# BIOINSPIRED OPTIMIZATION OF MOS2 2D MATERIAL WITH PRESENCE OF DEFECTS

**Wacław Kuś [1]*, Mohammed J. Akhter [2], Adam Mrozek [3], Tadeusz Burczyński [2]**

[1] Silesian University of Technology, Gliwice, waclaw.kus@polsl.pl
[2] Institute of Fundamental Technological Research Polish Academy of Science, Warszawa, tburczynski@ippt.pan.pl
[3] AGH University of Science and Technology, Cracow, Poland, amrozek@agh.edu.pl

**Keywords**: *Optimization, Atomic structure, $MoS_2$*

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 $MoS_2$ 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.

The research is funded within National Science Centre Poland project no. 2016/21/B/ST8/02450.

Calculations were performed in part at the Interdisciplinary Centre for Mathematical and Computational Modelling at the University of Warsaw under grant GB75-14.

## References

[1] Lammps Molecular Dynamics Simulator, accessed 24.09.2018, *http://lammps.sandia.gov*, 2018.

[2] M. Li, Y. Wan, L. Tu, Y. Yang and J. Lou. The Effect of VMoS3 Point Defect on the Elastic Properties of Monolayer MoS2 with REBO Potentials. *NanoscaleResearchLetters* 11:155, 2016.

[3] A. Mrozek. Basic mechanical properties of 2H and 1T MoS2 polymorphs. A short comparison of various atomic potentials. *International Journal for Multiscale Computational Engineering*, 2019 DOI: 10.1615/IntJMultCompEng.2019029100 (in press).

[4] F. H. Stillinger and T. A. Weber. *Physical. Review B,* 31:5262, 1985.