Ultrafast Dynamics of Excited Electrons in Semiconductors and Metals for Energy Applications

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How does an excited electron lose its energy? This problem is central in fields ranging from condensed matter physics to electrical engineering and energy. Recently, we developed and applied calculations to study the dynamics of out-of-equilibrium charge carriers – also known as hot carriers – in semiconductors and metals. I will present *ab initio* calculations of electron-phonon, electron-electron, and electron-defect scattering rates that are able to predict the relaxation times and mean free paths of hot carriers in materials.

The talk will discuss application of this framework to three problems: 1) Energy dissipation and hot carrier dynamics in the first picosecond after sunlight absorption in silicon. 2) Hot carrier scattering in GaAs, for which our results contribute to resolve experimental controversies and challenge the common notion that optical lattice vibrations are mainly responsible for hot carrier energy loss. 3) Hot carriers generated by surface plasmon polaritons in noble metals, a process of relevance in optoelectronics, photocatalysis, and photovoltaics, for which our results prescribe optimal conditions for hot carrier generation and extraction, and pave the way to accurate calculations of plasmonic losses in materials.

Taken together, the computational approach presented in this talk shines light on microscopic processes that are hard to capture both with experiments and calculations, and opens new avenues to compute excited electron dynamics in materials.