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A 3D Graph Neural Network-Based Approach to 3D Structure Analysis of XAS

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X-ray Absorption Spectroscopy (XAS) is an instrumental technique for elucidating the atomic-scale three-dimensional local structure of materials. Within XAS, the X-ray Absorption Near Edge Structure (XANES) region is particularly significant, as it provides insight into the three-dimensional structural characteristics. However, extracting quantitative three-dimensional structural information from XANES data necessitates a profound comprehension and precise assessment of structural nuances, often requiring the synthesis of multiple structural parameters—a feat that can be challenging to accomplish. Here, we develop Physics-Informed Graph Neural Network models capable of computing XANES spectra directly from inputted 3D structures. We improve the efficiency of the model based on the physical meaning of XAS. Initially, we focus on geometric features, specifically bond lengths, angles, and the dihedral angles between the absorbing atom and its surrounding atoms, which play a pivotal role in determining the fine structures observed within the spectrum. Consequently, these are deemed the most efficacious geometric parameters to be incorporated into our model. Furthermore, a judiciously selected feature function is implemented to augment the predictive efficacy of the model. Secondly, we examine the definition of a graph tailored for XAS analysis. In previous 3D GNN model, the typical approach adopts a uniform distance cutoff to define neighboring atoms around a central atom. But for XANES which primarily investigates the local environment surrounding the absorber atom, the topological significance of the graph edges associated with the absorber becomes critical. To address this, we introduce a customized graph extraction methodology in our XAS3Dabs model, which selectively focuses on the immediate vicinity of the absorber atom.

I plan to submit also conference proceedings

No

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