EFRC: CENTER FOR NEXT GENERATION OF MATERIALS BY DESIGN (CNGMD)

UPDATED: OCTOBER 2016

AWARDS: $14M (August 2014 – July 2018)

WEBSITES: http://www.energyfrontier.us/efrc/cngmd; http://www.cngmd-efrc.org/

TEAM: **National Renewable Energy Laboratory (Lead):** William Tumas (Director), John Perkins (Program Integrator), Dave Ginley (Chief Experimentalist), Stephan Lany, Andriy Zakutayev; **Lawrence Berkeley National Laboratory**: Gerbrand Ceder (Chief Theorist), Kristin Persson; **SLAC National Accelerator Laboratory:** Michael Toney; **Oregon State University:** Janet Tate; **Harvard University:** Daniel Nocera, Roy Gordon; **Colorado School of Mines:** Vladan Stevanovic, Brian Gorman; **Massachusetts Institution of Technology:** Alexie Kolpak, Tonio Buonassisi

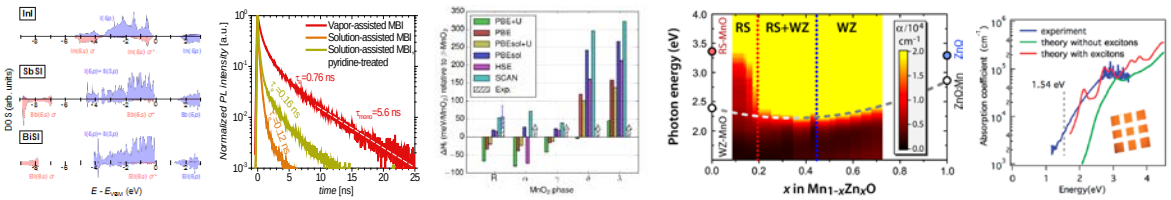
SCIENTIFIC MISSION AND APPROACH

The *vision* of the Center for Next Generation of Materials by Design (CNGMD) is to *dramatically transform the discovery of functional energy materials through multiple-property search, incorporation of metastable materials into predictive design, and the development of specific theory to guide materials synthesis.* The center integrates predictive theory with state-of-the-art high-throughput and directed synthesis and characterization including novel *in-situ* methods to understand and predict structure, properties, and phenomena at the molecular, nano, and meso scales. The focus is on semiconductor materials for renewable energy and energy efficiency applications including solar energy conversion, solid-state lighting, solar fuel production and piezoelectrics. Current research projects are:

1) **Pnictide Search** explores new metal nitrides to discover new functional semiconductor materials.
2) **Polymorphs and Synthesizability** aims to understand energy landscapes and identify synthetic pathways for specific polymorphs. The focus is on Mn, V and Ti oxides.
3) **Chalcogenide Alloys** predicts and guides synthesis of new functional semiconductor alloy materials.
4) **Defect Phase Diagrams** derives the defect energies and phase diagram to guide the synthesis of defect-functionalized materials.
5) **Perovskite-Inspired Materials Search** designs new materials based on the electronic features of defect tolerance and long carrier lifetimes observed in hybrid organic-inorganic halide perovskites.
6) **Piezoelectric Materials Search**, a new project started in 2016, is developing Pb-free piezoelectric materials, including new theoretically predicted metastable materials.

SELECTED SCIENTIFIC ACCOMPLISHMENTS

- Identified 9 promising materials classes for high defect tolerance based on features of hybrid organic/inorganic perovskites and experimentally showed 5 new materials have desired properties.
- Predicted a number of new nitride materials through theory. Using an activated N source, successfully synthesized metastable binary and ternary nitrides including new binary SnN.
- Predicted and experimentally validated qualitatively new phase diagrams for heterostructural alloys in the MnZnO and SnCaS systems.
- Developed first-principles approaches to predict polymorph stabilities and distributions.
- Predicted and experimentally verified new functionalities in metastable heterostructural alloys compared to isostructural alloys.
- Developed defect phase diagrams to address complex metastable defects and applied to effective electronic doping of Ga_2O_3 with potential applications for wide bandgap electronics.



