MINNESOTA LOCAL SECTION

SEPTEMBER 10TH: INEXPENSIVE, EFFICIENT APPROACHES FOR ENERGY PRODUCTION AND STORAGE

The Minnesota Local Section of the American Chemical Society is pleased to announce the upcoming September 10th, 2018 Meeting:

Inexpensive, Efficient Approaches for Energy Production and Storage

Presenter: **Dr. Amy L. Prieto**, Professor, Department of Chemistry, Colorado State University

We are interested in developing new synthetic methods for nanoscale materials with applications in energy conversion and storage. We work in three general areas: photovoltaics, hydrogen storage, and Li-ion rechargeable batteries. For this talk, I will focus on our work developing new architectures for rechargeable Li-ion batteries, with an eye toward the commercialization of this technology.

There are two main limitations to the rate of charging Li-ion batteries: slow diffusion of Li^+ into the electrodes and slow diffusion *between* them. The synthesis of high surface area electrodes has been shown to dramatically enhance performance because reducing the particle size of the electrode material reduces the distance the Li^+ ions have to diffuse. *The problem of decreasing the Li^+ diffusion length between electrodes has not yet been solved.* We are working to incorporate high surface area structures of a novel anode material into a new battery architecture wherein the current collector is conformally coated with an electrolyte made by electrochemical deposition, then surrounded by the cathode electrode. The significant advantage is that the diffusion length for Li^+ between the cathode and anode will be dramatically reduced, which should lead to much faster charging rates.

When: Monday, September 10th, 2018
No Executive Meeting
6:00-7:00pm - Social & Italian Dinner
6:50-7:00pm - Dr. Sijia S. Dong, post-doc travel grant recipient
7:00-8:00pm - Talk

Where: Bethel University
3900 Bethel Dr., St. Paul, MN 55112
Brushaber Commons
Park in the West Lot
Map (https://maps.bethel.edu/)

Cost: **$20 Meal Ticket/$5 Student Meal Ticket**
Talk is free. Please RSVP online

To purchase a meal ticket, go to the Web Store. To RSVP to only the talk, go to the RSVP page. Send any questions or comments to Arianna Ahl at amkooyman@gmail.com (mailto:amkooyman@gmail.com). Deadline to register is September 3rd.

Dr. Sijia S. Dong: Spectrum of the visual chromophore by multiconfiguration pair-density functional theory: Design of a strategy for automatic active space selection
Retinal is the chromophore in proteins that are responsible for vision. Its absorption maximum is sensitive to mutations of the protein. However, it is not easy to predict the absorption spectrum of retinal accurately, and questions remain even after

intensive investigation. Retinal poses a challenge for Kohn-Sham density functional theory (KS-DFT) because of the multireference character (strong correlation) in its excitations, and it poses a challenge for wave function theory because the size of the molecule makes multiconfigurational perturbation theory methods expensive. In this study, we demonstrate that multiconfiguration pair-density functional theory (MC-PDFT) provides an efficient way to predict the vertical excitation energies of 11-*Z* retinal, and it has accuracy better than complete active space second-order perturbation theory (CASPT2).

The procedure for selecting an active space for the reference wave functions of multiconfiguration methods is often nonsystematic. Here we demonstrate that the consistency between complete active space self-consistent field (CASSCF) and KS-DFT dipole moments is a useful and systematic criterion in selecting the active space. Based on this selection, we found that the nature of the terminal groups and the conformations of retinal play significant roles in the absorption spectrum. By considering a thermal distribution of conformations, we predict an MC-PDFT-based absorption spectrum of retinal that is consistent with experimental gas-phase spectrum and agrees better with experiments than the spectrum computed by CASPT2.