Electronic Supporting Information
for

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

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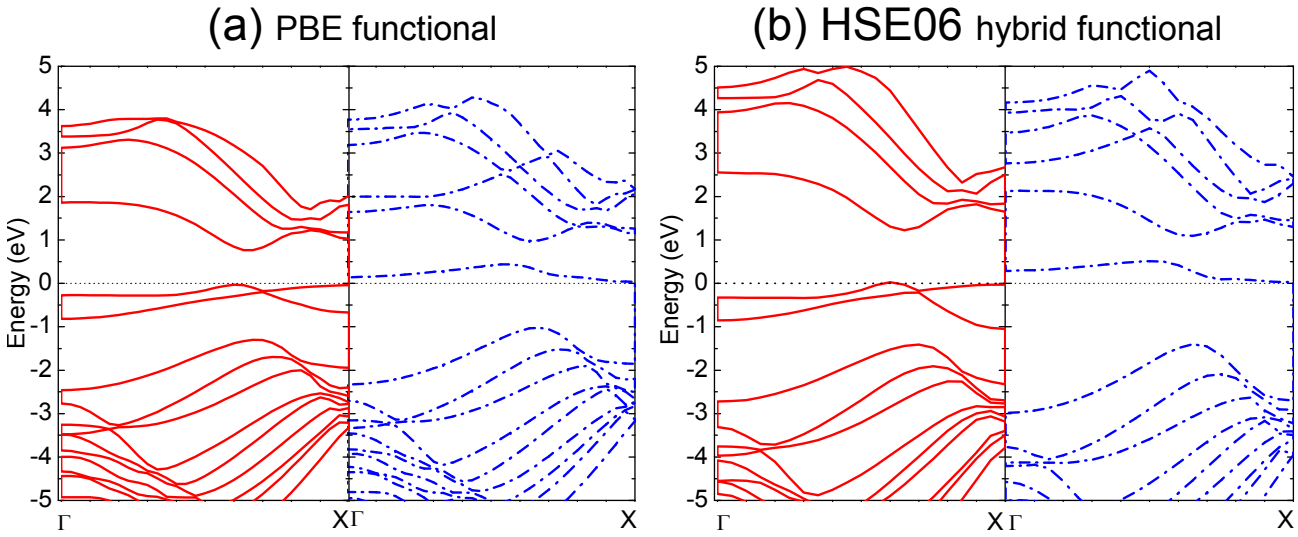

FIG. 1: (color online) Band structures of 2ZBNNR-N-(4,4)SWCNT with (a) PBE functional, (b) HSE06 hybrid functional, using Quantum-ESPRESSO package[3]. The red solid and blue dash-dotted lines denote the spin-up and spin-down bands, respectively. The Fermi level is set to zero.

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].

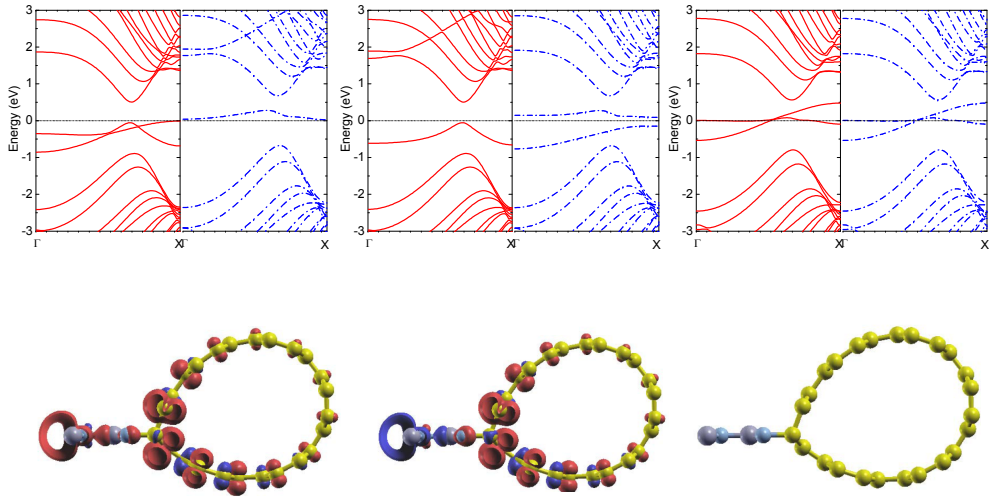

FIG. 2: (color online) Band structures, spatial distribution of the spin differences, and relative energies for 2ZBNNR-N-(6,6)SWCNT in (a) FM, (b) AFM, and (c) NM states, using OPENMX computer code[5]. The red and blue surfaces represent the spin-up (↑) and spin-down (↓). The isosurface of 0.003 $\mu_B/Å^3$ 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.

