Magnetism of Fe/BN-Nanotube Hybrid Structure

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Abstract:

A systematic study of Fe wires interacting with zig-zag boron nitride (BN) nanotubes is presented. Spin-polarized total-energy ab initio calculations based on the density functional theory are used to describe the structural, electronic and magnetic properties of all studied systems. The Fe wires, either outside or inside the nanotube, the most stable configuration is found to be over the centre of the hexagonal site. For all the investigated Fe structures adsorbed on the BN nanotubes, either high-spin or low-spin, the interactions between Fe atoms, between Fe and B and between Fe and N atoms become stronger as the Fe coordination number increases. The resulting magnetic moments for all adsorbed systems are found to be close to their original values for the corresponding free Fe structures. Some special magnetic properties resulting from the interaction between the Fe wires and zig-zag BN nanotubes are found. Our calculations suggest that for applications to spin transport devices, it is desirable to form magnetic nanostructures isolated by a non-magnetic material, i.e., BN walls, could be efficiently used for high-density data storage.