Condensed Matter / Biophysics Seminar

Predictive modeling of quantum processes in materials for energy

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4:00 P.M.

Rm 184 NSH

Quantum phenomena play an important role in the operation of modern electronic and optoelectronic devices. Predictive quantum calculations based on density functional theory can be applied to understand and design the properties of materials for new types of devices for energy applications. In this talk, I will show how predictive calculations of nonradiative Auger recombination in nitride materials were able to resolve the mystery of the reduced efficiency of blue LEDs at high power. Moreover, I will discuss how quantum confinement in ultrathin nitride nanostructures enables new types of visible and deep ultraviolet light-emitting devices. I will also show how calculations can predict the energy conversion efficiency of thermoelectric materials at high temperature for waste-heat recovery. Last, I will present results for the phonon-assisted absorption of visible light in silicon, which allows the operation of commercial silicon solar cells, and how light absorption in silicon can be improved by nanostructuring. These results highlight the impact of predictive modeling of quantum phenomena for the design of efficient materials for energy applications.

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