Self-doping in boron nanostructures: A route to structural design of metal boride nanostructures

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Superconductivity in one-dimensional nanostructures has become an appealing subject since the discovery of superconductivity in small-radius carbon nanotubes. In particular, metal boride nanotubes have attracted special attention in direct analogy with the superconducting bulk MgB_2. MgB_2 nanotubes are even argued to have higher superconducting temperature than bulk MgB_2 at 40K. However, the structures of atomically thin metal borides are largely unknown. Moreover, it is unclear whether the stoichiometry MgB_x with x=2 is the correct option for Mg or any other metal boride nanostructures. In order to elucidate these problems, a scheme is needed for finding the best structure at each MgB_x stoichiometry that greatly reduces the potentially enormous search space.

We present a novel self-doping picture in two-dimensional boron sheets. Using density functional theory, we show that for two-dimensional boron sheets adding or removing atoms does not change the number of bonding states but merely adding or removing electrons from the sheets. We demonstrate two applications of this self-doping picture. First, we propose a general design rule for boron, which explains many stable boron nanostructures discovered previously and provides a general method for construction of stable boron structures that may not have been considered before. Second, based on self-doping and simple charge transfer considerations, we develop an efficient scheme to search for stable metal boride nanostructures for arbitrary stoichiometry MgB_x. We apply this method to investigate the structures of atomically thin MgB_2 sheets and find a series of stable structures better than known or commonly accepted one. This new structure is thus more likely to be the precursor of atomically-thin MgB_2 nanotubes.

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[2] H. Tang and S. Ismail-Beigi, Phys. Rev. B **80**, 134113 (2009).