

Resolution-of-the-Identity and Beyond

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Achieving quantitative accuracy in the prediction of energetic and spectroscopic properties can become challenging as the size and complexity of molecules increase due to the accompanying rise in computational costs (i.e., computer time, memory, disk space). Developments by our group and applications that have provided insight about energetic predictions, the theoretical strategies used for the predictions (i.e., density functional approximations, and *ab initio* single and multi-reference strategies), and strategies for dramatically decreasing costs (i.e., resolution-of-the-identity, localization schemes) will be highlighted. Specifically, the correlation consistent Composite Approach (ccCA), which effectively has been utilized for many hundreds of main groups species, will be discussed, and its combination with routes for localizing and screening molecular orbitals have been considered. Recently, the domain-based local pair natural orbital methods (DLPNO) methods have been implemented within ccCA, and, here, the electronic energies, enthalpies of formation, and CPU times determined using ccCA, RI-ccCA, and DLPNO-ccCA are demonstrated for a set of 119 molecules consisting of first- and second-row main group atoms and linear alkanes. Several additional strategies are also discussed.