We are a multidisciplinary theory and computation group working at the intersection of physics, chemistry, and materials science. We interact closely with experimental groups to guide and be inspired by studies of new materials and phenomena in the context of nanoscience and renewable energy applications, and to validate and further develop our understanding of condensed phase systems. More »

We are part of the Theory of Nanostructured Materials Facility of the Molecular Foundry, a DOE nanoscience center at Lawrence Berkeley National Laboratory. Free access to our computational tools and expertise is available through the Molecular Foundry User Program.

**RESEARCH HIGHLIGHTS**

**Metal-Organic Frameworks for Small Molecule Adsorption**  
Florian Brown-Altvater posted on Apr 11, 2014

Predicted adsorption behavior of small molecules at open-metal sites in MOF-74 variants provides insight into gas storage and separation properties of nanoporous materials.

**WHAT'S NEW**

**Charge- and spin-transport in porphyrin-based molecular junctions**  
Florian Brown-Altvater posted on Feb 07, 2014

Sinead Majella Griffin posted on May 09, 2016

09.05.16
Self-energy corrected DFT calculation of spin-dependent transport, within non-equilibrium Green's function (NEGF) framework.

Complex Oxides for Solar Energy Conversion

2015-05-12
Alison Hatt posted on May 03, 2012
SrTiO₃ may be engineered for more efficient absorption of solar energy.

Metal-Organic Frameworks for Carbon Capture

10.4.15
Ligand choice can enhance carbon dioxide’s ability to bind to MOFs by a factor of 2 to 3, yielding clues for making better carbon-capture systems.

Congratulations to Josh Howe, who finished his PhD and is already off to Georgia Tech for a postdoc position.

Congratulations to Michele Kotluga who completed her PhD and has just started a postdoc at Rutgers. Best wishes Michele!

Welcome to Sinead Griffin, who recently joined our lab as postdoc!

Long overdue update: Congratulations to Peter Doak, who finished his PhD at the end of last year, and now has a postdoc position at Oak Ridge National Laboratory. Kyuho Lee accepted a position as Senior R&D Engineer at Synopsys for Media Tablet and TV. Warm welcome to Linn Leppert who recently joined the Neaton group as postdoc!
Visualizing optical excitations in a pentacene crystal reveals a delocalized exciton wavefunction with charge transfer character.

Sahar Sharifzadeh started her new job as assistant professor at Boston University. Best of luck, Sahar. We will miss you!


