EdgeALIGNN: Edge-centric graph neural networks for predicting bond-resolved properties in crystalline and disordered materials

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Abstract:
Quantum-chemical bonding descriptors are powerful tools for understanding and predicting material properties such as thermal conductivity and hardness [1-2]. However, computing descriptors such as the Integrated Crystal Orbital Bond Index (ICOBI) and the Integrated Crystal Orbital Hamilton Population (ICOHP) requires computationally expensive electronic-structure calculations, making large-scale studies of complex and disordered materials challenging. Materials can be represented as graphs, with nodes and edges corresponding to atoms and bonds, respectively, and this architectural representation is used in graph neural networks (GNNs). Here, we develop EdgeALIGNN, an edge-centric GNN based on ALIGNN [3], that predicts bond-resolved quantum-chemical descriptors directly from structures. Unlike most materials graph neural networks, which target graph-level properties, our model predicts edge-level quantities corresponding to individual chemical bonds. Pretrained on a large database of VASP-LOBSTER calculations, the model accurately predicts bond order (i.e., ICOBI) and bond strength (i.e., ICOHP), enabling efficient bonding analysis of chemically complex materials, interfaces, and amorphous systems. Furthermore, we demonstrate that the pretrained models can be fine-tuned with limited additional data, enabling accurate predictions of bonding descriptors across different levels of electronic-structure theory.

References:
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