Nanoscale Modelling of New 2D Materials

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KEYWORDS: *2D Materials, Interatomic Potentials, Nanoscale Modelling, Moire Pattern, AI Algorithms.*

2D materials play important role in engineering applications and the problem how to design new ones based on atomistic and nanoscale modelling is the subject of the paper.
The following problems are considered:
- for 2D Materials with p-orbitals, (graphene analogues), i.e. the case of materials where valence electrons are well spread as they reside on weakly correlated p-orbitals, we shall inquire how does the change of constituents towards heavier atoms affect structural properties;
- for 2D Materials with d-orbitals we shall explore whether our relatively simple method can be extended to capture systems with electrons correlations.
The main goal is to find stable arrangements of selected atoms of carbon, molybdenum, silicon and tin under certain imposed conditions. The total potential energy of an atomic system is minimized by AI in the form of a hybrid parallel evolutionary algorithm.
In the case of carbon 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 allotrppes obtained using the described metodology is presented, along with their mechanical properties [1,2].
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. The behavior and energy of the atoms is determined by the REAX-FF potential. Examples of such periodic SLMoS2 2H/1T heterostructures are presented with corresponding mechanical properties [3].
The ability of various interatomic potentials to reproduce the properties of silicene and tin, that is, 2D single-layer silicon and the stanene (2D tin), polymorphs are also examined [4], [5].
Finally, we present also mesoscopic scale superstructures, as a new tool to tailor properties of 2D materials. The simplest example here is Moire pattern in bi-layers, a generator of which is presented.

ACKNOWLEDGEMENT: This work was supported by the National Science Centre (NCN– Poland) Research Project: No. 2021/43/B/ST8/03207.

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