A density functional theory study of metalloporphyrin derivatives act as fluorescent sensor for rapid evaluation of trimethylamine

ABSTRACT

A fluorescent sensor based on metalloporphyrin was developed for trimethylamine (TMA) evaluation. Density functional theory (DFT) has been performed to investigate the design mechanism of fluorescent sensor. Fourteen metalloporphyrin (MP) models were selected to find the influence of metal atoms and substituent groups on the binding performance of fluorescent sensor. The optimized geometry structures, relative energies, mulliken charges, spin densities, and four frontier molecular orbitals together with binding energies of these fluorescent sensors were investigated. AgP sensor has the lowest relative energies before and after exposure to TMA, which make AgP sensor better than the others to go through more than one pathway. Binding energy results revealed that the metalloporphyrin sensors with different metal atoms and substituent groups cause remarkable changes in TMA binding performances. Thus, theoretical investigations can be used to extend the fluorescent sensor in to TMA related analytes in different detection requirements, and perhaps other molecule.

Keyword: Density functional theory; Fluorescent sensor; Metalloporphyrin; Trimethylamine