Effect of edge geometry and chemical structure on the electronic structure of graphene nanostructures

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The electronic structure of nanographene depends on its edge geometry. In the zigzag edges, nonbonding edge state localized around the edge region is created, while the electron waves form a standing wave in the vicinity of armchair edge, resulting in the gap formation. This is a consequence of massless Dirac fermion moving in the 2D hexagonal bipartite lattice in physics or Clar's aromatic sextet rule in chemistry. In addition, the electronic structure of graphene nanostructures depends on how the edge carbon atoms are terminated by foreign chemical species. We investigated the electronic structures of graphene nanostructures using STM/STS and AFM observations with graphene nanoislands embedded in graphene oxide sheets, and graphene nanoholes with their edges hydrogenated. The conductivity of graphene nanoislands increases upon the increase in their size. In addition, it is higher in zigzag edged nanoislands than in armchair edged ones. The STM current image shows that sextets observed as a bright spot is localized in the armchair edged islands, whereas they are migrating in the zigzag edged islands. These experimental findings demonstrate the presence of a standing wave with an energy gap in the energetically stabilized armchair edged islands in spite of the absence of such a standing wave in conducting zigzag edges ones. Zigzag edges of nanoholes with their edge carbon atoms being monohydrogenated have well localized edge states. Introducing dehydrogenated sites to a monohydrogenated zigzag edge makes the edge state disappear when the zigzag edge consists of repeating two monohydrogenated sites and one dihydrogenated site, and there are a variety of electronic structures depending on how the zigzag edges are decorated by a combination of mono- and dehydrogenated sites. We conclude that edge geometry together with edge chemical structure plays an important role in the electronic structure of graphene nanostructures.

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