CFEL SCIENCE

SEMINAR

November 25, 2015 - 2:00 p.m.

CFEL-bldg. 99, seminar room IV

Marco Bernardi

Caltech

Ultrafast Dynamics of Excited Electrons in Materials for Energy Applications

How does an excited electron lose its energy? This problem is central in fields ranging from condensed matter physics to electrical engineering and energy. The talk will discuss calculations of the dynamics of out-of-equilibrium charge carriers – also known as hot carriers (HCs) – in semiconductors and metals [1–3]. We will focus on first-principles calculations of electron-phonon, electron-electron, and electron-defect scattering that can predict the relaxation times and mean free paths of HCs in materials. This framework is applied to: 1) HC thermalization in the first picosecond after sunlight absorption in silicon. 2) HCs in GaAs, for which our results contribute to resolve experimental controversies and challenge the tenet that optical lattice vibrations are mainly responsible for energy loss. 3) HCs generated by surface plasmons in noble metals, a process of relevance in optoelectronics and photocatalysis, for which we predict optimal conditions for HC generation and extraction.

We will show how the concepts introduced in the talk can be extended to model electron transport and radiative recombination [4] from first principles. The talk will conclude with an outlook of the challenges to compute electron dynamics from first principles.

[1] M. Bernardi et al., *Phys. Rev.Lett.* 112, 257402 (2014).

[2] M. Bernardi et al., *PNAS.* 112, 5291 (2015).

[3] M. Bernardi et al., *Nature Commun.* 6:7044 (2015).

[4] M. Palummo, M. Bernardi, and J. C. Grossman, *Nano Lett.* 15, 2794 (2015).

Host: Angel Rubio – MPSD-CFEL Theory Department