

Design of new 2D materials using computational intelligence

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Abstract:

New potentially 2D materials based on carbon and molybdenum are generated by the intelligent memetic strategy combining the evolutionary algorithm and the conjugate-gradient optimization technique and molecular model [1,2]. The main goal of the optimal design is to find stable arrangements of carbon atoms under certain imposed conditions. The fitness function is formulated as the total potential energy of an atomic system. The optimized structure is considered as a discrete atomic model and interactions between atoms are modeled using the AIREBO potential. The parallel approach used in computations allows significant reduction of computation time. Validation of the obtained results of new 2D graphene-like materials obtained using the described algorithm are presented [3]. Apart from graphene one of the most prominent 2D material is the Single-Layered Molybdenum Disulfide (SLMoS₂), which reveals polymorphism at the nano-level. The paper presents optimization technique which allows to obtain SLMoS₂ heterostructures with desired mechanical properties. Proposed method combines the memetic global optimization of the potential energy of the nanostructure. The behavior and energy of the atoms is determined by the REAX-FF potential. Examples of such periodic SLMoS₂ 2H/1T heterostructures are presented [4].

References

[1] Burczyński, T. et al., *Intelligent Computing in Optimal Design*. Springer (2020).

[2] Burczyński, T. et al., *Multiscale Modelling and Optimisation of Materials and Structures*. Wiley (2022).

[3] Mrozek, A., Kuś, W., Burczyński, T., Nano level optimization of graphene allotropes by means of a hybrid parallel evolutionary algorithm. *Computational Materials Science*, Vol.106, pp.161-169 (2015).

[4] Kuś W., Akhter M., Burczyński T., Optimization of monolayer MoS₂ with prescribed mechanical properties. *Materials*, 15, 2812 (2022).

Biography of presenting author

Scientific degrees PhD and D.Sc. from Silesian University of Technology in Poland. He is member of Polish Academy of Sciences and European Academy of Science and Arts. He is the director of Institute of Fundamentals Technological Research of Polish Academy of Sciences. He has published in excess of 500 papers and 14 books.

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