

Electronic Structures of Graphene Edges and Nanographene

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The electronic structure of nanographene having open edges crucially depends on its edge shape. The circumference of an arbitrary shaped nanographene sheet is described in terms of a combination of zigzag and armchair edges. According to theoretical suggestions, nanographene has nonbonding π -electron state (edge state) localized in zigzag edges. This is reminiscent of the nonbonding π -electron state appearing in non-Kekulé-type aromatic molecules. The localized spins of the edge states can give rise to unconventional magnetism in nanographene, such as carbon-only ferromagnetism, magnetic switching phenomenon, spin glass state, etc. Nanographene can be prepared by heat-induced conversion of nanodiamond particles. Nanographene ribbons are found by chance around step edges of graphite. The detailed structures of individual nanographene ribbons thus found can be characterized by resonance Raman experiments, in which the graphitic *G*-band is used as a fingerprint. STM/STS investigations of well defined graphene edges which are hydrogen terminated in ultra-high vacuum condition confirm the presence of edge states around zigzag edges, in good agreement with theoretical works. Armchair edges are generally long and defect free, whereas zigzag edges tend to be short and defective. The feature of the edge state depends on the detailed geometry of the edge structures. The edge state in a short zigzag edge embedded between armchair edges becomes less localized due to state mixing with the adjacent armchair edges. The electrons in the edge state in a finite-length zigzag edge are subjected to electron confinement effect. Nanographene sheets are tailored by cutting along the direction which is chosen intentionally for designing functionality. Well defined edges can be prepared by chemical modifications with foreign atoms or functional groups. A combination of an atomic-resolution electron lithography technique and chemical modifications of the nanographene edges is expected to give nanographene-based molecular devices in the development of nanotechnology.

- [1] T. Enoki and Y. Kobayashi, *J. Mater. Chem. Highlight* **15**, 3999 (2005).
- [2] T. Enoki, Y. Kobayashi, and K. Fukui, *Inter. Rev. Phys. Chem.* **26**, 609 (2007).
- [3] T. Enoki and K. Takai, *Dalton Perspective*, 2008, submitted.