

Synthesis, structure and photoelectrochemical properties of the TiO₂–Prussian blue nanocomposite

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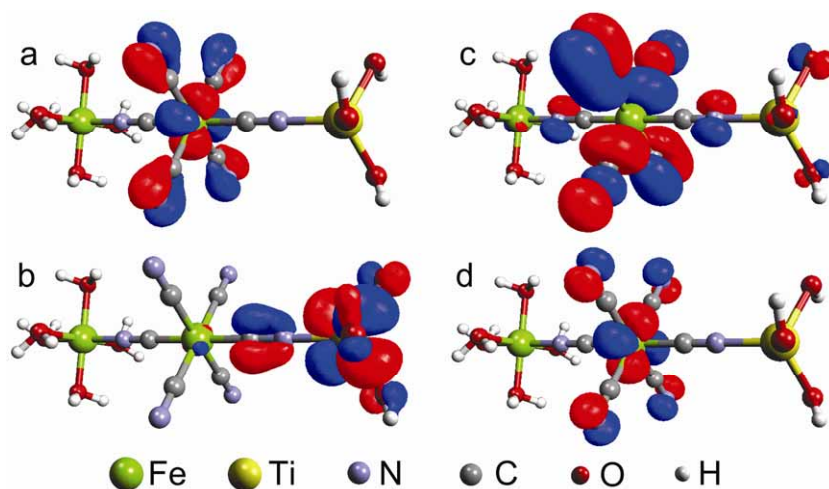


Fig. 8 Frontier molecular orbitals for the $[\text{Fe}(\text{H}_2\text{O})_5\text{--N}\equiv\text{C--Fe}(\text{CN})_4\text{--C}\equiv\text{N--Ti}(\text{OH})_3]_n$ ($n = -1, 1$) model compound: (a) $\text{Fe}^{\text{II}}\text{Fe}^{\text{III}}\text{Ti}^{\text{IV}}$, HOMO; (b) $\text{Fe}^{\text{II}}\text{Fe}^{\text{II}}\text{Ti}^{\text{IV}}$, LUMO; (c) $\text{Fe}^{\text{III}}\text{Fe}^{\text{III}}\text{Ti}^{\text{IV}}$, HOMO; and (d) $\text{Fe}^{\text{III}}\text{Fe}^{\text{III}}\text{Ti}^{\text{IV}}$, LUMO.