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Biomimetic Carbon Nanotube for Catalytic Hydrolysis of CO_2: First Principles Investigation of Role of Oxidation State and Metal Substitution DONGHWA LEE, Lawrence Livermore National Laboratory, YOSUKE KANAI, University of North Carolina — Reducing the amount of carbon dioxide (CO_2) in the atmosphere is one of the most important challenges we face in this century. Metallo-enzyme, carbonic anhydraze (CA), is known for its catalytic activity of CO2 hydrolysis, and a number of research groups have been experimentally working to mimic this activity in small molecules for the CO2 collection processes. Using accurate first principles electronic structure calculations, we investigate how the catalytic hydrolysis reaction of CA can be mimicked in a metal-porphyrin carbon nanotube system. Our work shows that the two-step catalytic process can be improved remarkably by controlling the oxidation state and also through the metal substitution in the porphyrin unit. Our work shows the feasibility of CO_2 hydrolysis in the metal-porphyrin carbon nanotube and also how the catalytic activity could be improved. This work is Prepared by LLNL under Contract DE-AC52-07NA27344.

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