HAJIM SCHOOL OF ENGINEERING AND APPLIED SCIENCES
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Department of Chemical Engineering presents

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March 6, 2019
Gavett Hall 202 @ 3:25pm

"*Theory-Guided Catalyst Design for Sustainable Energy Conversion and Chemical Production*"

Unprecedented climate change is undoubtedly the biggest challenge of the 21st century. Transitioning to sustainable sources of energy is an absolutely essential approach to reduce rising levels of CO_2 in the atmosphere. Renewable energy technologies such as fuel cells, metal-air batteries and electrolyzers are set to play an important role in replacing fossil fuels and transforming harmful chemicals to valuable/harmless compounds. There are, however, severe shortcomings in the present technologies, prohibiting them to become more economically attractive. One of the most important problems is the lack of active, selective and inexpensive catalysts for these processes. This calls for fundamental and applied research in this area, whereby catalyst development is a very exciting avenue with the potential for global impact. Revolutionary understanding of surface reactivity as well as identifying efficient catalysts have been facilitated by recent advances in theoretical tools, especially density functional theory (DFT), which combines computational efficiency with an acceptable accuracy. In this talk, I will present my recent research activities on atomic scale understanding of the frontiers of existing catalysts toward reactions of importance for clean energy processes and ultimately designing more efficient catalyst for energy conversion and chemical production. More specifically, I focus on 1) oxygen reduction reaction for fuel cells[1] and hydrogen peroxide (H_2O_2) synthesis,[2,3] 2) water oxidation reaction for H_2O_2 synthesis[4] and 3) electrochemical CO_2 reduction to produce valuable chemicals and fuels.[5,6]

References:

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