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Nanographene and Graphene Edges; Localized Edge State and Electron Wave Interference-Level Spectroscopies on Topological Insulators

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Graphene forms a 2D honeycomb bipartite lattice which consists of two independent sublattices. The electrons here move as massless Dirac fermion governed by relativistic Weyl equation $\hat{H} = v_F \sigma \mathbf{P}$. The linear **P** dependence in the kinetic energy gives cone-shaped π-valence and π*-conduction bands (Dirac cones), which touch each other at the Fermi level. The pseudo-spin σ effectively converted from the structural degree of freedom 2 couples with momentum **P**. The massless Dirac fermion feature brings about a variety of unconventional electronic phenomena. Chemists can understand this electronic structure simply in terms of tiling of aromatic sextets on the basis of Clar's aromatic sextet rule with sextet (benzene ring) as a fundamental unit. Infinite size graphene has three degenerate independent Clar's representations having $\sqrt{3}\times\sqrt{3}$ superlattice, in which the degeneracy causes the mobile π-electrons and their activities.

When graphene is cut into nanofragments, the created edges work as boundary conditions depending on the edge geometry. There are two independent geometry types; zigzag and armchair edges. The boundary condition at zigzag edge results in the broken symmetry of the pseudo-spins, creating a nonbonding edge state localized at zigzag edge. In chemistry, this can be understood as the existence of radical electrons moving around the zigzag edge on the basis of Clar's rule. As the edge state is strongly spin polarized, the localized edge-state spins strongly coupled with each other through exchange interaction play in giving a variety of magnetic cooperative phenomena. The electron scattering at armchair edge takes place as an inter-valley transition between two Dirac cones located at K and K' points at the Brillouin zone boundary. Accordingly, the transition brings about electron wave interference between K and K' points, giving a standing wave around the armchair edge. Clar's rule concludes the formation of a standing wave with a large energy gap as a consequence of the presence of a unique representation.

We discuss the edge-inherited unconventional electronic phenomena such as edge state and its magnetism, and electron wave interference, on the basis of experimental results of STM/STS, AFM, X-ray absorption (NEXAFS), Raman spectra, ESR, and magnetic susceptibility.