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Optimization of 2D materials based on Molybdenum

Tadeusz Burczyński 1 a),*, Wacław Kuś 2 b), Adam Mrozek 3 c)

[a)] Institute of Fundamental Technological Research, Polish Academy of Sciences, Warszawa, Poland
[b)] Silesian University of Technology, Gliwice, Poland
[c)] AGH University of Science and Technology, Cracow, Poland

tburczynski@ippt.pan.pl

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2D materials play important role in modern material science. Apart from graphene [1] based on carbon there is possible to create new 2D materials based on molybdenum. One of the most prominent 2D material is the Molybdenum Disulfide (MoS_2), which reveals polymorphism at the nanolevel. The 2H phase has semiconducting properties and approx. Young's modulus equals to 130 N/m, while the 1T polymorph reveals metallic or ferroelectric properties and two times lower stiffness [2]. Both phases of MoS_2 can exist simultaneously [3]. This paper presents an optimization approach enabling to obtain MoS_2 heterostructures with desired mechanical properties. The proposed memetic approach combines the global optimization, based on the bio-inspired algorithms (e.g. evolutionary algorithm) with the local conjugated-gradient minimization of the potential energy of the nanostructure [1, 4]. The behavior and energy of the atoms is determined by the REAX-FF potential [2].
Memetic optimization of MoS_2 with presence of defects [5] in the form of missing S atoms or the substitution of Mo atoms in place of S is also considered. The MoS_2 structure is modelled with the use of LAMMPS software [6] and the Stillinger-Weber interatomic potential is used during computations.

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