Calculations of the mechanism and rate of CO_2 electrochemical reduction to form fuel and/or chemical feedstock

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CO_2 can be reduced electrochemically to form chemical compounds that can be used as feedstock for chemical industry or as fuel. The challenge is to find electrode materials and dielectric solutions that can provide sufficiently high efficiency and selectivity in the electrochemical process. The morphology of the electrode surface as well as the chemical composition strongly affect the overpotential and product distribution. Nanostructuring of the electrode surface can offer avenues for optimization that are not available on flat crystal surfaces. Furthermore, the electrolyte solution can be tailored for the desired performance by nanostructuring, for example by forming clathrate clusters absorbing the CO_2 and by using mixtures of fluids such as water and acetonitrile. Due to the complexity of nanostructured electrodes and dielectric solutions, performance optimization can be assisted by theoretical calculations to guide experimental research and help interpret observations made in laboratory experiments. Calculations will be presented on the mechanism of electroreduction of CO_2 on various surfaces of copper electrodes to form C1 and C_2 products. Also, calculations of nanoparticle structure will be presented and the large effect subtle changes in cluster shape can have on electrochemical reactions.