Preface

Mechanisms of Catalytic and Electrocatalytic Reduction of Carbon Dioxide

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The behavior of carbon dioxide as a greenhouse gas, and the connection between rising levels of atmospheric CO₂ from the combustion of fossil fuels and the rising mean temperature of the atmosphere, has led to increased efforts to develop processes for CO₂ mitigation. This mitigation can be achieved by recycling CO₂ as liquid fuels or conversion to other value added chemicals. Many of these processes and approaches rely on catalysis, and in particular electrocatalysis and photoelectrocatalysis. In addition to process development, increased basic research focus on the mechanisms of these promising catalytic processes is occurring. A molecular level understanding of the mechanisms of CO₂ reduction under various conditions should lead to improved processes for carbon dioxide mitigation.

This special issue focuses on the question of the molecular level mechanism of CO₂ reduction to liquid fuels and value added chemicals, under both heterogeneous and homogeneous conditions. The majority of the work discussed concerns electrocatalytic processes. Both experimental and computational studies are included in the discussion, and the two approaches combine very well in

this field to provide a more complete mechanistic understanding. Six contributions are included in this special issue, ranging from a review of reaction mechanisms for direct carboxylation routes to the formation of acyclic carbonates, to original research contributions addressing the detailed mechanism of pyridinium and imidazolium catalyzed CO₂ electroreduction processes. A general review of molecular mechanisms of electrocatalytic reduction of carbon dioxide is included, as well as a detailed computational study of the mechanism of CO₂ reduction at semiconductor photoelectrode surfaces. The issue concludes with the description of a modeling study of the engineering feasibility of an integrated anodic/cathodic electrocatalytic process for large scale electrocatalytic CO₂ reduction. Each of these contributions illustrates the broadly interesting chemistry that CO₂ reduction must address, and illustrates the collaborations among electrochemists, computational chemists, molecular inorganic chemists, surface scientists and engineers that drives this field forward.

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