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Many-body effects on the zero-point renormalization of the diamond band structure

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The coupling of electrons to a bosonic field generally causes a renormalization of the energy levels. Whereas in vacuum, the electromagnetic fluctuations lead to the Lamb shift observed in the hydrogen atom levels, in condensed matter, the phonon field renormalizes the band structure, even at zero temperature. Being as large as several hundreds of meV, this renormalization is critical to the predictive power of *ab initio* calculations when it comes to absorption spectra, photovoltaic materials, or topological insulators. Following the early work of Fan and others in the 1950s, the problem was addressed by Allen, Heine and Cardona, whose theory provides perturbative expressions in terms of the electron-phonon coupling. Using semi-empirical methods, and later on, density functional theory (DFT), the temperature dependence of the band gap could be obtained for several semiconductors. Among those, diamond has become a case study where the zero-point renormalization is as much as half an election volt. The reliability of DFT for the electron-phonon coupling has however been challenged in recent years. Since the scattering of an electron by a phonon probes the excited states of a system, a theory describing this process should rely on an accurate unrenormalized band structure, unlike the one of DFT. A truly *ab initio* scheme however would rely on many-body perturbation theory. As such, we have demonstrated previously that such many-body treatment resulted in a significant increase of the electron-phonon coupling in C60 fullerene. In this presentation, I will report on how a careful treatment using many-body perturbation theory as implemented by the GW approach result in an enhancement of the electron-electron interaction causing a 40% enhancement in the zero-point renormalization (ZPR) in diamond with respect to the usual DFT treatment.

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