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A computational approach to the study of carbon nanodots for the determination of their structure and properties

Since their discovery in 2004, carbon nanodots (CNDs) have emerged as a promising class of carbon-based nanoparticles due to their properties: intense photoluminescence, low toxicity, excellent biocompatibility and easy surface functionalization.[1] Their synthesis employs straightforward bottom-up and top-down methods, which dictate the functional groups present on their surface, their size and their photoluminescent response.[2] As a result, CNDs have found numerous applications, particularly in biological and biomedical fields.[3] Despite extensive experimental and computational studies, a comprehensive atomic-level understanding of their structural features and their correlation with optical properties remains incomplete.[4] To fill this gap, an explicit treatment of the electronic degree of freedom is required, along with a compatible computational method that balances efficiency and accuracy. Here, we present results on the application of a computational multiscale approach based on ab-initio DFT (Density Functional Theory) and semi-empirical (TB-DFT, tight-binding density functional theory) methods to the class of CNDs. The challenge lies in identifying more effective starting models than the ones currently used, which are mostly based on polycyclic aromatic hydrocarbons (PAHs).[5] We propose that progressively larger carbon clusters (CCs) can serve as effective structural models for CNDs, as shown in the figure reported below.

Our investigation focuses on CNDs with an amorphous carbogenic core, which is the less explored variant in the literature. We present results on the structural investigation of pure, doped, and functionalized carbon clusters. Specifically, we explore nitrogen doping and functionalization with -OH, -NH_2, -COOH, and -$CONH_2$ groups, in agreement with the most common precursors used in the synthesis of CNDs. In addition, their optical properties are investigated using TD-DFT (time-dependent density functional theory), both for the pure and functionalized structures.

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