Mechanistic insight of metalloporphyrin-based fluorescence sensor reacting with volatile organic compounds

ABSTRACT

The theoretical design of a metalloporphyrin-based fluorescence sensor was developed for the discrimination of volatile organic compounds (VOCs). Molecular models of cobalt tetraphenylporphine (CoTPP) with small VOCs were investigated by the density functional theory (DFT) method at the Becke, 3-parameter, Lee–Yang–Parr (B3LYP) and LAN2DZ level. The relative energies of CoTPP and its complexes were calculated at three spin states (low, intermediate, and high) to obtain their optimized geometry structures. Singlets were found to be the most stable states for CoTPP and its complexes, except for CoTPP-oxygen and CoTPPpropanol at triplets. The binding performance was represented by the binding energy (BE), which showed the following order based on the most stable states: propane (L3) < oxygen (O2) < propanol (L2) < hydrogen sulfide (H2S) < propionaldehyde (L6) < nitrogen (N2) < butanone (L5) < ethyl acetate (L4) < trimethylamine (L1). We suggest that the CoTPP-based fluorescence sensor is sensitive to trimethylamine and ethyl acetate, and avoids the interference from propane and oxygen.