Synthesis of Heteroatom-Doped Carbon Dots with Enhanced Near-Infrared Fluorescence and Photothermal Properties toward Bioimaging and Photothermal Therapy Applications.

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Abstract

Cancer remains a critical global public health challenge, and conventional therapeutic strategies often cause substantial side effects. These limitations have motivated the development of multifunctional nanomaterials capable of both bioimaging and near-infrared (NIR) photothermal therapy, which offer deep tissue penetration and low background interference. In this study, nitrogen- and sulfur-doped carbon dots (N,S-CDs) were synthesized via a solvothermal approach using citric acid, urea, and DMSO to modulate defect states and bandgap structures for enhanced NIR absorption and emission. The carbon dots doped with 6 g of nitrogen precursor exhibited the highest absorption at 650 nm and superior photothermal conversion efficiency, followed by those doped with 12 g, which generated additional trap states. Optimization of solvent composition revealed that 5 mL of DMSO combined with 1 g of citric acid and 3 g of urea yielded the highest photothermal performance (PCE percentage at 61.8). Conversely, prolonged heating induced particle aggregation, diminishing both fluorescence intensity and photothermal behavior. Collectively, these findings demonstrate that the synthesized N,S-CDs possess favorable NIR-active properties for bioimaging and photothermal therapy, highlighting their potential as promising theranostic materials for integrated cancer diagnosis and treatment.

Keywords: Carbon Dots, Heteroatom Doping, Near-Infrared, Photothermal Therapy, Theranostics