Static dipole polarizabilities of icosahedral fullerenes from C\textsubscript{60} to C\textsubscript{2160} by all-electron density-functional theory

RAJENDRA ZOPE, TUNNA BARUAH, University of Texas at El Paso, MARK PEDERSON, Naval Research Laboratory, BRETT DUNLAP, Naval Research Laboratory —

The electronic response of C\textsubscript{60}, C\textsubscript{180}, C\textsubscript{240}, C\textsubscript{540}, C\textsubscript{720}, C\textsubscript{960}, C\textsubscript{1500}, and C\textsubscript{2160} fullerenes is characterized by determining their static dipole polarizabilities by all-electron density-functional theory. We first determine the dipole polarizabilities of C\textsubscript{60}, C\textsubscript{180}, C\textsubscript{240}, and C\textsubscript{540} fullerenes by the finite-field method, using 35 basis functions per atom (NRLMOL basis set), and using the PBE-GGA. In the second set of calculations the sum-over-states (SOS) polarizabilities for all fullerenes from C\textsubscript{60} through C\textsubscript{2160} are determined by our fully analytic formulation of density functional theory (ADFT). The 6-311G(d,p) basis set is used in the ADFT calculation, which amounts to 38800 basis functions for the largest fullerene in this series, namely C\textsubscript{2160}. The SOS polarizabilities are roughly 4 times larger than the finite-field polarizabilities. When scaled by a correction factor obtained within linear response theory, the SOS polarizabilities are within 1-3% of the finite-field polarizabilities. The polarizability per carbon atom increases from 1.34 Å\textsuperscript{3} in C\textsubscript{60} to 4 Å\textsuperscript{3} in C\textsubscript{2160} while the ratio of fullerene polarizability to its volume approaches unity pointing to quenching of quantum size effects by C\textsubscript{2160}. The results show previous tight-binding calculations greatly exaggerate the electronic response of large fullerenes.