University of Minnesota
Driven to Discover℠

Department of Chemistry

Special Seminar

9:45 a.m. Thursday, March 14, 2013 • 331 Smith Hall

Assistant Professor

Geoffrey Hutchison

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University of Pittsburgh

Rational Design of Molecular Materials: Molecular Springs, Solar Cells & More

Research interests focus on building electronic materials from molecular subunits, both organic and inorganic, using a variety of techniques to rationally design the desired properties. This encompasses chemical synthesis, characterization (both physical and chemical), combined with theoretical modeling and simulation.
Website: http://www.chem.pitt.edu/people/faculty/geoffrey-hutchison

Abstract

Present social and economic demands on energy sources are driving fundamental science and engineering research into alternative energy technologies. Our research focuses on combined experimental and efficient computational exploration of organic photovoltaics and piezoelectrics. We seek to find optimum or nearly-optimum materials properties through a combination of inverse design, genetic algorithms, and automated electronic structure calculations, combined with experimental synthesis and verification. With polymer solar cells, we have used a multi-objective genetic algorithm to uncover new design rules for highly-efficient targets. We also explore the charge transport in realistic, imperfect organic semiconductors to find design rules connecting nanoscale morphology with predicted current-voltage response. In piezoelectric materials, we have pioneered a new approach, using conformational distortions of individual molecules in an applied electric field to drive a “bottom-up” distortion, with greater piezoresponse than many conventional inorganics.

Host: Professor Aaron Massari