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Prediction of ELNES and Quantification of Structural Properties Using Artificial Neural Network

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ELNES observed using STEM is a promising technique for analyzing atomic and electronic structures with atomic resolution, thus it has been widely used for analyzing battery, catalysis and other functional materials. To extract materials information from the ELNES, namely, to interpret its spectral features, use of theoretical simulation is indispensable.

Theoretical simulation of ELNES is very powerful because it can be applied to unknown materials, however, in order to determine an atomic structure which reproduces the experimental ELNES, we have to perform a lot of calculations of candidate structures. Moreover, extracting materials information from their spectral features is not generally straightforward due to a complexity of relations between the spectral features and the atomic and electronic structures.

Here, to overcome those problems, we developed machine learning-based approaches for the ELNES characterization. Specifically, we used an artificial neural network to predict ELNES spectra [3] and quantify structural properties directly from ELNES [4-6]. We prepared O-K edge database of silicon oxides by a first principles calculation, CASTEP code, totally 1,189 spectra, and constructed the artificial neural network model. The crystal data of silicon oxides were obtained from Materials Project database [7]. Also, we prepared amorphous data for estimating our prediction model.

For construction of an ELNES prediction model, inexpensive information is suitable for input information. Therefore, we used partial density of states at a ground state as shown in Fig. 1 because they require much smaller computations than the ELNES calculation in which a core-hole introduction with a sufficiently large supercell is indispensable. Mean squared errors (MSE) of the crystalline silicon oxides data and one of the spectra are shown in Fig. 2(a,b). The predicted spectrum agrees well with its correct spectrum in Fig. 2(a). This implies that the artificial neural network has successfully trained the core-hole effect and it can predict the ELNES features only by its ground state electronic structure.

Then, the prediction model constructed by the crystalline silicon oxides was applied to predict the ELNES of the amorphous silicon oxides. Different from the crystalline materials, the amorphous data has much large errors as can be seen in Fig. 2(a,c). Detailed analysis revealed that the large errors are caused by a “underestimation” of the core-hole effects with comparison to the crystals. To improve the underestimation, we added bandgap information as input, resulting in excellent improvement in Fig. 2(a,d).

The details of the results and quantification of structural properties will be shown in our presentation [8].

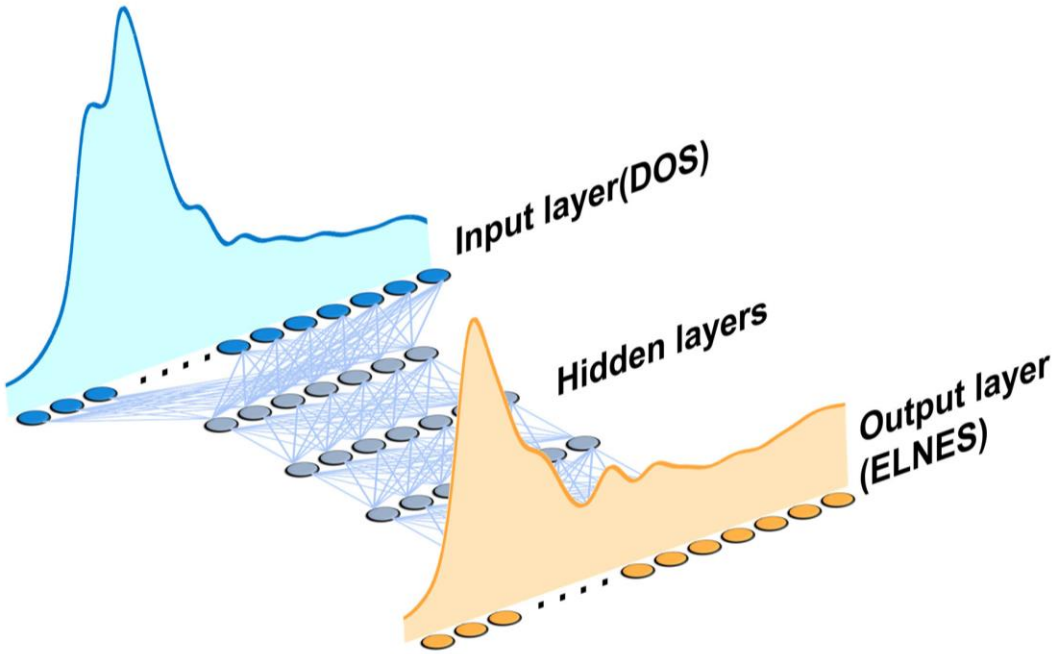

Figure 1. Neural network architecture for predicting ELNES.

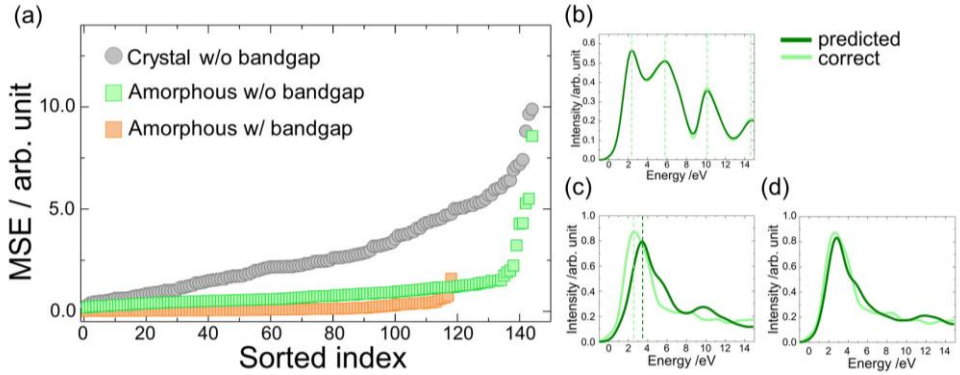

Figure 2. Prediction of crystal and amorphous test data. (a) Mean squared errors (MSEs) are plotted. Grey dots are crystals, and green and orange squares are amorphous with and without bandgap, respectively. (b,c) Predicted and correct spectrum of one of the crystal and amorphous, respectively. (d) Predicted and correct spectrum of the same amorphous data considering bandgap.

References
[1] F. Paruzzo et al., *Nature Communications*, **9** (2018), p. 4501.
[2] F. Oviedo et al., *npj Computational Materials*, **5** (2019), p. 60.
[3] S. Kiyohara et al., submitted.
[4] S. Kiyohara et al., *J. Phys. Mater.*, **2** (2019), p. 024003.
[5] T. Mizoguchi and S. Kiyohara, *Microscopy*, (2020), p. 1.
[6] S. Kiyohara and T. Mizoguchi, in preparation.
[7] A. Jain et al., *APL Materials*, **1** (2013), p. 011002.
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