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Mechanical and electronic properties of hybrid graphene-hBN monolayers under strain

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Abstract

Hybrid graphene-hexagonal boron nitride (hBN) monolayers have already been synthesized, but most investigations on their properties have only considered relaxed structures. In this talk, I will discuss the mechanical and electronic properties of two types of monolayers: in (i), we have a graphene sheet with hBN domains; in (ii), we have an hBN sheet with graphene domains. The results were obtained by combining density functional theory and molecular dynamics simulations. Regarding the mechanical properties, we find that we can control the Young´s modulus by adjusting the fraction of graphene and hBN in the hybrid monolayer, whereas the ultimate strength and strain are limited by the strength of the hybrid C-B and C-N bonds. Furthermore, the results show that the mechanical properties do not depend on the size of the considered structure. Concerning the electronic properties, we find that by combining composition and strain, we can produce hybrid sheets with band gaps spanning an extensive range of values (between 1.0 eV and 3.5 eV). Our results also show that the band gap depends more on the composition than on the external strain, particularly for structures with low carbon concentration.