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A Near Linear-Scaling Smooth Local Coupled Cluster Algorithm for Electronic Structure JOSEPH SUBOTNIK, ALEX SODT, MARTIN HEAD-GORDON, UC Berkeley, PITZER CENTER TEAM — We demonstrate near linear-scaling of a new algorithm for computing smooth local coupled-cluster singles-doubles (LCCSD) correlation energies of quantum mechanical systems. Full CCSD provides an excellent, size-consistent treatment of electron correlation, but is computationally expensive, scaling formally as $O(n^6)$; by contrast, our LCCSD algorithm recovers more than 99% of the CCSD correlation energy, while achieving near linear-scaling. Furthermore, previous domain-based LCCSD models had discontinuous potential-energy curves, with correspondingly infinite nuclear forces; by contrast, our domain-free algorithm's correlation energy is a rigorously differentiable function of nuclear coordinates, with correspondingly finite nuclear forces. Thus, our algorithm should allow, in the future, for the propagation of quantum dynamics on a highly correlated electron surface. We present applications to small polypeptide conformational energies, and demonstrate how one may smoothly dissociate two benchmark molecules (ethane and ketene) at the LCCSD level of electronic correlation using our algorithm.

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