Layered and two-dimensional materials explored from first-principles

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Abstract

Three-dimensional crystals with low dimensionality (*i.e.,* small effective electronic interactions in one or two dimensions) have a rich physical behavior that has been the subject of intense study over the last decades. Electronic instabilities in these systems play a crucial role in their properties, and simplified models have been used traditionally to predict and explain these properties. Their structural complexity has usually been an important difficulty for a fully first-principles approach for their study. However, current first-principles methods and computational facilities are now sufficiently powerful and efficient to allow us to attack problems which were formerly too complex to be tackled with these techniques.

Besides, layered materials are experiencing an impressive thrust due to the possibility of obtaining truly atomically-thin two-dimensional layers like in graphene. The unique properties of these layers, and the infinite possibilities offered by the formation of structures obtained from staking multiple layers of different materials, confer these systems a huge potential for devices with new functionalities.

I will describe some of our efforts in attacking some long standing problems in these materials using first-principles simulations. Examples are the prediction of Charge Density Waves in low dimensional metals originated from Fermi level instabilities, the electronic properties of two-dimensional materials like graphene containing impurities and disorder, and the interfaces of two-dimensional layers like graphene and MoS_2.