

Density functional study of electronic structure of hemes

–Roles of heme side chains and axial ligands–

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Heme is an ubiquitous cofactor in biomolecules and play a central role in biology, especially in electron transfer and enzyme catalysis. There are many types of heme, which have several heme side chains such as propionate groups. The differences in axial ligands and side chains yield many important functions of heme. In this study, we have investigated the roles of heme side chains by using density functional theory. The roles of heme side chains and axial ligands in the electronic structures and the function are discussed.