Electronic and Magnetic Properties of Hybrid Graphene Nanoribbons

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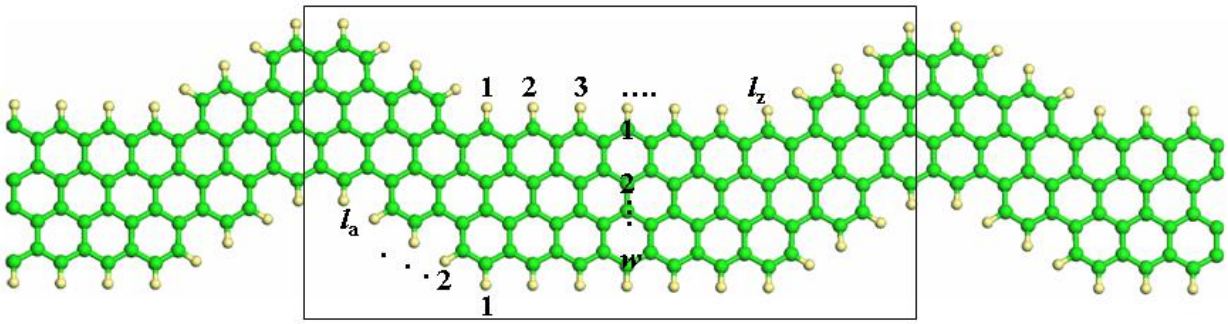
Using spin-polarized first-principles computations, we have systematically studied the electronic and magnetic properties of a new class of infinitely long hybrid graphene nanoribbons (HGNRs), which are constructed on the basis of experimentally-observed zigzag/armchair graphene nanoribbon heterojunctions.[1] HGNRs are initially nonmagnetic semiconductors, and then covert to magnetic semiconductors with increasing the length of zigzag segments. Interestingly, although the edge states of two zigzag edges in HGNRs are antiferromagnetically coupled to each other, the magnetization on two edges is not equal. Further investigation demonstrates that the electronic properties of HGNRs are mainly controlled by the zigzag segment length and the ribbon width. The electronic properties of nonmagnetic HGNRs are rather robust to the external electronic field. In contrast, the electronic properties of magnetic HGNRs are rather sensitive to external electronic field, and intrinsic half metallictiy can be realized under a critical value of 0.8 V/Å.

References

[1] Jia, X.; Hofmann, M.; Meunier, V.; Sumpter, B. G.; Campos-Delgado, J.; Romo-Herrera, J. M.; Son, H.; Hsieh, Y. P.; Reina, A.; Kong, J.; Science, **323** (2009), 1701–1705.

Figures



Atomic structure of HGNR (l_z,l_a,w). Carbon and hydrogen atoms are denoted with green and light yellow balls, respectively. The rectangle marks one-unit supercell in the ribbon axis direction.