Continuum modeling to advance the development of electrochemical synthesis devices

Justin C. Bui
Lawrence Berkeley National Laboratory, University of California – Berkeley

To allay the impacts of climate change, the decarbonization of the global economy is a scientific challenge of great urgency. Electrochemical synthesis technologies, which use electricity to power the conversion of abundant feedstocks (*i.e.*, water, air, and carbon dioxide (CO_2)) to value added products, present a promising pathway to decarbonize chemical manufacturing. Unfortunately, these devices often struggle with poor efficiency and selectivity when operating at industrially relevant rates. Continuum modeling enables the simulation of transport and catalysis in these systems to observe phenomena occurring at multiple length and time scales, beyond what is achievable experimentally, to better understand drivers of performance. In this talk, I will explore how continuum modeling can guide the design of devices performing the electrochemical reduction of CO_2 to form ethylene—a precursor to plastics and one of society's most sought-after chemicals. I will demonstrate how advances in modeling have elucidated the impact of transport and reactor design in these devices, particularly with respect to the nature of pulsed electrosynthesis and the effects of electrode micro-structuring. Ultimately, I will seek to highlight the role of continuum modeling in the development of devices that will advance the technology closer to realization, and by extension, our society to a sustainable future.