USING A ROBUST ΔSCF METHODOLOGY TO SIMULATE VIBRATIONAL SPECTROSCOPY OF EXCITED STATES

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The use of ΔSCF methods has a rich history in the computational study of electronic excited states. However, such calculations often suffer from a number of challenges including convergence difficulties and variational collapse. Addressing both of these concerns, we have recently developed a projection-operator based approach that significantly improves the robustness of SCF optimization. In this talk, we will describe this new SCF convergence method and demonstrate its ability for studying the vibrational spectroscopy of excited states. Our initial results show that our projection-based scheme provides reliable means for efficiently explore the structure and properties of molecules with electronic structures corresponding to excited states with the efficiency of ground state quantum chemistry models. Results using this method on a set of molecular systems will be compared with results obtained using the more expensive (linear response) time-dependent density functional theory, equation-of-motion coupled cluster, and configuration interaction methods.