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Energetics study of compressive, tensile and torsional stress in buckminsterfullerene

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Buckminsterfullerene is famous for its symmetrical structure which follows isolated pentagonal rule responsible for providing stability to the structure. However, defects can be introduced in fullerene to alter its structure and properties. Such defects can act as an active site for various reactions. Fullerene also acts as an additive to strengthen carbon composites. Hence energetics of defects needs to be studied. Tensile, compressive and torsional tests were simulated for a pair of diametrically opposite bonds, pentagonal and hexagonal rings. In addition to this, tensile and compressive tests were also simulated for diametrically opposite atoms. Opposite members were displaced by an equal amount in compressive and tensile tests. Torsional tests calculations were done for two cases. For the first case, only one end is twisted keeping opposite members fixed while for second case both opposite members were rotated by an equal amount. Selected atoms were frozen after incorporating aforementioned changes and rest all atoms were relaxed to obtain the optimized structure. Simulation experiments were carried out using Gaussian 09 under density functional theory framework, 6-31G(d) basis set and B3LYP hybrid exchange correlation functional. For small strain values, quadratic variation of strain energy U(ε) with ε was observed whereas transition to linearity between U(ε) and ε was observed for higher strain in compressive tests. In case of tensile stress, no such transition was observed and the relation between U(ε) with ε is quadratic for all sampled values of strain. Strain energy profile for torsional strain was found to be different for two cases. A new isomer of fullerene was formed when opposite bonds were twisted. The obtained fullerene molecule found to be violating the isolated pentagonal rule.

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