The Geometry of LJ Atomic Clusters

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The determination of the spatial conformation of an n–atom cluster with minimum Lennard–Jones (LJ) potential is tantamount, when all atoms are of the same type, to the problem of finding points $p_i = (x_i, y_i, z_i) \in \Re^3$, for $i = 1, \ldots, n$, so as to minimize

$$E = \sum_{i=1}^{n-1} \sum_{j=i+1}^{n} (r_{ij}^{-12} - r_{ij}^{-6}),$$

where r_{ij} is the Euclidean distance between points p_i and p_j. This global optimization problem has proved to be very difficult. In general, the best minima known for clusters of $n \leq 150$ atoms come from approaches as diverse as simulated annealing, lattice search followed by local minimization, and genetic algorithms, to name but a few.

We propose a method that combines a genetic algorithm with a stochastic search procedure on icosahedral lattices. Computational results up to $n = 309$ are presented, together with a discussion of the corresponding geometric characteristics. Although most of the optimal configurations found display well known geometries (icosahedral and decahedral), our study allowed us to discover a novel morphology for LJ atomic clusters.