GEOMETRIC, ELECTRONIC AND HYDROGEN PHYSISORPTION PROPERTIES OF BORON SHEETS AND NANOTUBES

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First principles calculations of the properties of the recently synthesized boron nanotubes (BNTs) [1] and sheets have been carried out. These nanostructures have a buckled surface, with a large buckling height of 0.8 Å (See Figures 1 and 2). This buckling stabilizes these structures, compared to the flat ones, by about 0.20 eV/B atom, and the buckling structure is identical to that of the quasi-planar B_{96} cluster, reported by Boustani et al. [2]. BNTs are metallic independently of their helical structure (armchair, zigzag and chiral), in contrast with the behaviour of carbon nanotubes (CNTs). Molecular hydrogen physisorption energies on different sites of the external buckled surface of the boron sheets and nanotubes are about 50-60 meV, smaller than on the external surface of graphene sheets and carbon nanotubes. This indicates that BNTs are not appropriate candidates for hydrogen storage. Chemisorbed states of the dissociated hydrogen on boron nanotubes have lower or similar energies than states corresponding to the physisorbed hydrogen molecule. The energy barrier from physisorption to dissociative chemisorption is about 1 eV, while this energy barrier is about 3 eV in CNTs.

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References:

[1] D. Ciuparu, R. F. Klie, Y. Zhu and L. Pfefferle, J. Phys. Chem. B **108**, 3967 (2004)
[2] I. Boustani, A. Quandt and A. Rubio, J. Solid State Chem. **154**, 269-274 (2000)

Figures:

Figure 1: Buckled boron sheet from different perspectives, with the structure and buckling height of 0.8 Å obtained in the relaxations of the geometry

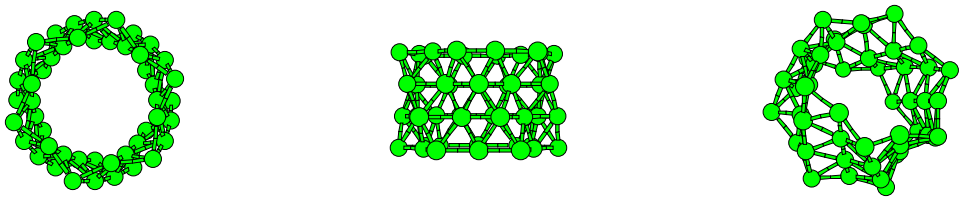

Figure 2: Buckled boron nanotubes from different perspectives, with the structure and buckling width of 0.8 Å obtained in the relaxations of the geometry