Global Optimization of Large Lennard-Jones Clusters with the Hidden Force Algorithm

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Global optimization of Lennard-Jones clusters up to size $N=350$ is carried out with our, so-called hidden force algorithm, implemented in a parallel, highly non-Markovian Monte Carlo program. The hidden force algorithm utilizes natural force patterns among particles to define Monte Carlo move sets, which can easily cross energy barriers and have been shown in our hands to find low-energy configurations without taking any symmetry constraints into account. The underlying Monte Carlo procedure is a mixture of independent parallel searches and periodically spawning new searches from the currently most successful process.