Linear scaling of *ab initio* theory to nano-clusters with molecular cluster perturbation theory

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Our recent work on the *ab initio* treatment molecular crystals and nano-clusters using our recently developed molecular cluster perturbation theory (MCPT) will be presented. This new methodology is designed to calculate arbitrarily large systems using explicit molecular wavefunctions. The MCPT framework uses coupled-cluster perturbation theory with the the product Hartree-Fock wavefunction in an intermolecular force expansion to compute infinite order monomer and dimer (including all products of dimers) interactions. The resulting perturbation theory has a standard $O(n^6)$ monomer computational scaling, but with the implementation of a range cutoff the total system size scaling is only $O(N)$. MCPT has been implemented to second-order to take advantage of the advanced dynamic memory control and fine grained parallelism in the new SIA/ACES parallel architecture. Benchmark crystal harmonic vibration modes, lattice site dipole moments and molecular energy shifts will be computed for several solid molecular crystals including 1,000 or more explicit molecules to demonstrate the scaling performance of the MCPT and SIA frameworks.