Title: Development and efficient implementation of algebraic diagrammatic construction theory for charged excitations in molecules and materials

Accurate simulations of charged electronic states are important for predicting many important properties of molecules and materials, such as ionization potentials (IPs), electron affinities (EAs), band gaps, and photoelectron spectra (PES). However, theoretical computations of charged excitations face several challenges associated with the description of charge distribution and open-shell electronic states that require accurate treatment of orbital relaxation and electron correlation effects. In this talk, I will describe an efficient and accurate approach for calculating electron attachment and ionization properties of molecules based on the algebraic diagrammatic construction (ADC) theory (EA/IP-ADC) and demonstrate the capabilities of our molecular implementation in the PySCF package for large systems (more than 1000 orbitals). I will also present our novel periodic ADC implementation for materials, which takes advantage of the translational symmetry of crystalline solids. The applications of periodic ADC to several semiconductors for obtaining band structures and band gaps will also be demonstrated.