NT2-005

Electronic Structures and Vibrational Spectra of Various Fullerene Structures and their Adducts: Density Functional Approach

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Using ab initio density functional theory, we investigate the electronic structures and the vibrational spectra of various fullerene structures, such as fullerene adduct and fullerene dimers. After performing the geometry relaxation to obtain their equilibrium structures, we calculate the dependence of their electronic structures on different configurations. We compare the electronic structures of [2+2] dumbbell C120 and the peanut-shaped coalescence products; and examine the dependence of the HOMO-LUMO gap of each fullerene adduct on the number of additives, or on their relative positions and orientations. The vibrational spectra of some structures are also calculated to compare with the available IR experimental data.