X-Breed Lecture

by Vicky V. T. Doan-Nguyen, Ph.D.

Advanced *operando* characterization of chalcogels for energy storage

日　時：平成２９年７月１３日（木）　１３：００～１４：３０
場　所：信州大学繊維学部 講義棟３１番講義室

Abstract:

Performance improvements in electrode materials for electrochemical energy storage rely upon in-depth understanding of the structure-property relations that evolve upon cycling. Nanostructured materials can be tailored to enhance metrics such as gravimetric capacity for energy storage. However, challenges remain in elucidating chemical and structural transformations that occur upon cycling. In this talk, I will discuss the use of advanced structural characterization techniques to guide materials design, in particular, *chalcogels*, for enhanced performance in energy storage.

The case study of chalcogels operates similarly to the typical Li-S conversion-type mechanism. Conversion reaction batteries operate by a different mechanism than that of intercalation materials, and they possess larger theoretical capacities. However, sulfur-based electrode materials suffer from parasitic polysulfide shuttling, which contribute to decreased capacity retention and cyclability. I demonstrate that transition metal polysulfide chalcogels

($MoS_{3.4}$) achieve high gravimetric capacity as electrode materials for lithium-ion batteries. Transition metal polysulfide chalcogels are amorphous, and comprise of polysulfide chains connected by inorganic linkers. The linkers appear to act as a "glue" in the electrode to prevent polysulfide shuttling. In the $MoS_{3.4}$ case study, the Mo polysulfide chalcogels function as electrodes in carbonate- as well as ether- based electrolytes and achieve an initial gravimetric capacity of 600 mAh/g. X-ray absorption spectroscopy and operando pair distribution function techniques were employed to elucidate the structural evolution of the electrode. Raman and X-ray photoelectron spectroscopy track the chemical moieties that arise during the anion redox-driven processes. The redox state of Mo remains unchanged across the electrochemical cycling even to 1 V and correspondingly, the redox is anion-driven. Chalcogels offer a new class of electrode materials for achieving high-capacity Li-ion batteries.

Biography:

Vicky Doan-Nguyen is University of California President's Postdoctoral Fellow and Elings Prize Fellow at the California NanoSystems Institute and the Materials Research Laboratory at the University of California, Santa Barbara and University of California, Los Angeles. Her research includes synthesis, *operando* structural characterization, and functional testing of advanced materials for energy storage and conversion. Vicky earned a B.S. in Chemistry and Women's and Gender Studies from Yale University and an M.S. and a Ph.D. in Materials Science and Engineering from the University of Pennsylvania. At UPenn, she has served as the Chair of the Penn Graduate Women in Science and Engineering (PGWISE) and led scientific demonstrations to the public and middle school girls to increase participation of women in science and engineering. During the Obama administration in 2013, Vicky interned at the White House Office of Science and Technology (OSTP). Her research at OSTP focused on science and engineering higher education policy at historically black colleges and universities (HBCUs). She has been recognized by the American Crystallographic Association for her work in powder diffraction with the Margaret C. Etter Student Lecturer Award.