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Research papers

Tuning interfacial interactions via nitrogen doping in sago bark-derived carbon dots for controlled curcumin release

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ABSTRACT

Carbon dot (CD)-based nanocarriers have garnered attention for drug delivery. However, a detailed understanding of heteroatom doping and pH-dependent interactions between drug molecules and nanocarriers remains limited. In this study, interactions between curcumin, used as a model drug, and sago bark-derived carbon dots (CDs) and N-doped carbon dots (NCDs) were examined under acidic (pH 5.5) and physiological (pH 7.4) conditions using both experimental and computational approaches. The results reveal that N-doping alters the nanocarrier's electronic environment, resulting in higher curcumin loading in curcumin-NCDs. Under different pH conditions, protonation and deprotonation processes alter the surface polarity of the nanocarriers, thereby influencing various interactions. At acidic pH, curcumin binding is primarily driven by van der Waals forces. Conversely, deprotonation at pH 7.4 introduces additional weak hydrogen bonds, resulting in slower release, as shown in the experimental data. These findings offer mechanistic insights into how heteroatom doping can tune pH-responsive surface interactions.