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.

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

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Research Archives >

WHAT'S NEW

2016 05 09
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
Alison Hatt
posted on May 03, 2012

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.
Visualizing optical excitations in a pentacene crystal reveals a delocalized exciton wavefunction with charge transfer character.

2019 15 PRM Leppert
Elizabeth Peterson posted on Dec 05, 2019

2019 14 PRL Schuler
Elizabeth Peterson posted on Sep 06, 2019

2019 13 ACS Nano Schuler
Elizabeth Peterson posted on Sep 06, 2019

2019 12 Nat Commun Barja
Elizabeth Peterson posted on Sep 06, 2019

Abstract


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