

**The Department of
Mechanical Engineering**
PRESENTS

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Winston Chung Hall 205/206
11:10-12:00PM

**Advances in Computing Charge Carrier Dynamics
in Materials from First Principles**

Abstract:

Calculations of charge transport and ultrafast dynamics have relied on heuristic approaches for the past several decades. Recent progress in combining density functional theory and related methods with kinetic equations, such as the Boltzmann transport equation (BTE), are enabling spectacular advances in computing carrier dynamics in materials from first principles. A special role is played by the interaction between charge carriers and lattice vibrations, also known as the electron-phonon (e-ph) interaction, which dominates carrier dynamics near room temperature and at energies within a few eV of the band gap. We will discuss our recently developed methods to compute e-ph scattering processes, and show how these developments enable accurate calculations of charge transport and ultrafast dynamics in materials, including:

- 1) Accurate calculations of the electron mobility, leading to new insight into charge transport in polar semiconductors [1], perovskite oxides, and organic materials [2]. We will also touch briefly on the computation of spin lifetimes.
- 2) The ultrafast dynamics of excited (so-called “hot”) carriers, with application to ultrafast spectroscopy and optoelectronics. A new parallel algorithm to propagate in time the BTE for excited electrons [2] and coupled electrons and phonons will also be presented. We will outline code development efforts, open problems and future directions.

Biosketch:

Marco Bernardi is Assistant Professor in the Department of Applied Physics and Materials Science at Caltech since Sept. 2015. He specializes in computational materials science and condensed matter theory. Marco obtained his Ph.D. in Materials Science from MIT, where he worked with Prof. Jeff Grossman on novel materials and physical processes for solar energy conversion. He was a postdoc in the Physics Department at UC Berkeley, where he worked with Prof. Steve Louie and Prof. Jeff Neaton on excited electrons in materials. His group at Caltech focuses on computing the dynamics of electrons and excited states in materials, with applications to electronics, optoelectronics, energy and ultrafast science. Marco received the NSF CAREER Award in 2018, the AFOSR Young Investigator Award in 2017, the Psi-K Volker Heine Young Investigator Award for electronic structure calculations in 2015, and the Intel Ph.D. Fellowship from Intel in 2013, among other awards. His research has been featured in several magazines and media outlets, including Nature, Scientific American, Wired and Technology Review.