Transfer Learning of a Universal Hamiltonian Graph Neural Network for Metal-Organic Frameworks

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Metal-organic frameworks (MOFs) are versatile materials with tunable crystal structures, morphologies, and chemical compositions, enabling a wide range of physical and chemical properties. Although most MOFs are intrinsically electrically insulating, carefully selected combinations of organic linkers and inorganic nodes can introduce electrical conductivity and redox activity [1]. Electronic structure methods, particularly Density Functional Theory (DFT), provide deep insight into the underlying chemistry and physics of these systems and are widely used to investigate their properties. However, the vast chemical design space of MOFs makes identifying optimal candidates for targeted applications a formidable challenge, further compounded by the computational cost of DFT [2], which limits its scalability for high-throughput discovery of novel electroactive MOFs. To tackle these challenges, in this work, we exploit a Universal Hamiltonian Graph Neural Network Model (Uni-HamGNN [3]), an E3-equivariant graph neural network for Hamiltonian prediction, to predict electronic properties of MOFs. We present a fine-tuning workflow for Uni-HamGNN, adapted for application to MOFs by using selective DFT-computed Hamiltonians as ground truth. The fine-tuned model achieves improved Hamiltonian matrix element accuracy compared to the pretrained baseline, making it reliable for electronic structure prediction.

References

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