World Academy of Science, Engineering and Technology
International Journal of Mathematical and Computational Sciences
Vol:14, No:12, 2020

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

Authors : Manju Verma, Parag A. Deshpande

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
Conference Title : ICSRD 2020 : International Conference on Scientific Research and Development
Conference Location : Chicago, United States
Conference Dates : December 12-13, 2020