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Ab initio study on the effect of phenyl substitution on the binding of carbon dioxide to salcomine

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Metal-organic complexes, such as metal-porphyrins, can function as homogeneous catalysts for electrochemical reduction. In this work we present ab initio electronic structure calculations for a reaction involving carbon dioxide and salcomine, a coordination complex consisting of a salen ligand and a cobalt (II) atom. Changes to the binding energy due to substitutions on the phenyl ring by different functional groups are also studied. Cases where a shrinking HOMO-LUMO gap decreases the overpotential and increases the catalytic efficiency of the complex are analyzed. This study provides a theoretical basis for possible salen complex candidates as electrocatalyst for the reduction of carbon dioxide.

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