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Modeling Amorphous Silicon Using Neural Networks

Wednesday 9 June 2021 13:00 (3 minutes)

In this work, we present a method based on deep learning (DL) to predict the structure of amorphous silicon (a-Si). The accuracy of our approach is validated through training networks to estimate the potential energy. Two architectures, multilayer perceptron (MLP) and convolutional neural network (CNN), have been examined for this purpose.
The models have been trained on a dataset generated by molecular dynamics (MD) simulations. The dataset consists of 216-atom a-Si configurations.
The performances of the two architectures over the test set are compared while they have the same total number of parameters and layers.
The results of training these two neural networks yield a
root mean square error of the order of 0.1 meV/atom. This error was reported in the range of 2-6 meV/atom in previous works [1-3], which confirms the accuracy of our models. Calculation of the average error shows that CNN performs better than MLP.
After validation of our approach, we trained a generative model, variational autoencoder (VAE), to generate a-Si configurations. The generated structures and their structural properties are comparable to the real ones. In general, the performances of our models are quite satisfactory, and this suggests that they could be used to approximate the potential energy and generate a-Si structures, and thus be a viable model for investigating disordered systems.

References:
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2. Comin, M. and Lewis, L.J., 2019, Deep-learning approach to the structure of amorphous silicon, Physical Review B 100, 094107.
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Authors: Dr FADAIE, mojde (University of Montreal); Prof. LEWIS , Laurent (University of Montreal)

Presenter: Dr FADAIE, mojde (University of Montreal)

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