AB INITIO STUDY OF STRUCTURAL, ELECTRONIC AND OPTICAL PROPERTIES OF EDGE-FUNCTIONALIZED GRAPHENE QUANTUM DOTS

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Abstract

Graphene quantum dots (GQD) are nano-particles small enough to exhibit unique electronic and optical properties that results from quantum confinement and edge effects. Unlike graphene they exhibit opening of the HOMO-LUMO band gap responsible for their unique optoelectronic properties high photoluminescence (PL) quantum yield, excellent photobleaching resistance and photostability, low citotoxicity, good biocompatibility, high solubility in various solvents, exceptional electrochemical activity and physicochemical stability. These characterisics of the GQDs make them suitable for a wide range of applications from biomedical applications such as diagnostics and therapy, to susteanable agricultural and environmental appications. In this respect carbon-based quantum dots such as GQDs, present promising candidates for usage in biosensing and fluorescence bioimaging applications, allowing a fast, more sensitive and more selectable detection and diagnosis. As biocompatible nanoparticles, they also have the potential to revolutionize the prospects of photodynamic therapy (PDT) in clinical treatments of cancer [1] and other diseases, antibacterial [2] and preventive antivirus PDT [3], being applied as photosensitizer agents. In a meanwhile comprehensive biomedical studies should pave the way for safe and efficient use of carbon-based quantum dots in clinical applications. In the present work, we investigate the effects of size and shape variation, as well as edge-functionalization on the structural and optical properties of GQDs, using the first-principles study based on the density functional theory (DFT) and time-dependent density functional theory (TD-DFT). We investigate edge-functionalized GQDs, with oxygen-containing –OH and –COOH groups, different shapes, such as hexagonal, triangular and rectangular and zigzag/armchair edge configuration, as well as variation of size, in tailoring the optoelectronic properties and photoluminescence behaviour of GQDs leading to a wide variety of applications.

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