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Investigation of Bond Strain Effects on XANES Spectra by Supervised Machine Learning

Content

A recently published method [1] enables the decoding of X-ray absorption near edge structure (XANES) spectra of nanoparticles to obtain important structural descriptors: coordination numbers and bond distances. Utilizing supervised machine learning (ML), the method trains an artificial neural network (ANN) to recognize a relationship between the nanoparticle structure and the XANES spectrum. Once trained, the ANN is used to "invert" an unknown spectrum to obtain the corresponding descriptors of the catalyst structure. Bond strain is known to be an important catalytic descriptor, yet, its accurate determination in reaction conditions is hampered by high temperature and low weight loading of real catalysts. ML–assisted XANES analysis offers a promising new direction for extracting the bond strain information from XANES — and not from extended x-ray absorption fine structure (EXAFS) analysis. Using simulated XANES spectra of Au nanoparticles, we have developed an ANN capable of "inverting" an unseen XANES spectrum and predicting structural disorder in the form of mean squared displacement. The utility of the method was demonstrated on both the computer-simulated nanoparticles of different sizes and degrees of disorder as well as on experimental data of disordered nanoparticles.

[1] J. Timoshenko, D. Lu, Y. Lin, and A. I. Frenkel, The Journal of Physical Chemistry Letters 8, 5091 (2017).

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