UIC COLLOQUIUM
Department of Physics

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"*Electron Dynamics in Materials from First Principles*"

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Recent progress in combining density functional theory and related methods with the Boltzmann transport equation are enabling spectacular advances in computing electron dynamics in materials from first principles. The interaction between electrons and lattice vibrations (phonons) plays a central role as it governs carrier dynamics near room temperature and at low energy. I will present our recently developed methods to compute electron-phonon scattering processes from first principles, and show how these advances enable calculations of charge transport and ultrafast dynamics in materials, including:

1) First-principles calculations of the carrier mobility, providing new insight into the mechanisms governing charge transport in semiconductors [1,2] and oxides [3,4]. I will discuss various challenges, including treating materials with polar bonds, structural phase transitions, strong electron-phonon interactions leading to polaron formation, spin-orbit coupling [5], and crystallographic defects.

2) Accurate simulations of the ultrafast dynamics of materials out of equilibrium, with application to ultrafast spectroscopy and optoelectronics [6]. We will focus on a recently developed approach to propagate in time the Boltzmann equation for coupled nonequilibrium electrons and phonons, and its application to 2D materials. We will outline our efforts to develop an open source code, PERTURBO [7], to make these new computational methods and workflows available to the community.

[1] J.-J. Zhou and M. Bernardi Phys. Rev. B (Rapid Commun.) 94, 201201 (2016)
[2] N.-E. Lee, J.-J. Zhou, L. Agapito and M. Bernardi Phys. Rev. B 97, 115203 (2018)
[3] J.-J. Zhou, O. Hellman and M. Bernardi Phys. Rev. Lett. 121, 226603 (2018)
[4] J.-J. Zhou and M. Bernardi Phys. Rev. Research 1, 033138 (2019)
[5] J. Park, J.-J. Zhou and M. Bernardi Phys. Rev. B 101, 045202 (2020)
[6] V. Jhalani, J.-J. Zhou and M. Bernardi Nano Lett. 17, 5012 (2017)
[7] J.-J. Zhou, J. Park, I.-T. Lu, I. Maliyov and M. Bernardi arXiv 2002.02045

To join this colloquium, please go to:
https://uic.zoom.us/j/88270605693?pwd=RzRrUkVJVnhnbVE4SDNJWmVRWlNOQT09

The Department of Physics Colloquium will be held via Zoom.