[1] J. P. Perdew, K. Burke, and M. Ernzerhof, *Phys. Rev. Lett.* 1996, **77**, 3865.
[2] J. Heyd, G. E. Scuseria and M. Ernzerhof, *J. Chem. Phys.* 2006, **124**, 219906.
[3] P. Giannozzi, S. Baroni, N. Bonini, M. Calandra, R. Car, C. Cavazzoni, D. Ceresoli, G. L. Chiarotti, M. Cococcioni, I. Dabo, A. Dal Corso, S. Fabris, G. Fratesi, S. de Gironcoli, R. Gebauer, U. Gerstmann, C. Gougoussis, A. Kokalj, M. Lazzeri, L. Martin-Samos, N. Marzari,F. Mauri, R. Mazzarello, S. Paolini, A. Pasquarello, L. Paulatto, C. Sbraccia, S. Scandolo, G. Sclauzero, A. P. Seitsonen, A. Smogunov, P. Umari, and R. M. Wentzcovitch, *J. Phys.: Condens. Matter* 2009, **21**, 395502.
[4] H. J. Monkhorst and J. D. Pack, *Phys. Rev. B* 1976, **13**, 5188.
[5] OpenMX Website. T. Ozaki, H. Kino, J. Yu, M. J. Han, N. Kobayashi, M. Ohfuti, F. Ishii, T. Ohwaki and H. Weng, http://www.openmx-square.org/.

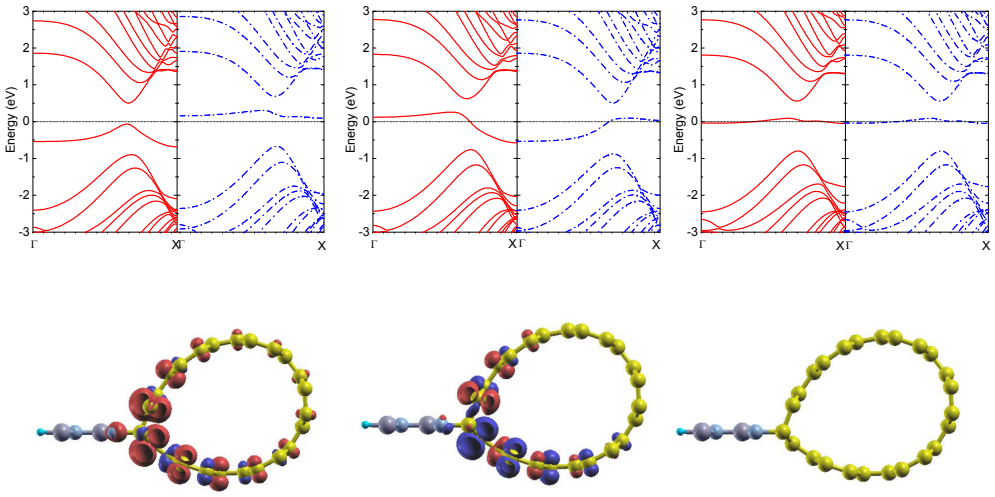

FIG. 3: (color online) Band structures, spatial distribution of the spin differences, and relative energies for H-2ZBNNR-N-(6,6)SWCNT in (a) FM, (b) AFM, and (c) NM states, using OPENMX computer code[5]. The red and blue surfaces represent the spin-up (↑) and spin-down (↓). The isosurface of 0.003 $\mu_B/Å^3$ 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.

