Reinforced Learning in Optimization of Interatomic Potential

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ABSTRACT

The analysis of nanostructures at the atomic level requires knowledge of interatomic interactions. There is a lot of data available in the literature for potentials, but it is often necessary to adjust the parameters of interatomic interactions for unusual structures, e.g. two dimensional materials. The aim of this work is to present a method for the optimal selection of interatomic parameters using machine learning techniques. Reinforced learning is one of the groups of methods that allow the use of artificial intelligence in the selection of parameters or models of real systems. The article uses the Monte Carlo Tree Search method [1,2] combined with local and global optimization algorithms for the optimal selection of silicon potential parameters for two dimensional structures.

The research used Molecular Dynamics (MD) to simulate nanostructures, and based on the results, nanostructure parameters were determined and compared with standard data from the literature. The aim of the optimization was to ensure the greatest possible compliance of the nanostructure parameters with the reference data. MD analyses were performed using the LAMMPS package [3].

The full article presents a description of the method as well as numerical examples for the two dimensional structure of silicon – silicene.

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