Title: Improvements to the Efficiency of Coupled-Cluster calculations for Excited States

Abstract:

Equation-of-motion coupled-cluster(EOM-CC) calculations can provide an accurate description of excited states of molecular systems. These calculations carry a large cost however, particularly when one is interested in the high energy states associated with core-level process such as those involved in X-ray absorption spectroscopy. This work considers the utility of two methods of reducing the computational cost of such calculations; the short iterative Lanczos integration method and the core valence separation (CVS) approximation wherein excitations are only considered if they involve at least one core orbital. These approximations greatly reduce the cost of calculating molecular excitations, particularly core-level features such as K and L-edges.