Recent progress in electron-phonon calculations from first principles

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Electron-phonon interactions (EPIs) are ubiquitous in condensed matter physics and materials science, as they underpin the electrical and optical properties of metals, semiconductors, and superconductors. In this context the ability to study EPIs from first principles represents a key step towards predictive materials modelling and design. In this talk I will describe two recent methodological advances in the calculation of EPIs, namely the calculation of temperature dependent phonon-assisted optical absorption spectra [1], and the calculation of Frölich electron-phonon interactions in polar materials [2]. In the case of phonon-assisted optical absorption we have found a way to go beyond the textbook theory by Hall, Bardeen, and Blatt which does not incorporate the temperature dependence of band structures in the spectra. I will demonstrate how this new technique performs by discussing the temperature-dependent indirect optical absorption of silicon. In the case of polar materials the electron-phonon matrix elements diverge at long wavelengths due to the electric fields associated with the LO phonons. This is commonly known as the Frölich interaction. Here we found a way to capture the polar singularity exactly by separating the short- and long-range contributions to the matrix elements in a manner analogous to what is routinely done in calculations of LO-TO splittings. Using the example of anatase titanium dioxide I will show how the Frölich interaction can have important consequences on the lifetimes of photoexcited carriers.

[1] M. Zacharias, C. E. Patrick, and F. Giustino, Phys. Rev. Lett. 2015, in press.
[2] C. Verdi and F. Giustino, Phys. Rev. Lett. 2015, in press.