## CHEMICAL ENGINEERING

## SEMINAR SERIES



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Monday, January 28, 2019 Professor of Materials Science and Chemical Engineering

Stony Brook University

A Neural Network Approach for Operando Characterization of Catalysts: from Ultra-Small Clusters to Nanoparticles

ABSTRACT: The quest for unlocking the elusive nature of catalytic active sites in nanometer-scale catalysts often dictates the make-up of a research team. It includes chemists, able to make well-defined nano-structures that can range from shape-controlled nanoparticles to size-selected clusters to single site catalysts. Characterization experts develop new methods, required for their atomic-level characterization in operando conditions. The interpretation of such data should result in the desired structural details, but that last step is often the most difficult to make, because extracting the real-space structure from experimental spectra is often an ill-posed problem. Here we report on the use of X-ray absorption spectroscopy (XAS) and supervised machine learning (SML) for determining the three-dimensional geometry of metal catalysts. In our method, artificial neural network is used to rapidly unravel the hidden relationship between the XAS features and catalyst geometry. As a result, computers can be trained to invert the experimental spectrum and obtain the underlying structural descriptors on the fly, during the chemical reaction. I will demonstrate our approach by taking the SML to the task of reconstructing the average size, shape, compositional motifs and morphology of mono- and hetero-atomic nanoparticles that range in size from hundreds of atoms to just a few, from their experimental spectra.

RECEPTION 3:30 • LECTURE 4:00 - 5:00 PHYSICS ASTRONOMY BLDG. Knowledge and solutions for a changing world

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, having joined in the Fall of 2016. Prior to his appointment at SBU, he has held a number of different positions, including a Professor and Chair, Physics Department at Yeshiva University and a Research Scientist in Materials Research Laboratory of the University of Illinois at Urbana-Champaign. 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 the University of Washington. 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 emphasis on catalysis, electromechanical materials, filtration materials, quantum dots, physico-chemical properties of nanoparticles, as well as machine learning methods for structural analysis and design of nanomaterials. He is a founding Principal Investigator and the Spokesperson for the Synchrotron Catalysis Consortium at Brookhaven National Laboratory. He is a Fellow of the American Physical Society and the author of over 300 peer-reviewed publications, which have been cited over 15,000 times.