X-ray absorption fine structure spectroscopy has been used to study short range order in mono- and bimetallic nanoparticles for four decades. Due to their role in catalysis, we briefly revisit their structural and compositional descriptors that affect their reactivity. Among the most frequently used descriptors are various attributes of structure, shape and compositional motifs (e.g., core-shell, random or cluster-by-cluster). While the synthesis methods are improving to provide well controlled catalytic ensembles, characterization methods lag behind, being unable to either provide accurate three-dimensional structural details of well-defined nanoparticles or do so in real working (*operando*) conditions. The main limitations are the strong asymmetry of the radial distribution function, typical for nanoparticles, and short data range due to the high temperature and low metal loading, typically used in *operando* conditions. This talk will review new methods of data analysis and modeling of nm-scale nanoparticles and sub-nm clusters that extend beyond conventional fitting of experimental EXAFS spectra. Such methods rely on the ability to theoretically generate XANES or EXAFS spectra for candidate structures and directly compare with the experiment. I will compare our approaches developed in the last 2 years in which we used Molecular Dynamics (MD)[1,2] or DFT[3] simulations, reverse Monte Carlo simulations,[1,2] blind signal separation[4] and supervised Machine Learning for XANES and EXAFS data analyses.[5] These methods were applied to a set of experimental standards of well defined mono- and bimetallic nanoparticles.

In conclusion, the new methods of data analysis and modeling of metal nanoparticles and small clusters were developed. The talk discusses the advantage of the new methods in addressing limitations of existing analysis and modeling approaches.

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