Advances in the chemical processing industry have led to increased use of small alkanes over traditional oils. The dehydrogenation of ethane is critical for the production of alkenes, which can be used to synthesize different chemicals and fuels. Oxidative dehydrogenation of ethane to produce ethylene is a key reaction in this field (Scheme 1). However, ethylene can be formed with carbon dioxide instead of hydrogen to create efficient carbon monoxide and syngas (Scheme 2). There are three important benefits of utilizing this reaction pathway instead of the first. The first benefit is that carbon dioxide only reacts with ethane, which can improve selectivity for dehydrogenation and prevent ethane conversion into undesired products. The second benefit is that such processes allow efficient production of alkenes, thereby reducing the energy required for ethylene production. The third benefit is that carbon dioxide is a greenhouse gas, which means using this reaction pathway can help mitigate climate change.

Cobalt molybdate was chosen as a catalyst in this reaction (Scheme 2) because it was found to be promising in experimental studies. Catalysts can lower the activation energy for a reaction by either orienting the reacting particles in such a way that successful collisions are more likely or reacting with the reactants to break their bonds. The second benefit is that carbon dioxide only reacts with ethane, which can improve selectivity for dehydrogenation and prevent ethane conversion into undesired products. The third benefit is that such processes allow efficient production of alkenes, thereby reducing the energy required for ethylene production. The third benefit is that carbon dioxide is a greenhouse gas, which means using this reaction pathway can help mitigate climate change.

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The dehydrogenation of ethane using carbon dioxide as the oxidant was studied using density functional theory (DFT) based molecular simulations. The goal of this project was to understand the mechanisms of such carbon dioxide assisted dehydrogenation reactions on cobalt molybdate catalysts using density functional theory (DFT) based molecular simulations.

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