Computational Chemistry Study on the Catalytic CO_2 Fixation and Cyclic Carbonate Synthesis

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A molecular modeling methodology has been applied to explain several experimental results of the catalytic CO_2 fixation and cyclic carbonate synthesis. Carbon dioxide is known as a primary greenhouse gas and could be removed by the reaction with an epoxide to produce carbonates. However, due to a huge activation barrier (55~59 kcal/mol) of this reaction, the use of catalysts is inevitable. Among various types of catalyst, we have studied in zeolitic imidazolate framework (ZIF)-90, ionic liquid immobilized ZIF-90, polystyrene-supported quaternized ammonium salt, KI/KI-glycine, and dimethylethanolamine (DMEA). For each catalyst, the most probably reaction pathway was proposed based on the calculated energetics including reaction and activation energies. The proposed reaction mechanisms were then used for the interpretation of experimental results.