TDDFT Studies of the Excited State Electronic Structure tetraphenylporphyrin and Iron(II)-tetraphenylporphyrin

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Abstract

Density functional theory (DFT) and time-dependent density functional theory (TDDFT) were used to analyze the absorption spectra for tetraphenylporphyrin (H2TPP) and iron(II)-tetraphenylporphyrin (FeTPP). The ground state of FeTPP is known to be the spin-triplet although the quintet is nearly degenerate. The predicted main features in the absorption spectra are nearly the same for the two spin systems. The results are used to analyze the experimental absorption spectra of H2TPP, FeTPP and iron(II)-tetraphenylporphyrinsulfonate(FeTPPS).