**Abstract**

The present study highlights the structural and electronic spectra of Sn(IV)tetrakis(4-pyridyl) porphyrins (SnTP) using density functional theory (DFT) and time-dependent density functional theory (TDDFT). The impact of axial ligands (OH− , Cl− , and H2O) and protonation at pyridine sites on the excitation properties of SnTP is also explored. The considered SnTPs were optimized at B3LYP/6-31+G\* level of theory with LANL2DZ basis set for Sn metal. The effects of tetrahydrofuran (THF) and dimethylformamide (DMF) solvents were also assessed employing conductor-like polarizable continuum (C-PCM) model. The observed structural effects correlate well with the experimental data and clearly depict the impact of axial ligands on the SnTP ring. The absorption spectra along with the frontier orbitals in all three phases show noticeable dependence of axial ligation on the photophysical properties of SnTPs. The transition character of molecular orbitals and their respective density of states (DOS) were explored to infer the orbitals involved in electronic transitions.