Nanostructure Design of Catalysts for Hydrogenation of Carbon Dioxide

Principal Investigator: Xiao Cheng Zeng, Chemistry
http://ascweb.unl.edu/possibilities/xiao.html

Abstract

The goal of this proposal is to develop a class of nanostructured cooperative catalysts on crystallographically-defined oxide support for the hydrogenation of carbon dioxide (CO_2) into methanol. Conversion of CO_2 into low molecular weight hydrocarbon such as methanol provides an alternative means to recycle CO_2 into the carbon fuel cycle. Methanol has similar density as that of water, but with a high octane number. An additional energy-science benefit is that methanol can be easily stored and recycled as a chemical feed stock and portable fuel for vehicles. Our proposed nanostructure design catalyst system consists of sub-two nanometer copper (Cu) nanoclusters on crystallographically defined zirconium oxide (ZrO_2) nanotube support. Advantages of the ZrO_2 over other supporting oxides are that it adsorbs much less water and the specific metal/oxide interface can enhance CO_2 adsorption. Nanostructured hybrid materials often exhibit unusual chemical reactivities than their bulk forms, partially because of the strong metal support interactions (SMSI). The joint experimental (Cheung) and theoretical (Zeng) effort will be directed towards the exploration of size-dependent catalytic activities, active sites on copper nanoclusters in the sub-2 nm size range, as well as effects of various nanostructured oxide (ceria, ZnO, and alumina) supports. Knowledge of structure/support-activity relationship will be invaluable to the design of optimal copper nanoclusters/nanostructured oxide support hybrid materials and to assist energy-related industries respond to federal climate change initiatives.

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The negative long-term environmental impact of increasing carbon dioxide in the atmosphere, caused by burning of fossil fuels for energy, will ultimately necessitate the development of new renewable energy sources. To harness alternative energy sources and to create more energy-efficient and environmentally friendly technologies require a concerted effort for developing novel catalytic materials. In a recent report "Catalysis for Energy" by the Department of Energy (DOE) (*www.er.doe.gov/bes/reports/files/CAT_rpt.pdf*), the importance of catalysis is stated as the following: "Catalysis—the essential technology for accelerating and directing chemical transformation—is the key to realizing environmentally friendly, economical processes for the conversion of fossil energy feedstocks. Catalysis also is the key to developing new technologies for converting alternative feedstocks, such as biomass, carbon dioxide, and water." The goal of this collaborative seed project is to search and explore a new class of nanostructured cooperative catalysts on crystallographically-defined oxide support for the hydrogenation of carbon dioxide (CO_2) into methanol. Expected outputs from the project are the synthesis and characterization of copper nanoclusters decorated zirconia nanotube catalyst. Simulation of chemical kinetics for the targeted chemical reactions – conversion of CO_2 into methanol - will be carried out using the state-of-the-art density functional theory methods. Catalytic capability of nanotube supports made of various metal oxide such as ceria, zinc oxide and alumina, and doped metal nanoclusters (e.g. chromium doped copper nanoclusters) will be also investigated. Other nanostructured oxide supports including *nanowires* and *nanoparticles* will be explored for comparison. These studies are expected to offer a wide range of possible catalytic sites and oxidation potentials for interested catalytic reactions. Success of this project will lay the pathway to strengthen current effort in catalyst development at the University of Nebraska-Lincoln, and attract future scientists and engineers into energy science research, which in turn will promote infrastructure development between disciplines and institutions in Nebraska. Convincing preliminary results attained from this seed project will be valuable for attracting new external funding.