Electronic Supporting Information
for

Hybrid structures of BN nanoribbon/single-walled carbon nanotube: ab initio study

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FIG. 1: (color online) Band structures of 2ZBNNR-N-(4,4)SWCNT with (a) PBE functional, (b) HSE06 hybrid functional, using Quantum-ESPRESSO package[3]. The red solid and blue dash-dotted lines denote the spin-up and spin-down bands, respectively. The Fermi level is set to zero.

Computational Details of PWSCF code of the Quantum ESPRESSO

Fig. 1 displays the band structures with PBE functional[1] and Heyd-Scuseria-Ernzerh screened hybrid functional (HSE06)[2], which is carried out by means of the density functional theory (DFT), as implemented in the Quantum-ESPRESSO package[3], with the plane wave cutoff energy of 60 Ry. The BZ integration has been performed with $61 \times 1 \times 1$ $k$-point sampling points in the Brillouin zone integration[4].

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FIG. 2: (color online) Band structures, spatial distribution of the spin differences, and relative energies for 2ZBNNR-N-(6,6)SWCNT in (a) FM, (b) AFM, and (c) NM states, using OPENMX computer code[5]. The red and blue surfaces represent the spin-up ($\uparrow$) and spin-down ($\downarrow$). The isosurface of $0.003 \mu\text{B/Å}^3$ is adopted. The red solid and blue dash-dotted lines denote the spin-up and spin-down bands, respectively. The Fermi level is set to zero.

FIG. 3: (color online) Band structures, spatial distribution of the spin differences, and relative energies for H-2ZBNNR-N-(6,6)SWCNT in (a) FM, (b) AFM, and (c) NM states, using OPENMX computer code[5]. The red and blue surfaces represent the spin-up (↑) and spin-down (↓). The isosurface of 0.003 μB/Å³ is adopted. The red solid and blue dash-dotted lines denote the spin-up and spin-down bands, respectively. The Fermi level is set to zero.

FIG. 4: (color online) Band structures and spatial distribution of the spin differences, and relative energies for 3ZBNNR-B-(6,6)SWCNT in (a) FM, (b) AFM, and (c) NM states, using OPENMX computer code[5]. The red and blue surfaces represent the spin-up (↑) and spin-down (↓). The isosurface of 0.003 μB/Å³ is adopted. The red solid and blue dash-dotted lines denote the spin-up and spin-down bands, respectively. The Fermi level is set to zero.
FIG. 5: (color online) Band structures and spatial distribution of the spin differences, and relative energies for H-3ZBNNR-B-(6,6)SWCNT in (a) FM and (b) NM states, using OPENMX computer code[5]. The red and blue surfaces represent the spin-up (↑) and spin-down (↓). The isosurface of 0.003 $\mu_B/\text{Å}^3$ is adopted. The red solid and blue dash-dotted lines denote the spin-up and spin-down bands, respectively. The Fermi level is set to zero. There is no stable AFM phase.