

Utilization of Local Methods to Reduce Computational Cost within ccCA

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The Resolution of the Identity (RI) approximation and the domain-based local pair natural orbitals (DLPNO) methods have been used to lower the computational cost while targeting the energetics of post-HF calculations. These methods were utilized within the ccCA framework to reduce the computational cost (disk space, CPU time, memory) and the results are calibrated with experimental enthalpies of formation. These investigations provide insight into development of more cost-effective methods throughout the periodic table.