple University
SCAN+rVV10: A Promising Density Functional for Layered Materials
24. **John H. Perepezko**, University of Wisconsin, Madison
A Combined Experiment and Simulation Approach to the Design of New Bulk Metallic Glasses
25. **Warren Pickett**, University of California, Davis
Discovering Insulating Topological Insulators
26. **Darrin Pochan**, University of Delaware
Programmable Peptide-Based Hybrid Materials
27. **Thomas Proffen**, Oak Ridge National Laboratory
Center for Accelerating Materials Modeling from SNS Data
28. **Karin Rabe**, Rutgers University
High-Throughput Mapping of Functional Dielectric/Metallic Heterostructures
29. **Aldo Humberto Romero**, West Virginia University
Search for Magneto-electronic Behavior in Complex Fluoride-based Interfaces
30. **Sapna Sarupria**, Clemson University
An Integrated Multiscale Modeling and Experimental Approach to Design Fouling-Resistant Membranes
31. **Darrell Schlom**, Cornell University
Closing the Loop to Make the World's Strongest Ferromagnetic Ferroelectric
32. **Jan Schroers**, Yale University
High-Throughput Simulations and Experiments to Develop Metallic Glasses
33. **Sergei Sheiko**, University of North Carolina, Chapel Hill
Acoustically Transformative Materials

34. **Joern Ilja Siepmann**, University of Minnesota
Nanoporous Materials Genome: Methods and Software to Optimize Gas Storage, Separation, and Catalysis
35. **Randall Snurr**, Northwestern University
Simulation-Driven Design of Highly Efficient MOF/Nanoparticle Hybrid Catalyst Materials
36. **Volker Sorger**, The George Washington University
Theory-Enabled Development of 2D Metal Dichalcogenides as Active Elements of On-Chip Silicon-Integrated Optical Communication
37. **Frank Spano**, Temple University
Developing Design Rules for Enhancing Mobility in Conjugated Polymers
38. **Eric Toberer**, Colorado School of Mines
Computationally Driven Targeting of Advanced Thermoelectric Materials
39. **Zachary Trautt**, NIST
Facilitating the Development of Modular Data Models in Materials Science
40. **Mark Tuckerman**, New York University
Development of Design Rules for High Hydroxide Transport in Polymer Architectures
41. **Yasutomo Uemura**, Columbia University
Designing, Understanding and Functionalizing Novel Superconductors and Magnetic Derivatives
42. **Chris Van de Walle**, University of California, Santa Barbara
Design and Fabrication of Wide-Band-Gap Nitride-Based Alloys
43. **Anton Van der Ven**, University of California, Santa Barbara
Integrated Computational Framework for Designing Dynamically Controlled Alloy-Oxide Heterostructures
44. **David Vanderbilt**, Rutgers University
Enhanced Functionalities in 5d Transition-Metal Compounds from Large Spin-Orbit Coupling
45. **Michael Weinert**, University of Wisconsin, Milwaukee
Emergent Functionalities at the Epitaxial Interfaces of Correlated and Spin-Orbit Materials
46. **Steven White**, University of California, Irvine
Speeding Up Strongly Correlated Calculations: Wavelet Coarse Graining and Machine-Learned Density Functionals
47. **Lian Yu**, University of Wisconsin, Madison
Engineering Organic Glasses
48. **Ji-Cheng Zhao**, The Ohio State University
Design Knowledge Base of Low-Modulus Titanium Alloys for Biomedical Applications
49. **Alex Zunger**, University of Colorado – Boulder
Theory-Guided Experiments in Search of Designed Topological Insulators and Band-Inverted Insulators
50. **William Tumas**, NREL
Center for Next Generation of Materials by Design