A Neural Network Approach for Structural Characterization of Metal Nanoparticles and Clusters

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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 near edge structure (XANES) spectroscopy and artificial neural network for refining the three-dimensional geometry of metal catalysts. Neural network is used to unravel the *hidden* relationship between the XANES features and catalyst geometry. To train the neural network, we rely on the *ab-initio* XANES simulations by theoretical spectroscopy codes. Our approach allows one to solve the structure of a metal catalyst from its experimental XANES, as demonstrated here by reconstructing the average size, shape and morphology of well-defined mono- and bimetallic nanoparticles.1 In the case of ultra-small clusters their average size can be estimated. This method is applicable to the determination of the structure of metal catalysts in *operando* studies and can be generalized to other nanoscale systems. It also allows “on-the-fly” XANES analysis, which is a required step for high-throughput and time-dependent studies, including the “reaction on demand” capabilities.



**Figure 1.** Illustration of the Machine Learning approach: feature space (absorption coefficient values) is mapped by neural network to nanoparticle-averaged coordination numbers that for well-defined particles can be interpreted in terms of specific sizes, shapes and structures.

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**References**

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