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Interplay between structural and electronic properties of various fullerene derivatives, and their absorption spectra SORA PARK, JEUNG SUN AHN, YOUNG-KYUN KWON, Kyung Hee University — Using density functional theory (DFT), we investigate the geometrical structures and electronic properties of various fullerene derivatives formed by attaching several kinds of addends on C_{60} through [2+2] cycloaddition. Various forms of such derivatives are modeled by considering different kinds, different positions and different numbers of addends to study how structural configurations will affect their electronic structures. Our results reveal that some derivatives with certain symmetries determined by the configuration of addends may have wider energy gap than that of pristine C_{60} . This suggests that absorption properties could be adjusted by controlling the addends configurations. To describe the excited state properties, such as absorption spectra, of various C_{60} derivatives more accurately, we performed time-dependent (TD) DFT calculations. We find the position and the intensity of the peak of absorption spectra of derivatives are affected by the specific symmetry of the derivatives defined by the configurations of the addends. To explore such peculiar effects, we analyze the charge distribution and orbital mixing characters.

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