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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 $\mathcal{O}(3N)$ 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 $\mathcal{O}(1)$ 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 H_2 to C_{60}. Adiabatic ionization potentials and relaxed Hubbard U parameters are presented as an example of the method.
[1]D.V. Porezag and M.R. Pederson, Phys. Rev. B **54**, 7830 (1996).
[2]B.J. Powell, M.R. Pederson and T. Baruah (submitted).
[3] J.F. Janak, Phys. Rev. B **18**, 7165 (1978).

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