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On the fullerene formation mechanism by means of Benzene combustions: MD study

O Biswajit Saha, Stephan Irle, Keiji Morokuma
Fukui Institute for Fundamental Chemistry, Kyoto University, Kyoto 606-8103, Japan
saha@fukui.mbox.media.kyoto-u.ac.jp

Although subject to intensive studies, the formation mechanism of buckminsterfullerene C_{60} and related higher fullerenes has long evaded discovery. To elucidate their atomistic self-assembly mechanism, we have previously performed high-temperature quantum chemical molecular dynamics simulations on carbon vapor model systems initially consisting of C_2 molecules. Our simulations revealed a coherent mechanism how highly ordered fullerene cages are naturally self-assembled under nonequilibrium conditions, following a series of irreversible processes from the polymerization of C_2 molecules to vibrationally excited giant fullerenes, which then shrink by C_2 evaporation down to the smallest spherical, isolated pentagon rule obeying species C_{70} and C_{60} as the smallest and kinetically most stable species of the shrinking process. We showed that the potential energy surface associated with giant fullerene cage growth, measured by an average cluster curvature, is downhill all the way, and in agreement with high level energetics from density functional theory. The fullerene formation mechanism turned out to be a good example for dynamic self-assembly leading to dissipative structures far from thermodynamic equilibrium, and the shrinking hot giant road provides a natural explanation for the observed cage size distributions. Here, we present new simulations with benzene molecules as carbon feedstock instead of C_2 molecules.