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Prediction of a Nanostructure Called Porphyrin-Like Buckyball, Using Density Functional Theory and Investigating Electro Catalytic Reduction of Co_2 to Co by Cobalt– Porphyrin-Like Buckyball

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Abstract : The transformation of carbon dioxide into fuels and commodity chemicals is considered one of the most attractive methods to meet energy demands and reduce atmospheric CO_2 levels. Cobalt complexes have previously shown high faradaic efficiency in the reduction of CO_2 to CO. In this study, a nanostructure, referred to as a porphyrin-like buckyball, is simulated and analyzed for its electrical properties. The investigation aims to understand the unique characteristics of this material and its potential applications in electronic devices. Through computational simulations and analysis, the electrocatalytic reduction of CO_2 to CO by Cobalt-porphyrin-like buckyball is explored. The findings of this study offer valuable insights into the electrocatalytic properties of this predicted structure, paving the way for further research and development in the field of nanotechnology.

Keywords : porphyrin-like buckyball, DFT, nanomaterials, CO_2 to CO
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