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A highly selective fluorescent probe for cyanide ion and its detection mechanism from theoretical calculations

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Abstract

A new cyanide probe has been prepared by one-step synthesis and evaluated by UV-*vis* and fluorescent method. This probe is combined by a fluorene part and a hemicyanine group through a conjugated linker, which is found to show rapid response, high selectivity and sensitivity for cyanide anions with significant dual colorimetric and fluorescent signal changes in aqueous solution. An intramolecular charge transfer (ICT) effect plays a key role in the CN⁻ sensing properties, and the details of this mechanism are further supported by DFT and TD-DFT calculations. The theoretical study shows that the introduction of CN⁻ twists the original plane structure and blocks the ICT process in the whole molecule, which brings about the absorption blue-shift and the fluorescence quenching.

Graphical abstract

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