School of Natural Sciences
Physics Colloquium Series

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Computational Simulations of Solar-Energy Materials: Amorphous Silicon and Solar Thermal Fuels

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Abstract:

Computational theory has an important role to play in increasing our understanding of current materials and enabling rational design of new materials. Building on recent advances in theoretical formalisms, algorithms, and code development for high-performance computing, we can bring to bear a toolbox of first-principles methods such as density-functional theory (DFT), its time-dependent form (TDDFT), and the GW/Bethe-Salpeter (BSE) approach. I will present two examples of work for solar-energy applications.

(1) Hydrogenated amorphous silicon (a-Si:H), is useful for photovoltaics and a good model system for amorphous materials. In a joint theoretical/experimental study, we found the changes of Raman spectra under stress, which can be used to characterize devices, and used the results to create a multiscale model for complex Si materials.

(2) Solar thermal fuels (STFs) are an unconventional paradigm for integrated solar-energy conversion and storage. A material absorbs sunlight and stores the energy chemically via an induced structural change, which can later be reversed to release the energy as heat. We developed and implemented a new efficient approach for forces in the excited state to study the dynamics after light absorption for prototype STF molecules.

Bio

David Strubbe received his bachelor's degree in physics and chemistry from the University of Chicago, and Ph.D. from the University of California, Berkeley in 2012 in physics with designated emphasis in nanoscale science and engineering. His thesis in condensed-matter theory, advised by Professor Steven Louie, focused on methods and applications for calculations of optical and transport properties of organic molecules. As a postdoctoral researcher, he studied materials for solar energy in the group of Professor Jeffrey Grossman in the Department of Materials Science and Engineering at the Massachusetts Institute of Technology. He began this summer as assistant professor of physics at UC Merced.