

A Density Functional Theory Study of Metal-Porphyrin Graphene for CO₂ Hydration

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Abstract : Electronic structure calculations of hydrogen terminated metal-porphyrin graphene were carried out to explore the catalytic activity for CO₂ hydration reaction. A ruthenium atom was substituted in place of carbon atom of graphene and ruthenium chelated carbon atoms were replaced by four nitrogen atoms in metal-porphyrin graphene system. Ruthenium atom created the active site for CO₂ hydration reaction. Ruthenium-porphyrin graphene followed the mechanism of carbonic anhydrase enzyme for CO₂ conversion to HCO₃⁻ ion. CO₂ hydration reaction over ruthenium-porphyrin graphene proceeded via the elementary steps: OH⁻ formation from H₂O dissociation, CO₂ bending in presence of nucleophilic attack of OH⁻ ion, HCO₃⁻ ion formation from proton migration, HCO₃⁻ ion desorption by H₂O addition. Proton transfer to yield HCO₃⁻ ion was observed as a rate limiting step from free energy landscape.

Keywords : ruthenium-porphyrin graphene, CO₂ hydration, carbonic anhydrase, heterogeneous catalyst, density functional theory

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