Substitutional doping in MoS_2

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Planar materials, such as graphene [1,2], have recently raised a great deal of interest due to the exceptional electronic properties, in particular a high electron mobility [3], which render them very attractive as the channel material for a field effect transistor (FET). On the other hand, graphene has a semimetallic character, with the bands crossing at the Fermi point, which causes a residual non-negligible conductivity even in the off state. Thus, great efforts have been made to generate a gap in graphene by the action of external biases, fabrication of bilayered structures, molecular adsorption, strains, etc.; but that has been at a cost to the electronic transport properties [4].

A different approach is to choose a different planar material with a semiconductor character from the onset in order to fabricate an FET channel, such as Radisavljevic *et al.* have recently made [4]. They have used MoS_2, which is similar to graphene in the sense that it is a layered hexagonal material with strong covalent intralayer bonding and a weak van der Waals interlayer bonding. This lies at the root of the extremely good properties of MoS_2 as an industrial solid lubricant, as well as the facility with which it can be exfoliated into single layers, with a structure shown in Fig. 1. The semiconductor character of the MoS_2 single layer is clear in Fig. 2, with a direct GGA band gap of 1.67 eV, comparing to the experimental value of 1.8 eV [5].

Of course, the addition of dopant impurities to a semiconductor is what enables the fabrication of a multitude of interesting devices. We will present first-principles calculations of dopant activation energies of different single substitutional impurities into the MoS_2 lattice, in order to identify promising candidates for shallow p- and n-type doping, using a method that we have recently developed [6,7] to correct for the spurious interactions arising from the periodic boundary conditions.

References

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Figures

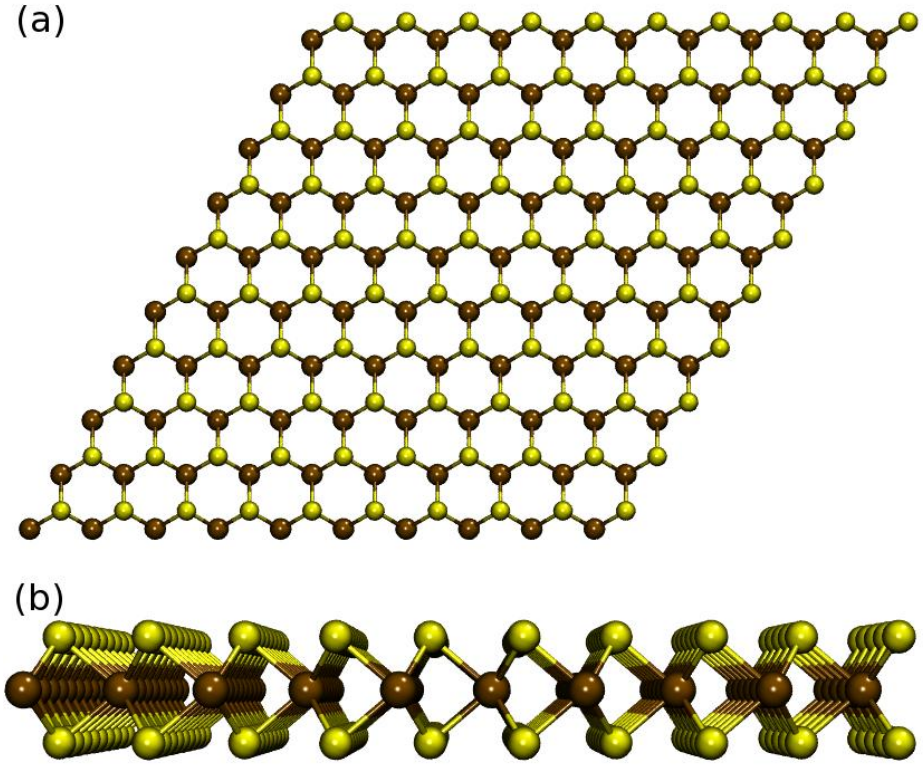

FIG. 1: *(a) Top and (b) side view of a single layer of MoS_2.*

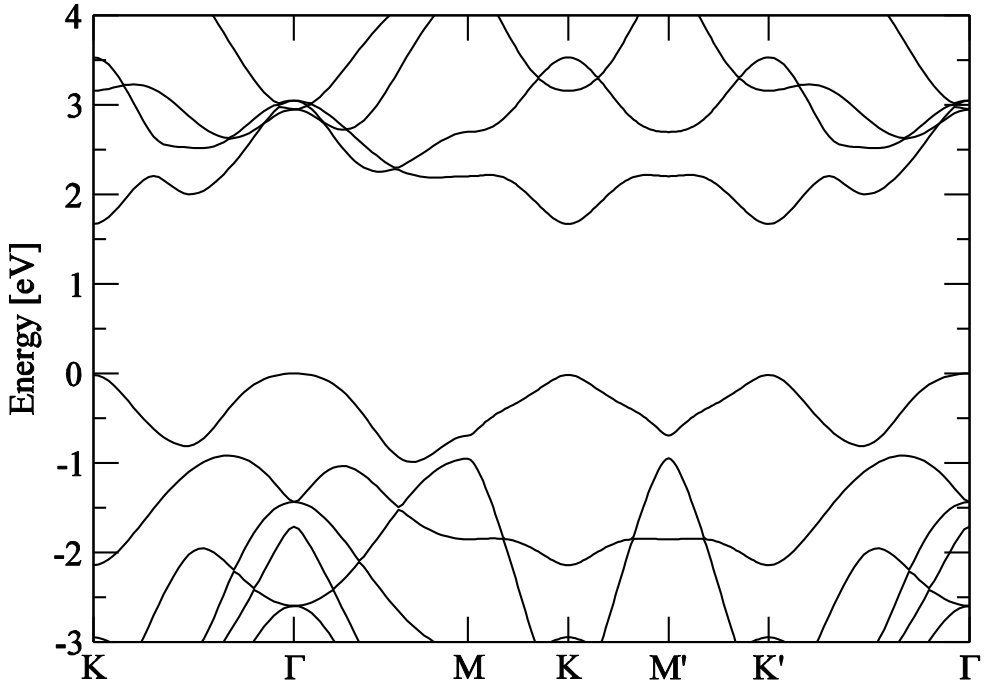

FIG. 2: *Band structure of a single layer of MoS_2.*