The influence of different metal atoms on the performance of metalloporphyrin-based sensor reaction with propanol

ABSTRACT

Density functional theory (DFT) method was carried out to investigate the molecular interaction between metalloporphyrin-based sensor and propanol. The relative energies were used to determine the most stable state of metalloporphyrin and its complexes at three different spin states for further theoretical studies. The low-spin states were found to be the most stable states for cobalt porphyrin (CoP), tin porphyrin (Sn), and zinc porphyrin (ZnP) before exposure to propanol and CoP, SnP, ZnP, iron porphyrin (FeP), ruthenium porphyrin (RuP) after exposure to propanol. The intermediate-spin state was found to be the most stable states for the other metalloporphyrins and their complexes, except for manganese porphyrin (MnP) after exposure to propanol. The calculated binding energies were shown the following order for metalloporphyrin-based sensor-binding propanol: MnP>ZnP>CoP>RuP>SnP>FeP>AgP>CuP. This calculated result may be useful for the theoretical design of metalloporphyrin-based sensor for propanol determination and perhaps other analyte.

Keyword: Metalloporphyrin; Sensor; Density functional theory; Propanol