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Fröhlich electron-phonon coupling from first-principles in anatase TiO_2[1] CARLA VERDI, FELICIANO GIUSTINO, University of Oxford — The calculation of electron-phonon properties in polar materials from first principles remains largely unexplored despite their ubiquitous role in many technological applications, such as light-emitting devices and transparent electronics. In polar semiconductors and insulators the electrons can be strongly coupled to the macroscopic electric field induced by longitudinal optical (LO) phonons at long wavelength, leading to the so-called Fröhlich interaction. In our work we develop a general formalism for calculating the Fröhlich vertex from first principles, which can be used as a powerful tool in conjunction with *ab initio* interpolation based on maximally localized Wannier functions [1]. We demonstrate our method by computing the electron lifetimes in anatase TiO_2 and we establish quantitatively the importance of the inclusion of the *ab initio* Fröhlich coupling. Finally, we address the problem of investigating the properties of polaronic quasiparticles, i.e. electrons dressed by a phonon cloud, that can easily form in polar materials and affect their charge transport properties.

[1] C. Verdi and F. Giustino, Phys. Rev. Lett. **115**, 176401 (2015).

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