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Computational Study on the Structural and Electronic Properties of Various Fullerene Derivatives[1] SORA PARK, JEUNG SUN AHN, Department of Physics, Kyung Hee University, YOUNG-KYUN KWON, Department of Physics and Research Institute for Basic Sciences, Kyung Hee University — Using *ab initio* density functional theory, we investigate the structural and electronic properties of various fullerene derivates. The equilibrium structures of various additives adsorbed on a fullerene molecule forming fullerene adducts are computed through the geometry relaxation. For a given fullerene adduct, we also calculate the optimum configuration with a different number of additives. In tandem with the structural studies, we calculate the dependence of the HOMO-LUMO gap of each fullerene adduct on the number of additives, and on their relative positions and orientations. Further, using the GW approximation, we also examine the quasiparticle electronic structure of various fullerene derivates.

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