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Computational Intelligence in Design of New Nanostructures

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ABSTRACT

New potentially 2D nano-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].

The main goal of the optimization 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, along with their mechanical properties.

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 with corresponding mechanical properties.

REFERENCES

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