Physics Colloquium

Thursday, February 6, 2020 at 4:25pm in LL. 316

"Importance of Disorder in Experimentally Relevant Models"

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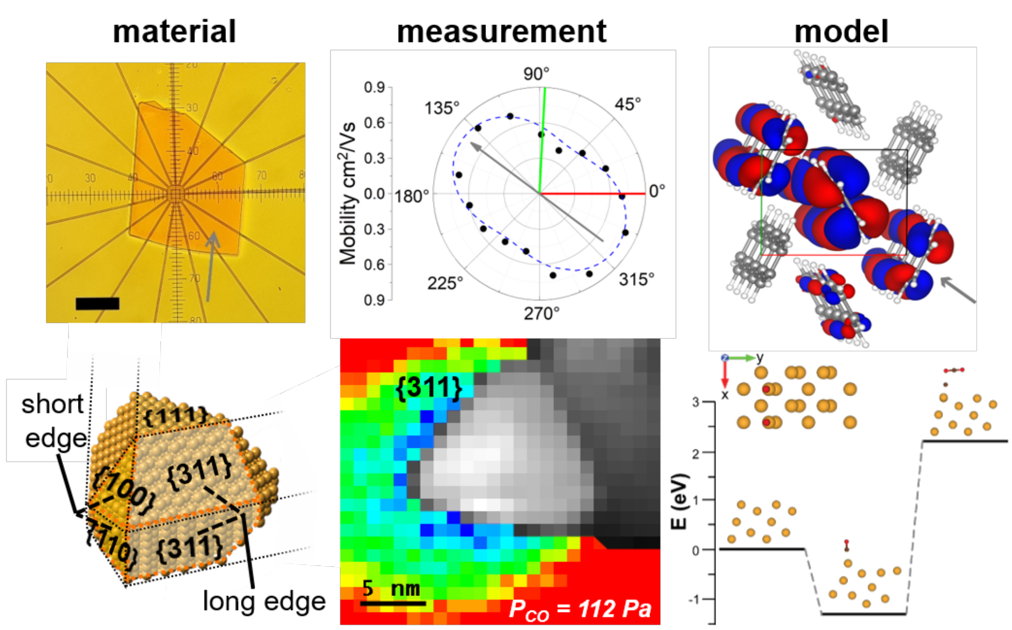
With limited natural resources and a growing global population, new materials that lower our energy consumption and its cost are critical. Understanding the fundamental properties of materials that combine to provide desired performance is essential to predicting new materials for a given application. To this end, the fundamental processes that drive electronic materials, for applications like photovoltaics, transistors, light-emitting diodes, photosynthesis, water-splitting, catalysis, and batteries, can be understood in terms of fundamental excitation, oxidation, reduction, energy transfer, electron or hole transfer or transport. Quantum chemical tools allow us to study these processes in terms of geometric and electronic changes in a system.

Focusing on the development of models at the interface of experiment and theory, we use quantum chemistry to interrogate the chemical physics of materials and improve fundamental understanding of structure-function relationships in a range of electronic, energy harvesting, and catalytic processes. Combining molecular and materials perspectives, we seek to uncover insights into the fundamental properties of a broad range of atomic to nanoscale materials and build computational models that are both descriptive and predictive. In this talk I will describe our recent efforts to develop models of the effect of inherent molecular vibrations on transport in tetracene single crystals as well as light-driven reactions on faceted gold particles.



Lisa Fredin earned a doctorate in chemistry at Northwestern University, and a bachelor's in chemistry, biochemistry and applied mathematics (minor in computer science) at the University of Texas at Austin. Before coming to Lehigh, Fredin served as a research chemist at the National Institute of Standards and Technology in Gaithersburg, Maryland. Her research draws on her background combining experiment and theory to develop computational and theoretical models of fundamental electronic properties to design materials with targeted properties. The Fredin group develops models of the chemistry and physics of a broad range of disordered materials, bridging physical chemistry, material science, nanoscience, and computation; as well as, probing the boundaries of the particle and wave approximations of electrons in materials.