

## SMS Spring 2022 Seminar Series

Friday Feb 25 | 2:30pm | Virtual

### Tuning the Properties of Catalysts for the Reduction of CO<sub>2</sub> with Metals, Ligands, and Applied Electric Fields

Catalysts for the reduction of CO<sub>2</sub> are of interest in the production of solar fuels, and as a means of mitigating atmospheric CO<sub>2</sub>. The question of which solar fuels should be made from CO<sub>2</sub> is an important one. Unlike water splitting ( $\text{H}_2\text{O} \rightarrow \text{H}_2 + \frac{1}{2} \text{O}_2$ ) where a single reduced product (H<sub>2</sub>) is obtained, the reduction of CO<sub>2</sub> can produce a variety of different chemical reduction products, CO, HCOOH, H<sub>2</sub>CO, CH<sub>3</sub>OH, CH<sub>4</sub>, to name a few, as well as C<sub>2</sub> and higher products. Which product(s) will be produced from solar energy, and then be used as building blocks to manufacture higher fuels and specialty chemicals is not presently known. Indeed, the question of whether CO<sub>2</sub> should be reduced electrochemically to an organic molecule, or instead, hydrogen produced by water splitting, should be used to hydrogenate CO<sub>2</sub> to organic products is not clearly understood at this time. There are very few known catalysts for the efficient hydrogenation of CO<sub>2</sub>, so whether electrochemical reduction or hydrogenation of CO<sub>2</sub> is ultimately practiced on an industrial scale, the development of new catalysts will be required to enable new technology. Several recent advancements in the activation and electrochemical reduction of CO<sub>2</sub> have been achieved. These include the use of earth-abundant metals including manganese, in place of rhenium and ruthenium, and the use of artificial co-factors to promote catalysis. The general properties of molecular catalysts on conducting substrates under bias as probed by surface spectroscopies pose challenges to researchers attempting to do catalysis at an electrified interface. Surface spectroscopies can provide detailed information about the electronic structure and environmental effects of catalysts operating within the diffusion layer of an electrode under bias. Recent studies of the effects of high electric fields on molecular catalysts supported on electrode surfaces will be presented. The rates of catalysts operating at different applied voltages (without current flow) will be discussed within the context of Stark Effect tuning of catalyst orbital energies. Recent results of achieving highly active hybrid electrocatalyst materials based on molecular catalysts and graphitic carbon supports for selective reduction of CO<sub>2</sub> in water at neutral pH will also be presented.

### Cliff Kubiak, PhD

*Professor, University of California, San Diego*

Clifford P. Kubiak received the Sc. B. degree with honors in chemistry from Brown University (1975) and the Ph. D. (1980) in chemistry from the University of Rochester, where he worked with Richard Eisenberg. Kubiak was a postdoctoral associate with Mark S. Wrighton at M. I. T. (1980-81). He began his independent career as a faculty member at Purdue University from 1982 – 1998. He moved to UCSD in 1998 as Harold C. Urey Professor, and served as Chair of the Department of Chemistry & Biochemistry (2002-2006). He was named Distinguished Professor at UCSD in 2008. He has held visiting appointments at Tohoku University, University of Chicago, University of Erlangen, and University of Paris - Diderot. He was Visiting Associate in Chemistry – JCAP at California Institute of Technology 2012- 2015. He was the recipient of the ACS Award in Inorganic Chemistry (2012), Inter-American Photochemical Society Award in Photochemistry (2013), Basolo Medal for Outstanding Research in Inorganic Chemistry (2015), ACS Award in Organometallic Chemistry (2018) and he was elected to the American Academy of Arts & Sciences (2014), and National Academy of Sciences (2020). He has served on the Editorial Advisory Boards of Accounts of Chemical Research, Inorganic Chemistry, and Materials Science in Semiconductor Processing. He is the author of 300 scientific articles. Kubiak's research is in catalytic transformations of CO<sub>2</sub>, artificial photosynthesis, and ultrafast electron transfer within the ground states of inorganic mixed valence systems.

