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Machine Learning Based Molecular Properties Discovery for Quantum-chemical Simulations

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ABSTRACT

In molecular quantum mechanics, mappings between molecular structures and their corresponding physical and chemical properties greatly influence the accuracy of simulation for chemical interactions at the quantum level. Based on the information of molecular structure-property mappings, researchers could use the mappings to assemble and build new materials with certain molecular properties in the future. Scientists used density functional theory (DFT)-based methods for predicting material behavior. However, the accuracy of using DFT-based models is highly restricted since the methods are usually designed based on specific molecules, and thus when it is applied to large-scale simulations, the accuracy is unpredictable. Recently, machine learning became a popular way to figure out mappings that can minimize the prediction deviations by training with large-scale datasets and constructing unique neural networks to easily extract features from input representations. The networks that we mainly used include convolutional neural networks (CNN) and fully connected neural networks. A simulation tool called *Molecular Quantum Machine* is built based on the machine learning model we designed. It will be published on nanoHUB.org and could be used to get a value of predicted atomization energy when it is given an organic molecule structure. The tool can give users an immediate prediction with an error rate of below 0.8%. The efficiency with which the simulation tool could bring is useful for engineers and scientists to get accurate molecular structure-atomization energy predictions with low computation costs immediately.

KEYWORDS

molecular properties, machine learning, convolutional neural network