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Electron-phonon interaction using Wannier functions: from single-layer graphene to cuprate superconductors[1]

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The interaction between electrons and phonons is central to many phenomena, including electrical and thermal transport and superconductivity. Recently the electron-phonon (e-ph) interaction has been the focus of intense research efforts in the physics of high-temperature superconductivity and nanoscale transport. Despite the continued interest in the e-ph problem, first-principles calculations remain challenging due to the large computational effort required to describe e-ph scattering processes in the proximity of the Fermi surface. In this talk I will present a method based on Wannier functions which greatly reduces the computational cost of e-ph calculations [1,2]. The underlying idea is to exploit the spatial localization of electrons and phonons in the maximally localized Wannier representation. After describing the method I will review recent applications to materials of current interest. I will discuss how the e-ph interaction affects the dynamics of Dirac fermions in graphene [3], the origin of superconductivity in boron-doped diamond [1], and the relation between Fermi surface topology and superconductivity in super-hard carbides. I will conclude this presentation by discussing the role of phonons in the angle-resolved photoemission spectra of cuprates [4].

[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, Phys. Rev. B 76, 165108 (2007).
[3] C.-H. Park, F. Giustino, M.L. Cohen, and S.G. Louie, Phys. Rev. Lett. 99, 086804 (2007).
[4] F. Giustino, M.L. Cohen, and S.G. Louie, http://arXiv:0710.2146.

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