Mechanistic Studies of CO_2 Cycloaddition with Propylene Oxide (PO) to form Propylene Carbonate (PC): A Density Functional Theory Study

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Chemical fixation of CO_2 with propylene oxide (PO) to produce propylene carbonate (PC) is an attractive way to convert CO_2 into valuable chemicals. The rate-limiting step of the reaction is the CO_2 ring-opening step with the activation energy of ~30 kcal/mol. High temperature/pressure is necessary for this reaction to move forward because of the high activation barrier of the rate-limiting step of the reaction. Towards this end, development of a catalyst that can lower the activation barrier of the ring-opening reaction for CO_2 cycloaddition reaction can help lower the operating cost of the reactor and is a highly active area of research. In this work, we carried out DFT calculations on Zn-/Co-ZIF-71 to evaluate the effect of different transition metals on ring-opening mechanism for CO_2 cycloaddition reaction.