Deciphering experimental spectroscopic data using machine learning

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Understanding the structure of working functional materials remains a challenge, because the choice of experimental techniques that provide atomic-level information and are also suitable for operando studies is extremely limited. Among those few, an invaluable tool is X-ray absorption spectroscopy (XAS). XAS provides unique information about the environment around the absorbing atoms, but the accuracy of conventional approaches for XAS data analysis is, however, limited, when they are applied to heterogeneous, disordered structures, which are common for functional materials.

Recent developments in data-enabled discovery methods provide a key to this problem. Machine learning methods can be successfully used to correlate XAS features with the descriptors of 3D local structure.[1] Here we demonstrate the potentiality of this method on the example of studies of particle size and shape effect on X-ray absorption near edge structure (XANES) spectra of monometallic nanoparticles,[2] and operando extended X-ray absorption fine structure (EXAFS) studies of alloy formation in Cu-Zn nanocatalysts for CO_2 electroreduction.[3]

[1] J. Timoshenko, A. I. Frenkel, *ACS Catal.*, **9**, 10192 (2019)

[2] J. Timoshenko, D. Lu, Y. Lin, A. I. Frenkel, *J. Phys. Chem. Lett*., **8**, 5091 (2017)

[3] J. Timoshenko, H. Jeon, I. Sinev, F.T. Haase, A. Herzog, B. Roldan Cuenya. *Chem. Science* **11**, 3727 (2020)