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The equilibrium and electronic structure of large icosahedral fullerenes using an all-electron fully analytic density functional theory

RAJENDRA ZOPE[1], University of Teaxs at El Paso, BRETT DUNLAP, US Naval Research Laboratory — We have recently developed a fast, variational and fully analytic density functional theory (ADFT). Instead of numerical integration it employs analytic integration using Gaussian basis sets and the calculus of variations to express the molecular orbitals as well as the Kohn-Sham potential in linear-combination of atomic orbital form. We first parametrize the ADFT to provide the experimental geometry of C_{60} fullerene. Using this parametrization, the triple zeta 6-311G(d,p) orbital basis, and density fitting with exchange-correlation bases that include up to f functions, the geometries of C_{240}, C_{540}, C_{960}, C_{1500}, and C_{2160} fullerenes are optimized. The equilibrium structures of these fullerenes are polyhedral in nature, confirming the previous predictions by tight-binding methods. Bond distances are converging towards those of graphene. The evolution of electron removal energies, electron affinities, and singlet excitation energies from C_{60} to C_{2160} is studied using the ΔSCF and transition-state methods.

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