BIOINSPIRED OPTIMIZATION OF MOS2 2D MATERIAL WITH PRESENCE OF DEFECTS

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The article is devoted to the optimization of the atomic structure of two-dimensional MoS₂. The purpose of optimization is to determine the material structure with given mechanical properties. The design variables are microstructure parameters. The purpose of optimization is to obtain not only a structure with given material properties but also a stable system of atoms with minimal energy (minimum local energy). Due to the frequent occurrence of defects [2] in the form of missing S atoms or the substitution of Mo atoms in place of S, the analysis considers the effect of such errors. The MoS₂ structure is modelled with use of LAMMPS software [1,3] and the S-W interatomic potential [4] is used during computations. Optimization is carried out using biologically inspired algorithms to determine the global optimum. The algorithm based on combined evolutionary algorithm, artificial immune system and particle swarm optimization is used.

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References