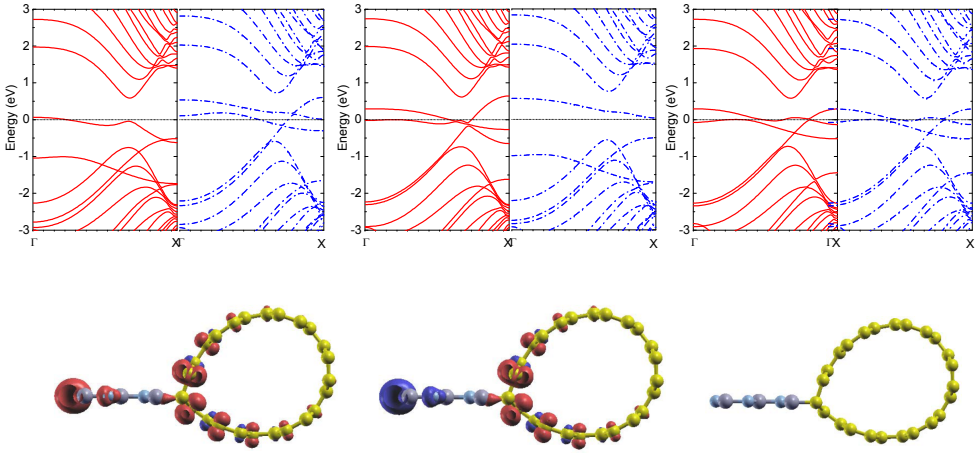

FIG. 4: (color online) Band structures and spatial distribution of the spin differences, and relative energies for 3ZBNNR-B-(6,6)SWCNT in (a) FM, (b) AFM, and (c) NM states, using OPENMX computer code[5].T he red and blue surfaces represent the spin-up (↑) and spin-down (↓). The isosurface of 0.003 $\mu_B/Å^3$ 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.

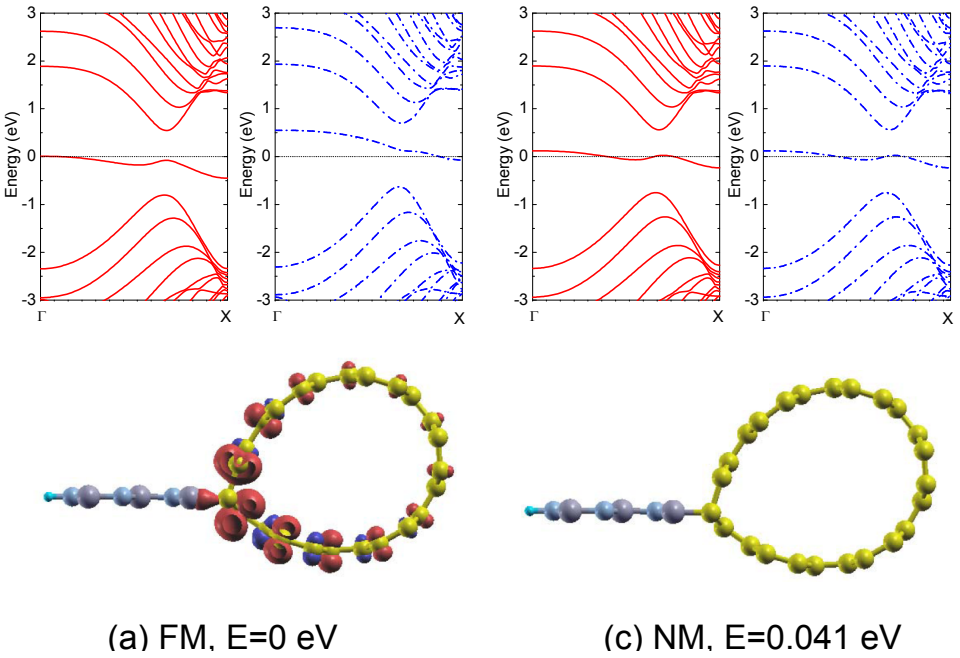

FIG. 5: (color online) Band structures and spatial distribution of the spin differences, and relative energies for H-3ZBNNR-B-(6,6)SWCNT in (a) FM and (b) NM states, using OPENMX computer code[5]. The red and blue surfaces represent the spin-up (↑) and spin-down (↓). The isosurface of 0.003 $\mu_B/Å^3$ 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.