Algebraic Diagrammatic Construction Theory For Charged Excitations Of Solids

Samragni Banerjee, Alexander Yu. Sokolov
Department of Chemistry and Biochemistry,
The Ohio State University, Columbus, OH, 43210
E-mail: banerjee.156@osu.edu

Recently, there has been a rapid increase in the development of wavefunction-based highly accurate quantum chemistry methods for simulating charged excitations of crystalline solids. Accurate simulations of charged excitations are important for computing ionization potentials (IPs) and electron affinities (EAs), which are useful for predicting band gaps, band structures and other spectroscopic properties of materials.

In this poster, I will describe an efficient and accurate approach based on the algebraic diagrammatic construction (ADC) theory for calculating electron attachment and ionization properties of crystalline materials. The ADC approximations are derived from the perturbative expansion of a propagator, poles and residues of which provide information about excitation energies and transition intensities. Our ADC implementation for materials uses periodic boundary conditions, thus taking advantage of the translational symmetry of crystalline solids. I will briefly discuss the theory for this new approach and show our numerical results for quasiparticle band structures and band gaps of several semiconductors and insulators computed using periodic ADC(n) at different orders of perturbation theory ($n \leq 3$).