DEPOSITION, ALLOYING AND STACKING OF 2D HONEYCOMB MATERIALS: A VIEW FROM FIRST PRINCIPLES*

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Graphene provided the impact and excitement to explore isolated two-dimensional (2D) crystals, such as hexagonal boron nitride (*h*-BN), transition-metal dichalcogenides (TMDCs), phosphorene, and many others, providing a rich variety in composition, electronic structure and properties. Their unique optical, electronic and mechanical properties make them the next frontier in advanced materials for optical and electronic thin flexible devices applications based solely on 2D layers. Therefore, considerable effort has recently been directed to the synthesis and modification of 2D materials for band gap engineering.

In this talk, I discuss, by means of first-principles electronic structure calculations, the possibilities of synthesizing 2D crystals on a substrate and altering their electronic band structures via different approaches, as alloying and stacking 2D materials vertically, the known van der Waals (vdW) heterostructures. In this context, the following systems are systematically discussed:

(i) The deposition of Sn atoms on top of a Si-terminated 4H-SiC(0001) surface. The influences of the Sn overlayer geometry, the surface passivation by H and F as well as the chemical functionalization of the Sn layer by fluorine and hydrogen, and their topological character are investigated in detail. The explicitly calculation of Z2 invariant shows that the passivation of the substrate is mandatory for obtaining tin based 2D topological insulators.

(ii) The alloying among the group-IV elements [1] and between graphene and *h*-BN are studied considering different local atomic configurations and a statistical method to account for disordered effects, discussing their phase stability through temperature versus composition phase diagrams and predicting the electronic and optical properties.

(iii) The coincidence lattice method derived from surface studies is developed to predict new possibilities for the simulation of vdW heterostructures [2]. This includes finding supercells that require little computational effort to simulate, despite being incommensurable, and assessing combinations with specific rotation angles. This enables theoretical studies to explore deeper possibilities within vdW-bonded systems, effects due to interlayer twist, or Moiré patterns despite limited computational resources. Theoretical structures can be easily created to emulate real-world samples. Results are given and discussed for a variety of the most interesting TMDCs, group IV dichalcogenides, graphene, and group III− V compounds.

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Keywords: first-principles calculations; 2D materials; deposition; alloys; phase separation; van der Waals heterostrutures

References

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