Population based random search and the topology of the potential energy surface of Lennard-Jones clusters

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Abstract

Low-energy configurations of Lennard-Jones atomic clusters are determined by population based random search. Using a combination of evolutionary computations and Monte Carlo simulation, the topology of the potential energy surface is elucidated and the probabilities of convergence to the global minimum and saddle points are analyzed. An understanding of this phenomenon can lead to the glass formation, protein folding, and the other problems with competing minima. Some empirical results are given for Lennard-Jones clusters 6 to 13 particles.