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Investigation of the performance of T-carbon nanostructure as optical absorbing material under hydrostatic stress

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Abstract
In this research, we use first-principles calculations based on density functional theory (DFT) to investigate the electro-optical performance of a three-dimensional T-carbon nanostructure. In addition to analyzing the dynamic and static stability of the optimized structure of the T-carbon unit cell, as new research, the electro-optical properties of T-carbon, under the effect of omnidirectional hydrostatic stress on the unit cell up to 9 GPa, were simulated by using computational codes. The obtained results indicate the acceptable performance of this nanostructure as a suitable optical absorbent material. This three-dimensional nanostructure can be used to design innovative components such as electro-optical sensors, light intensifiers, optical detectors, and organic perovskite solar cells.

Keywords: density function theory, carbon allotrope, three-dimensional T-carbon nanostructure, electro-optical properties

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