ARTIFICIAL INTELLIGENCE IN DESIGN OF NEW NANOSTRUCTURES

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The intelligent computing method based on a memetic strategy combining the evolutionary algorithm and the conjugate-gradient optimization technique and molecular model is used to design new potentially 2D nanostructures based on carbon, molybdenum and silicon [1].

The main goal is to find stable arrangements of atoms under certain imposed conditions. The fitness functions are formulated as the total potential energy of an atomic system. The optimized nanostructure is considered as a discrete atomic model based molecular dynamics. Interactions between atoms of carbon, molybdenum and silicon are modeled using the diferent potentials. Validation of the proposed methodology was performed for new 2D graphene-like materials using AIREBO potential [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 behaviour and energy of the atoms is determined by the REAX-FF potential. Examples of such periodic SLMoS2 2H/1T heterostructures are presented [3].

New nanostructures based on silicon are also presented using the presented intelligent methodology and interatomic potentials [4].

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