**Abstract**

This paper is proposed to understand the interaction of porphyrin layers with diatomic molecules interacting at their interior regions by applying ab initio and density functional theory (DFT) methods. We have used NO, CO, and O2 diatomic molecules to interact with the porphyrin layers. The most common Fe-centered metalloporphyrin structure with tetra-pyrrlic rings having N4 core is chosen for the study. The optimization of Porphyrin-Porphyrin (PI-PII) and Porphyrin-Diatomic molecule-Porphyrin (PI-AB-PII) (AB = NO, CO, and O2) complexes are performed using HF method. In order to understand the planarity and appropriate stacking size of porphyrins and also to infer the separation of diatomic molecules between porphyrin layers the behavior of PI-AB-PII complexes (where AB = NO, CO, and O2) are analyzed using structural properties and molecular electrostatic potentials (MEP). The MEPs are calculated using hybrid exchange correlation functional B3PW91 of DFT along with 6-31+G\* basis set for the PI-PII and PI-AB-PII complexes obtained from HF method.