Contribution ID: **34**　　　　　　　　　　　　　　　　Type: **Oral Presentation**

Unlocking Hidden Functionality Descriptors in Nanomaterials with Machine Learning –Driven XAFS

Tuesday 6 January 2026 09:00 (40 minutes)

Understanding how nanomaterials work requires identifying their active units, pinpointing active sites, and providing data that inform theoretical models. Two major challenges are the intrinsic heterogeneity of active species and their dynamic restructuring in reactive environments. In the first part of my talk, I will introduce a descriptor-based approach that bridges structure and function in nanomaterials. X-ray absorption spectroscopy (XAS) is ideally suited to probe such descriptors in operando, yet their identities and numbers are often "hidden" within the spectra. I will describe the machine learning –based methodology our group has developed over the past decade to extract structural, compositional, electronic and dynamic descriptors from X-ray spectra and link them to material's function. I will also discuss extensions of this approach to other structural techniques.

Presenter: Prof. FRENKEL, Anatoly (Stony Brook University)

Session Classification: Advanced Approaches to EXAFS Analysis