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Pushing the limits of first-principles electron-phonon calculations: from photoemission kinks to band

gaps

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The electron-phonon interaction is key to some of the most intriguing and technologically important phenomena in condensed matter physics, ranging from superconductivity to charge density waves, electrical resistivity, and thermoelectricity. Starting from the late nineties first-principles calculations of electron-phonon interactions in metals have become increasingly popular, mainly in connection with the study of conventional superconductors and with the interpretation of angle-resolved photoemission experiments. In contrast, progress on first-principles calculations of electron-phonon interactions in insulators has been comparatively slower. This delay is arguably due to the conventional wisdom that the signatures of electron-phonon interactions in semiconductor band structures are so small that they fall within the error bar of the most accurate electronic structure calculations. In order to fill this gap we developed, within the context of state-of-the-art density-functional techniques, a theory proposed by Allen and Heine for calculating the temperature dependence of band gaps in semiconductors [P. B. Allen, V. Heine, *J. Phys. C: Solid State Phys.* 69, 2305 (1976)]. This methodology allows us to calculate both the temperature dependence of the quasiparticle energies and the renormalization due to zero-point quantum fluctuations. In order to demonstrate this technique an application to the intriguing case of diamond will be discussed [F. Giustino, S. G. Louie, M. L. Cohen, *Phys. Rev. Lett.* 105, 265501 (2010)]. In this case the calculated temperature dependence of the direct band gap agrees well with spectroscopic ellipsometry data, and the renormalization due to the electron-phonon interaction is found to be spectacularly large (>0.6 eV). This unexpected finding might be only the tip of the iceberg in a research area which remains largely unexplored and which, from a first glimpse, appears rich of surprises.