Efficient Method for Electron-Phonon Coupling in Molecules and Nanoscale Systems

BEN POWELL, University of Queensland, Brisbane, Queensland 4072, Australia, MARK PEDERSON, Naval Research Laboratory, TUNNA BARUAH, University of Texas El Paso — The coupling between electrons and phonons plays important roles in physics, chemistry and biology. However, the accurate calculation of the electron-phonon coupling constants is computationally expensive as it can involve solving the Schrödinger equation for $O(3N)$ nuclear configurations, where $N$ is the number of nuclei. In analogy to the efficient field-induced extraction of IR and Raman spectra in molecules,[1] consideration of charge-induced changes in Hellman-Feynman forces as a function of electronic charge allows determination of all HOMO and LUMO electron-phonon coupling constants, including isotope dependencies, with only two SCF calculations regardless of system size.[2] The approach can also be used for electron-phonon interactions associated with other electronic states. The relation of this method to Janak’s theorem[3] is discussed. This $O(1)$ approach is numerically very stable and produces accurate results for electron-phonon coupling constants in tests on approximately 15-20 molecules ranging in size from $\text{H}_2$ to $\text{C}_{60}$. Adiabatic ionization potentials and relaxed Hubbard U parameters are presented as an example of the method.