
Density Functional Study of the Structural and Electronic Properties of Various Fullerene Derivatives

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Density functional theory (DFT) calculations have been performed to investigate the structural and electronic properties of various fullerene derivatives consisting of a fullerene molecule and several kinds of addends combined through [2+2] cycloadditions. We have considered various geometrical configurations of addends combined with C_{60} , such as different numbers, different positions giving different symmetries. Our calculations indicate that the HOMO-LUMO gap becomes wider than that of pristine C_{60} only when addends locate on C_{60} with specific symmetries. This suggests that absorption properties could be adjusted by controlling the addends configurations on C_{60} . For further investigation of this peculiar dependence, we have carried out analysis of the charge distribution and orbital mixing characters.

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