Molecular and Ab-initio Approaches in Computational Design of New 2D Nano-Structures

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Computational design of nano-structures belongs to challenging problems of interdisciplinary modeling and can be considered in terms of big data analysis and optimization issues.

Potentially new, single-atom thick nano-structures based on carbon are generated by the two stage searching strategy linking molecular and ab-initio approaches.

In the first stage optimal searching for new stable atomic arrangements of 2D carbon lattices with predefined mechanical properties is presented using the memetic method combining the evolutionary algorithm and the conjugate-gradient optimization. The main goal of the optimization is to find stable arrangements of carbon atoms revealing desired mechanical properties. The semi-empirical potential (AIREBO) is used in these molecular simulations.

The nano-structures derived from the first stage are then profoundly analyzed in the second stage using the first-principles density functional theory from the structural, mechanical, phonon and electronic properties point of view.

Finally, the proposed nano-structure is mechanically, dynamically and thermally stable and can be considered as semiconducting-like with a direct band gap of 0.829 eV.

Some results in this paper are unique and we trust will be verified by other works. The synthesis of the proposed structure is a separate task and goes beyond the area of this work.

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