A Computational Mechanistic Study on Catalytic CO_2 Fixation Reactions with Epoxides Producing Cyclic Carbonates

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The carbon dioxide (CO_2), occupying most of the greenhouse gases, continues to be reduced according to international treaties. One of the methods to remove CO_2 is producing cyclic carbonates using epoxides and CO_2 as reactants. But this reaction inherently needs the use of catalysts because it has a significantly high activation barrier (55~59 kcal/mol). Meanwhile, the computational chemistry has been applied to explain experimental results mechanistically. We thus introduce the molecular modeling methodology to suggest the most probable reaction pathways for several catalytic CO_2 fixations with epoxides and support their experimental results. Among the catalysts, we have chosen zeolitic imidazolate framework (ZIF)-90, polystyrene-supported quaternized ammonium salt, KI/KI-glycine, and dimethylethanolamine (DMEA) to provide their catalytic activities with mechanistic explanation. The approach in this study is very general to be used in other various chemical processes.