One-shot calculation of temperature-dependent optical spectra and phonon-induced band-gap renormalization

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The calculation of the electronic and optical properties of solids is usually performed by describing the nuclei as classical particles clamped to their equilibrium positions. This approximation inevitably misses the dependence of electronic and optical properties on temperature, quantum zero-point effects, and phonon-assisted optical processes [1]. In this talk I will introduce a recent development, the Williams-Lax theory, which enables the calculation of the temperature-dependent optical spectra and band gaps of solids by seamlessly including quantum nuclear effects and phonon-assisted transitions [2]. The optical absorption coefficients of common semiconductors calculated using this technique are in remarkable agreement with experiments over several orders of magnitude, both for direct-gap semiconductors like gallium arsenide and for indirect-gap semiconductors like silicon. I will show how the Williams-Lax theory is related to the theory of temperature-dependent band structures by Allen and Heine, and provides an adiabatic approximation to the classic theory of phonon-assisted optical absorption by Hall, Bardeen, and Blatt. I will also discuss how this theory relates to imaginary-time path integrals. The main advantage of this new approach is that it enables the calculation of optical properties of solids at finite temperature using a single supercell calculation (one-shot) [3]. Since the Williams-Lax method is agnostic to the theory employed for describing electronic and optical excitations, it can also be used for performing systematic GW/BSE calculations at finite temperature.

[1] F. Giustino, Rev. Mod. Phys. 2017, in press; arXiv:1603.06965.

[2] M. Zacharias, C. E. Patrick, and F. Giustino, Phys. Rev. Lett. 115, 177401 (2015).

[3] M. Zacharias and F. Giustino, Phys. Rev. B 94, 075125 (2016).