

Orientation Dependence of O₂ Dissociation from Heme-O₂ Adduct

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From an environmental viewpoint, much attention has been focused on polymer electrolyte fuel cells (PEFCs) as an alternative electronic power source of the future. However, PEFCs are too expensive for widespread use because of the large amount of platinum used for both anode and cathode electrode catalysts. Many researchers have tried to design alternative catalysts to platinum, e.g., platinum-based alloys and platinum-group metals, for many years [1]. Regardless of their great efforts, however, both cheaper and more active materials than platinum have not been discovered yet. New breakthroughs for catalyst-design may be possible using ideas other than such conventional ideas as mentioned above.

It is well known that hemoglobin (Hb) can transport oxygen and carbon dioxide in the vascular systems of animals. Heme, which has been considered as the active site of Hb, is constructed from at least one iron-porphyrin (FeP) complex. We think that the catalytic activity of FeP may be used for cathode electrode application in PEFCs, where the oxygen reduction reaction (ORR) takes place [2]. We evaluate how the orientations by which O₂ molecule binds to heme affect the O-O bond cleavage from heme-O₂ adduct using *ab initio* calculations based on density functional theory (DFT), as a first step toward better understanding of the ORR on heme [3]. Here, we consider some configurations of O₂. We will discuss the details at the symposium.

References

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