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Local Correlation Calculations Using Standard and Renormalized Coupled-Cluster Methods PIOTR PIECUCH, WEI LI, JEFFREY GOUR, Department of Chemistry, Michigan State University — Local correlation variants of the coupled-cluster (CC) theory with singles and doubles (CCSD) and CC methods with singles, doubles, and non-iterative triples, including CCSD(T) and the completely renormalized CR-CC(2,3) approach, are developed. The main idea of the resulting CIM-CCSD, CIM-CCSD(T), and CIM-CR-CC(2,3) methods is the realization of the fact that the total correlation energy of a large system can be obtained as a sum of contributions from the occupied orthonormal localized molecular orbitals and their respective occupied and unoccupied orbital domains. The CIM-CCSD, CIM-CCSD(T), and CIM-CR-CC(2,3) algorithms are characterized by the linear scaling of the total CPU time with the system size and embarrassing parallelism. By comparing the results of the canonical and CIM-CC calculations for normal alkanes and water clusters, it is demonstrated that the CIM-CCSD, CIM-CCSD(T), and CIM-CR-CC(2,3) approaches recover the corresponding canonical CC correlation energies to within 0.1 % or so, while offering savings in the computer effort by orders of magnitude. By examining the dissociation of dodecane into $C_{11}H_{23}$ and CH_3 and several lowest-energy structures of the $(H_2O)_n$ clusters, it is shown that the CIM-CC methods accurately reproduce the relative energetics of the corresponding canonical CC calculations.

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