Abstract

A robust and accurate method of modeling carbon nanostructures is proposed using a simulated annealing Monte Carlo algorithm via TransRot by modeling clusters of buckyballs, \((C_{60})_n\). A new set of force parameters for carbon-carbon interactions were determined and reproduced structures for the dimer that were previously only obtainable through expensive quantum calculations. The resulting model is called the Quantum-fit Lennard-Jones Interacting Atoms (QLIA) potential and can model the order-disorder rotational transitions of solid \(C_{60}\) unlike existing potential models. After optimizing the \((C_{60})_n\) and determining the appropriate Lennard-Jones potential and TransRot parameters, clusters ranging from \(n = 3\) to \(n = 8\) were optimized. Global minima for each cluster and local minima for \(n = 7\) and \(n = 8\) were determined and their symmetry was analyzed and compared to the Cambridge Lennard-Jones clusters database. The slip-staggered geometry common in systems of polycyclic aromatic hydrocarbons was observed and determined to be a result of dispersion and Pauli exclusion forces. Lastly, the resulting model introduces a novel way to analyze more complicated carbon nanostructures, such as other fullerenes, carbon nanotubes, and graphene-graphene sheets.