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Decoding Reactive Structures in Catalysts

Abstract: Tracking the structure of catalysts under operando conditions is a challenge due to the paucity of experimental techniques that can provide atomic-level information for active metal species. As a result, the search of activity descriptors – attributes of structure, dynamics and electronic properties of working nanoscale devices that are responsible for their functionality – relies almost exclusively on theoretical prediction and human expertise. X-ray absorption fine structure spectroscopy (XAFS) stands out as an element-specific method that is very sensitive to the local geometric, dynamic and electronic properties of the metal atoms and their surroundings and, is, therefore, able to track local structure modifications in operando conditions. Here we report on the use of X-ray absorption near edge structure (XANES) spectroscopy and supervised machine learning (SML) for investigating the information content "hidden" in the spectra. Using an autoencoder-based approach, we zoom in on the latent space for obtaining the information on the number of key descriptors that affect the X-ray absorption spectrum. Using a multilayer perceptron, we determine the values of key descriptors in monometallic and bimetallic nanocatalysts and size-selective clusters. In both cases, we train the artificial neural network on theoretical XANES simulations and use it to "invert" the experimental spectrum and obtain the corresponding structural properties. An application of these methods to the determination of catalytic descriptors in operando conditions, such as studies of reactivity of dilute Pd-in-Au catalysts will be demonstrated.

Biography: Anatoly Frenkel is a Professor in the Department of Materials Science and Chemical Engineering at the Stony Brook University and a Senior Chemist (Joint Appointment) at the Division of Chemistry, Brookhaven National Laboratory. He received M.Sc. degree from St. Petersburg University and Ph. D. degree from Tel Aviv University, all in physics, followed by a postdoctoral appointment at University of Washington (Seattle). His research interests focus on development and applications of in situ and operando synchrotron methods to solve a wide range of materials problems, with most recent emphases on catalysis, ranging from nanoparticles to "single-atom" catalysts, electromechanical materials, filtration materials, quantum dots, as well as machine learning methods for structural analysis and design of nanomaterials. He is a founding Principal Investigator for the Defense Synchrotron Consortium, and the Spokesperson for the Synchrotron Catalysis Consortium, both - at Brookhaven National Laboratory. He is a Fellow of the American Physical Society. He is the author of over 400 publications.

Tuesday, September 14, 2022
12:00 PM – 1:00 PM

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