CNGMD research, from left: Calculated electronic structure of perovskite-inspired PV absorbers; Photo-excited carrier life time measurements for $MA_3Bi_2I_9$; Computed and experimental formation energies of MnO_2 polymorphs; Measured absorption coefficient and calculated band gaps for MnZnO alloys; Calculated and measured optical absorption of metastable Sn_3N_4.

IMPACT

- *Impact on Materials Genome Initiative (MGI):* CNGMD work on *Perovskite-Inspired Materials* to identify and test promising, non-toxic alternatives to perovskite solar materials called out by White House in *The First Five Years of the Materials Genome Initiative: Accomplishments and Technical Highlights.* CNGMD developed methods being used for applied MGI research including Solar Energy Institute of India and US (http://www.seriius.org), the NIST-led High-Throughput Experimental Materials Science Virtual Laboratory (https://mgi.nist.gov) and several emerging DOE Energy Materials Network consortia (e.g. HydroGEN, Duramat).
- *Outreach, Education and Training:* Organized 2016 Spring MRS symposium "Materials, Interfaces and Devices by Design". Three CNGMD PI's were instructors for the associated tutorial attended by 100+ people. Two CNGMD PI's were lecturers at the International School for Materials for Energy & Sustainability IV (2015) and V (2016). More than 30 invited talks presented by CNGMD scientists. Currently, 13 graduate students and 13 post-docs are working with CNGMD.
- *Publically Released Research Tools and Data: Substrate Picker*, a CNGMD developed tool to guide substrate selection for targeted materials synthesis is now available via the Materials Project (https://materialsproject.org). Results of CNGMD first-principles material property calculations are available through NREL MatDB (http://materials.nrel.gov) and the Materials Project. New *in-situ* experimental tools developed at SLAC now available for general use.

PUBLICATIONS AND INTELLECTUAL PROPERTY

As of October 2016, CNGMD had published 20 peer-reviewed publications cited over 130 times and filed 1 US patent application. The following is a selection of impactful papers:

- Sun, W., Dacek, S.T., Ong, S.P., Hautier, G., Jain, A., Richards, W.D., Gamst, A.C., Persson, K.A., Ceder G., The thermodynamic scale of inorganic crystalline metastability, *Science Advances,* **2**, e1600225, 10.1126/sciadv.1600225 (2016). [**0 citations**].
- Peng, H., Ndione, P. F., Ginley, D. S., Zakutayev, A. & Lany, S. Design of semiconducting tetrahedral $Mn_{1-x}Zn_xO$ alloys and their application to solar water splitting. *Physical Review X*, **5**, 021016, doi:10.1103/PhysRevX.5.021016 (2015). [**12 citations**]
- Brandt, R. E., Stevanovic, V., Ginley, D. S. & Buonassisi, T. Identifying defect-tolerant semiconductors with high minority-carrier lifetimes: beyond hybrid lead halide perovskites. *MRS Communications*, **5**, 265, doi:10.1557/mrc.2015.26 (2015). [**44 citations**]
- Brandt, R. E., Kurchin, R.C., Hoye, R.L.Z. *et al.* Investigation of bismuth triiodide (BiI_3) for photovoltaic applications, *J. Phys. Chem. Lett.,* **6**, 4279, doi:10.1021/acs.jpclett.5b02022 (2015). [**11 citations**]
- Huynh, M., Shi, C., Billinge, S. J. L. & and Nocera, D. G. Nature of Activated Manganese Oxide for Oxygen Evolution. *J. American Chemical Society*, **137**, 14887, doi:10.1021/jacs.5b06382 (2015). [**20 citations**]
- Kitchaev, D. A., Peng, H., Liu, Y., Sun, J., Perdew, J. P. & Ceder, G. Energetics of MnO_2 polymorphs in density functional theory. *Physical Review B*, **93**, 045132, doi:10.1103/PhysRevB.93.045132 (2016). [**5 citations**]
- Ding, H., Dwaraknath, S., Garten, L., Ginley, D. S. & Persson, K. A. Computational approach for epitaxial polymorph stabilization through substrate selection. *ACS Applied Materials and Interfaces,* **8**, 13086, doi:10.1021/acsami.6b01630 (2016). [**2 citations**]