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Advances in Computing Charge Carrier Dynamics from First Principles

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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 at room temperature and for carrier energies within a few eV of the band edges.
We will discuss our recently developed methods to compute and interpolate e-ph scattering processes on ultra-fine Brillouin zone grids, and then show how these developments enable new computations of charge transport and ultrafast dynamics, including:
1) Accurate calculations of the carrier mobility in polar semiconductors [1] and oxides, including new methods to treat complex materials with structural phase transitions (e.g., perovskites) and new insight into charge transport in organic molecules.
2) The ultrafast dynamics and detailed scattering mechanisms of excited (so-called "hot") carriers. We will discuss the application of this framework to solar energy conversion, the interpretation of ultrafast spectroscopy results, and open problems in gallium nitride light emission technologies. A new parallel algorithm to propagate in time the BTE [2] will be introduced.

BIO:

[1] J.-J. Zhou and M. Bernardi Phys. Rev. B (Rapid Commun.) 94, 201201 (2016).
[2] V. Jhalani, J.-J. Zhou and M. Bernardi Nano Letters 17, 5012 (2017).

Marco Bernardi is Assistant Professor in the Department of Applied Physics and Materials Science at Caltech since September 2015. He specializes in theoretical / computational materials science and condensed matter physics. Marco holds a B.S. from the University of Rome "La Sapienza", and a M.S. in Materials Science from the University of Rome "Tor Vergata" in Italy. He obtained his Ph.D. in Materials Science from MIT, where he worked with Prof. Jeff Grossman on novel materials and physical processes in 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 transport and ultrafast dynamics of electrons and excited states in materials, with applications to energy conversion, novel electronics and optoelectronics, and ultrafast spectroscopy.

Marco has received a number of awards, including the 2015 Psi-K Volker Heine Young Investigator Award for electronic structure calculations, the Intel Ph.D. Fellowship from Intel, and the Endeavour Research Fellowship from the Australian Government, among others. His research has been featured in a number of magazines, including Wired, Nature, Scientific American, and Technology Review.