Determination of Catalytic Descriptors from Operando Experiments Using Machine Learning

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Detecting active species and active sites in functional nanomaterials is a major challenge due to the paucity of experimental techniques that can provide atomic-level information in working conditions. We have recently demonstrated that machine learning methods can be used to decipher information about the three-dimensional geometry of mono- and bimetallic nanoparticles and clusters encoded in their X-ray absorption spectroscopy (XAS) data.[1,2] In other words, we trained a computer to learn how to '*invert*" the spectrum of a nanoparticle and map it onto the underlying structural and electronic descriptors. We have also learned how to estimate the *a priori* unknown number of these descriptors by feeding the X-ray spectrum into an autoencoder neural network and minimizing the number of nodes in the latent space of the autoencoder. These methods are gaining recognition due to their ability to extract not only descriptors that are related to the coordination numbers and interatomic distances but, in principle, all relevant descriptors that are derived from the atomic coordinates, and study their correlations. Examples will range from the determination of compositional motifs in dilute bimetallic alloys (Pd in Au) studied under operando hydrogen - deuterium exchange conditions to analysis of morphological descriptors in monometallic nanoparticles. I will discuss the extension of these applications to other techniques, beyond XAS, such as small angle X-ray scattering (SAXS) and electron energy loss spectroscopy (EELS).

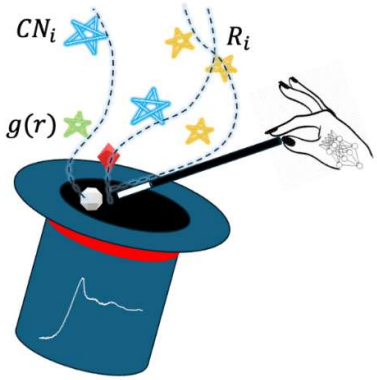

Figure 1 – Information, hidden in experimental spectra, and its "extraction" using machine learning methods

REFERENCES

1. J. Timoshenko, D. Lu, Y. Lin, A. I. Frenkel. Supervised machine learning-based determination of three-dimensional structure of metallic nanoparticles. J. Phys. Chem. Lett., **8**, 5091-5098 (2017)
2. J. Timoshenko, A. I. Frenkel "Inverting" X-ray Absorption Spectra of catalysts by machine learning in search for activity descriptors. ACS Catalysis (Perspective) **9**, 10192-10211 (2019)