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Conversion of Carbon Dioxide to Oxygenates by Plasma Catalysis

Abstract.

Direct production of methanol and complex oxygenates from carbon dioxide (CO_2) and hydrogen (H_2) has been exalted as a valuable means to reuse CO_2 as energy-storing and valued-added chemicals. However, the high thermal stability of CO_2 posts challenges to transform this molecule with high efficiency. The emerging use of plasma (or a gas discharge) to excite CO_2 to far-from-equilibrium vibrational states is promising for surmounting the high-temperature requirements in traditional thermocatalytic reactions. Though plasma reactions have been shown to convert CO_2 to carbon monoxide with high energy-efficiency (>80%), reported plasmas-based conversions of CO_2 with H_2 so far yield methanol with both low conversion- and energy-efficiency. New catalyst design principles for plasma catalysis are thus critically needed to understand the complex synergy of excited chemical species with the catalyst surface for overcoming current limitations.

The major goal of this proposal is to gain insights into the roles of oxygen vacancy defects in reducible transition metal oxide catalysts in the synthesis of methanol and C_2+ oxygenates from CO_2 and H_2 through plasma reactions. These defects are hypothesized to enhance the CO_2-activation and reduce detrimental side reactions by scavenging atomic oxygen produced in the plasma. By using an experiment-theory approach, we aim to understand how excited species in the plasma react with CO_2 adsorbed onto these catalysts for methanol production. Through spectroscopic experiments, we will quantify excited chemical species in the reaction and measure the reaction kinetics as a function of catalyst structures and reaction conditions. Computation modeling will be applied to predict possible chemical species and the kinetics for each micro-step reaction. Combined experimental and computation parameters will be used to construct kinetic models for elucidating reaction mechanisms. The obtained models will be employed to pin-point the energy-efficiency or reaction steps and guide the design of multifunctional metal oxide plasma catalysts.