Electronic structure of solids, including vibrational effects : Temperature dependence and zero-point motion

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Modifications of electronic eigenenergies due to vibrational effects and electron-phonon coupling are sizable in many materials with light atoms. While often neglected, they have been recently computed from first principles using different formalisms, among which the perturbation-based Allen-Heine-Cardona (AHC) approach, considering both the adiabatic and the non-adiabatic harmonic approximation. Electron-phonon coupling can be obtained from density-functional perturbation theory (DFPT) as well as from many-body perturbation theory (MBPT), e.g. the GW approximation.
I will provide a brief overview of the concepts and formalisms, and present recent progresses, including : the validation of AHC theory implementation in two different software applications, with an agreed DFPT zero-point motion correction of 0.4 eV for the direct bandgap of diamond[1] ; the MBPT result for the same material, 40% higher[2]; the breakdown of the adiabatic AHC theory for infrared-active materials, and fix of this problem in the non-adiabatic AHC theory[3,4], with results for diamond, Si, LiF, AlN, BN, and a dozen oxydes; the connection with the Frohlich Hamiltonian and polaron physics.

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