Ab Initio Calculations of Metallotetrabenzoporphyrins

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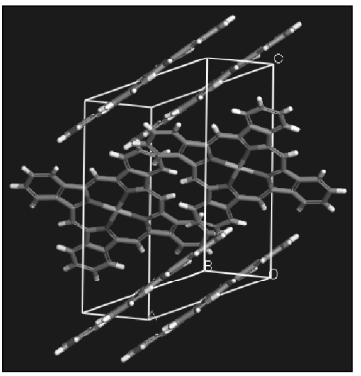
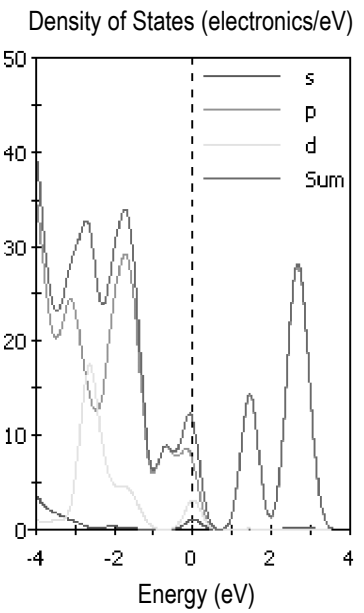
Tetrabenzoporphyrin (C36H22N4, TBP) is a solution processable polycrystalline small molecule organic semiconductor. By substituting different metal atoms in the core of the TBP molecule, such as Cu, Zn, Ni, we can modify the electrical performance and thin-film morphology of the organic semiconductor. In this project, we used the CAmbridge Serial Total Energy Program (CASTEP) and DMol^3, based on density functional theory (DFT) to calculate the energy band structure, density of states (DOS), optical properties, HOMO, LUMO and Fermi level of various metallotetrabenzoporphyrin (MTBP) molecules. This project seeks to explore the relation between the core atom and the electronic structure of the MTBP, and to further predict what core atom would be beneficial to the electrical performance of the organic semiconductor. Another goal of this project is to study the adsorption of H_2O and O_2 onto the MTBP molecules, which models the degradation of MTBP OTFTs stored in ambient. By applying DFT calculations, we hope to explain the observed increase in thin-film conductivity when the Organic Thin-Film Transistors (OTFTs) are exposed to air. This project is conducted in very close collaboration with Professors N. Ono and H. Yamada from Ehime University, Japan.



MTBP unit cell.



CuTBP DOS simulation result.