Half Metallicity in BC_2N Nanoribbons: Stability, Electronic Structures, and Magnetism

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1 Supporting Information - Evaluation of the Exchange-correlation Functional

To evaluate the accuracy of the results obtained with the PBE exchange-correlation functional, we have examined the electronic structures of the C^BC^N-4-BC_2NNR with both the GGA-PBE[1] functional and the HSE[2–4] hybrid functional. The HSE functional has recently shown great improvement in prediction of band gaps of semiconductors, for example graphene nanoribbons and boron nitride nanoribbons. The calculations were performed with the Vienna ab initio simulation package (VASP)[5–8], and the same configurations (relaxed with PBE functional) were used in this test. In all the simulations, we have employed the projector-augmented plane-wave (PAW)[9,10] to model the electron-ion interactions, a cutoff energy of 400 eV, and a $1 \times 1 \times 5$ kpoint mesh in the Monkhorst–Pack[11] scheme.

We present the spin-resolved band structures of ferromagnetic and anti-ferromagnetic states for the C^BC^N-4-BC_2NNR in Fig. 1. We only tested two states of one typical BC_2N nanoribbon because calculations with the HSE exchange-correlation functional were very time consuming, and the convergence of the self-consistent field (SCF) cycle is hard to achieve. However, for the purpose of comparison, the present results are deemed sufficient. The results have demonstrated that the band structures obtained with the PBE functional qualitatively agree with those calculated with the HSE hybrid functional. As shown in Figure 1, both functionals predict that the ferromagnetic and anti-ferromagnetic states of the C^BC^N-4-BC_2NNR are metallic and semiconducting, respectively. As expected, the band gaps calculated by the PBE functional are underestimated. It is only 0.05 eV, which was only one third of the energy gap predicted by the HSE functional (0.15 eV). In addition, several narrow states (with small energy dispersion) have been shifted away from the Fermi level in the band structure obtained with the HSE functional. This is attributed to the self-interaction between the localized edge states, which is not correctly introduced in the PBE simulations.

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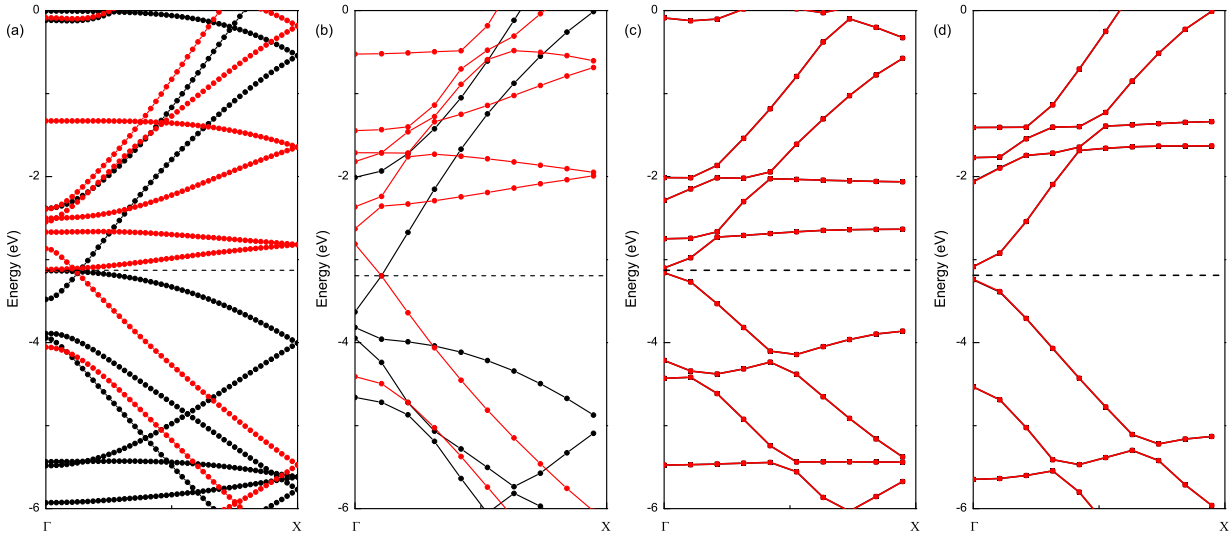

Fig. 1 Comparison between the spin-resolved band structures of the ferromagnetic (a, b)and antiferromagnetic (c, d) states for the C^BC^N-4-BC_2NNR calculated with the PBE (a, c) and HSE (b, d) exchange-correlation functionals. Band structures in spin-up and spin-down directions are shown in red and black, respectively.