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Energy Colloquium and Computational Materials Science Seminar

Electronic Structure of Solids: Temperature Dependence and Zero-Point Motion Effect

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ABSTRACT:

Electronic and optical properties of materials are affected by atomic motion through the electron-phonon interaction. This interaction has two noticeable effects on the electronic structure: variation of band gaps as a function of temperature (usually, a decrease of the gap with increasing temperature), but also so-called band-gap renormalization even at absolute zero temperature, due to zero-point motion. Ignored in most calculations of the electronic structure, zero-point effects and temperature dependence have been evaluated recently from first principles for several materials.

I will provide a brief overview of the available formalisms, and cover recent progresses in this field. In particular, many of these calculations relied on the adiabatic approximation, reasonably valid for materials without infrared-activity, but eagerly applied to other materials. I will present the first large-scale (29 materials) first-principles evaluation of the zero-point renormalization of band edges beyond the adiabatic approximation. For materials with light elements (F, O, N, C or lighter), the band gap renormalization is often larger than 0.3 eV, and up to 1.1 eV. This effect cannot be ignored if accurate band gaps are sought. For infrared-active materials, global agreement with available experimental data (within 15%) is obtained only when dynamical effects are taken into account. The dynamical effects even dominate zero-point renormalization for many materials. The connection with the Fröhlich Hamiltonian, used for decades to describe large polarons, will be discussed.