Molecular Design of Efficient Catalysts for Greenhouse Gas Utilization

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Carbon dioxide reduction is a promising approach to produce fuels, while mitigating the environmental impact of greenhouse gas emissions in the atmosphere and securing the United States' energy future. In conjunction with technologies such as carbon capture and sequestration, carbon dioxide reduction closes the carbon cycle and produces useful products such as methanol or methane. However, many technical challenges must be overcome before carbon dioxide reduction can be deployed commercially. In particular, we must quantify the factors governing the rate and efficiency of the initial carbon dioxide activation and dissociation, and the role of the catalyst in the reaction dynamics. We have developed a quantum dynamics model following the time-dependent wavepacket approach to simulate the dynamics of gas-phase carbon dioxide photodissociation, and now compare our calculated absorption cross sections to experimental measurements on related systems. We demonstrate how this model may be extended to the study of photocatalytic carbon dioxide reduction at surfaces. We also present our molecular models of carbon dioxide adsorption to reduced ceria surfaces and methane dehydrogenation on platinum nanoclusters, and propose an integrated process to convert greenhouse gases to chemicals and fuels.