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ACCEPTED MANUSCRIPT

Carbon Quantum Dots-Ag Nanoparticle Complex as a Highly Sensitive "Turn-On" Fluorescent Probe for Hydrogen Sulfide: A DFT/TD-DFT Study of Electronic Transitions and Mechanism of Sensing

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Carbon Quantum Dots-Ag Nanoparticle Complex as a Highly Sensitive "Turn-On" Fluorescent

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Scheme. 1. Proposed mechanism of the CQDs-AgNPs nanoprobe for H₂S sensing.

Highlights:

- A fluorescent nanoprobe based on efficient carbon quantum dots (CQDs)-modified silver nanoparticles (AgNPs) (CQDs-AgNPs) for effective monitoring of H₂S is presented.
- DFT/TD-DFT investigations were conducted on the electronic structures, absorption and emission spectra of CQDs-AgNPs complex as well as the sensing mechanism.

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