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Structure and Properties of Carbon Dots

Carbon dots (CDs) are extensively studied nanomaterials with broad application potential due to their bright, tunable photoluminescence (PL), high (photo)stability, low toxicity, and excellent biocompatibility, as well as their emerging promise in photocatalysis. However, understanding the origins of their PL and photocatalytic (PC) behavior remains incomplete [1,2], largely due to the structural complexity and variability of CDs. To address this, we employ a comprehensive suite of computational chemistry methods to explore their structure–property relationships. Using ab initio calculations, we investigated the reaction mechanisms underlying CD formation from simple precursors such as citric acid and ethylenediamine, successfully identifying early-stage pathways that align with experimental results [3]. Reactive molecular dynamics simulations provided further insights into intermediate structures formed during later synthesis stages. Classical all-atom molecular dynamics simulations revealed the structural organization of CDs [4], including the localization of molecular fluorophores [5] formed during synthesis. Additionally, quantum mechanical and hybrid QM/MM calculations demonstrate how the optical properties of prototypical fluorophores are modified through dimerization, and noncovalent and covalent confinement within the CD structure [6]. The developed models can be further used to understand behavior of CDs, e.g., in sensing applications [7,8]. This work underscores the power of combining state-of-the-art theoretical approaches with modern experimental techniques to unravel the complex structural and optical properties of CDs and similar nanomaterials.

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