Electron-Phonon Interaction with Wannier Functions

Feliciano Giustino[†]

Department of Physics, University of California at Berkeley, Berkeley, California 94720, USA, and Materials Sciences Division, Lawrence Berkeley National Laboratory, Berkeley, California 94720, USA

The electron-phonon interaction plays a central role in a variety of phenomena, including for example electrical resistivity, superconductivity, Peirls instability, and polaronic transport in conducting polymers. Despite the continued interest in the electron-phonon problem, modern first-principles calculations are still limited to simple bulk systems with a few atoms per unit cell, and only sporadic attempts have been made to address complex materials such as nanostructures or doped superconductors. The current situation is at least partly due to the significant computational burden in the study of phenomena involving electron-phonon coupling, where a detailed account of the electron and phonon scattering processes in proximity of the Fermi surface is required. In this talk I will present a methodology based on electronic and lattice Wannier functions which reduces by several orders of magnitude the computational cost of such studies [1]. The underlying idea is to exploit the spatial localization of electrons and phonons in the Wannier representation in order to compute from first-principles only a limited set of electronic and vibrational states and electron-phonon matrix elements. The results thus obtained are then used to calculate the corresponding quantities at arbitrary electron and phonon momenta in the Bloch representation through a Wannier-Fourier interpolation. In most practical cases the final results carry the same accuracy of a direct first-principles calculation, while the computational cost is comparable to that of a standard phonon dispersion calculation. In the first part of the talk I will describe how we calculate the electron-phonon vertex in the joint electron/phonon Wannier representation. The localization properties of the vertex will be analyzed by making connection with the electronic Hamiltonian in the Wannier basis and with the matrix of the Interatomic Force Constants [2]. By considering a simple virtual crystal model of boron-doped diamond, I will demonstrate the accuracy of the Wannier-Fourier interpolation in Bloch space, and discuss the convergence of the electron and phonon self-energies with the sampling of the Brillouin zone. In the second part of the talk I will review a few recent applications to systems of technological relevance. I will discuss the mechanism of superconductivity in boron-doped diamond [1], show how the electron-phonon interaction affects the carrier lifetimes and the velocity of Dirac fermions in graphene [2], and clarify the relation between the superconducting properties of superhard transitions metal carbides and the Fermi surface topology in these materials [3].

[†] Work done in collaboration with J. R. Yates, I. Souza, C.-H. Park, J. Noffsinger, M. L. Cohen, and S. G. Louie

[1] F. Giustino, J. R. Yates, I. Souza, M. L. Cohen, and S. G. Louie, Phys. Rev. Lett. **98**, 047005 (2007).

[2] F. Giustino, M. L. Cohen, and S. G. Louie, *unpublished*.

[3] C.-H. Park, F. Giustino, M. L. Cohen, and S. G. Louie, *unpublished*.

[4] J. Noffsinger, F. Giustino, S. G. Louie, and M. L. Cohen, *unpublished*.