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Electronic and magnetic functions of nanographene-based host-guest system

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The electronic structure of nanographene having open edges crucially depends on its edge shape. According to theoretical predictions, nanographene has nonbonding π-electron state (edge state) localized in zigzag edges. We investigated the electronic structure of graphene edges, the magnetism of the edge-state spins in nanographene and the effect of host-guest interaction on the magnetism. For magnetic investigations, we employed nanoporous activated carbon fiber (ACF) having a 3D disordered network of nanographite domains, each of which is a stack of 3-4 nanographene sheets. STM/STS investigations of hydrogen-terminated graphene edges confirm the presence of edge states around zigzag edges, in good agreement with theoretical works. The feature of the edge state depends on the detailed geometry of the edge structures. The magnetism of nanographene in ACF has a ferrimagnetism feature with a net magnetic moment, for which the cooperation of ferromagnetic intra-zigzag-edge and ferromagntic/antiferromagnetic inter-zigzag-edge interactions is responsible. Heat-treatment, which induces an insulator-metal transition, brings about spin glass state of the edge-state spins in the vicinity of the transition. Physisorption of guest species such as water, organic molecules, rare gas in the ACF nanopores generates a high-spin/low-spin magnetic switching phenomenon, in which a discontinuous reduction of the magnetic moment takes place. This is explained in terms of the strengthening of the inter-graphene-sheet antiferromagnetic interaction, which is induced by the mechanical compression of nanographite domains by the condensed guest molecules. The magnetic oxygen molecules physisorbed in the nanopores work seriously to decrease the magnetoresistance in ACF as a consequence of the interaction between the oxygen molecule spins and edge-state spins.