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The First Picosecond after Sunlight Absorption in Si, GaAs, and CdTe from First-Principles Calculations MARCO BERNARDI, JEFFREY B. NEATON, Lawrence Berkeley Natl Lab, STEVEN G. LOUIE, University of California Berkeley — Sunlight absorption in semiconducting materials generates out-of-equilibrium electron populations – also known as hot carriers – relaxing towards equilibrium through a host of scattering processes at the subpicosecond time scale. While such dissipation processes typically result in the loss of more than half of the energy associated with the absorbed sunlight, a microscopic understanding of this ultrafast regime is still missing. In this talk, we provide a detailed picture of the first picosecond after sunlight absorption in semiconductors of wide use in photovoltaics (PV) such as Si, GaAs, and CdTe. Our results are based on ab initio calculations combining density functional theory and the GW plus Bethe-Salpeter Equation (GW-BSE) approach together with electron-phonon interactions. We computed the lifetimes and k-space dependence of electron-electron and electron-phonon scattering events responsible for ultrafast solar energy dissipation. Using this information, we simulated the ultrafast dynamics of hot carriers using an empirical-parameter-free formulation of the Boltzmann equation. A clear understanding of hot carrier dynamics emerges for several materials of interest in PV, and novel engineering paradigms are suggested.

Marco Bernardi
Lawrence Berkeley Natl Lab

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