



The Hebrew University Center
for Nanoscience & Nanotechnology



האוניברסיטה
העברית
בירושלים

Nano Seminar

Determination of Nanocatalyst Structure “on-the-Fly” by a Neural Network

Prof. Anatoly I. Frenkel

Department of Materials Science and Chemical Engineering, Stony Brook University, USA
Division of Chemistry, Brookhaven National Laboratory, USA

Abstract:

Tracking the structure of heterogeneous catalysts under *operando* conditions remains a challenge due to the paucity of experimental techniques that can provide atomic-level information for catalytic metal species. Here we report on the use of X-ray absorption spectroscopy (XANES and EXAFS) and supervised machine learning (SML) for determining the three-dimensional geometry of metal catalysts. Artificial neural network (NN) is used to unravel the *hidden* relationship between the XANES features and catalyst geometry. In the case of EXAFS, NN is used to obtain the radial distribution function directly from the spectra. Our approach allows one to solve the structure of a metal catalyst from its experimental XANES or EXAFS spectra. These applications are demonstrated by reconstructing the average size, shape and morphology of well-defined platinum nanoparticles¹ and monitoring structural changes in bulk Fe during its structural phase transition from BCC to FCC upon heating.² This method is applicable to the determination of nanomaterial structure in *operando* studies. It also allows on-the-fly analysis, and is a promising approach for high-throughput and time-dependent studies.

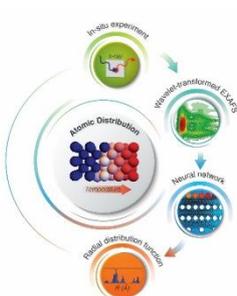
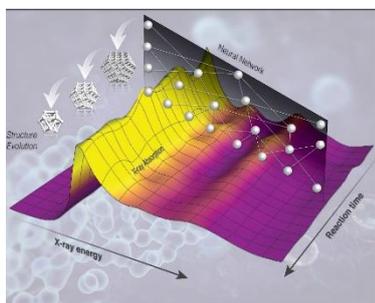


Figure 1. Illustration of the Machine Learning approach: an X-ray absorption spectrum is mapped by neural network to structural descriptors of nanoparticles (coordination numbers or radial distribution function).

References

- ¹ J. Timoshenko, D. Lu, Y. Lin, A. I. Frenkel, *J. Phys. Chem. Lett.* **8**, 5091-5098 (2017).
- ² J. Timoshenko, A. Anspoks, A. Cintins, A. Kuzmin, J. Purans, A. I. Frenkel, *Phys. Rev. Lett.* **120**, 225502 (2018).

Gathering & Refreshments at 10:50

Thursday, July 12th 2018, 11:00 at the Seminar Hall
Los Angeles Building, entrance floor.