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Diverse Electronic and Magnetic Properties of Fluorine-Doped Graphene Nanoribbons. KHANH NGUYEN DUY[1], MING-FA LIN[2], Natl Cheng Kung Univ, YU-HUANG CHIU COLLABORATION[3], YU-TSUNG LIN COLLABORATION[4] — The feature-rich electronic and magnetic properties of fluorine-doped graphene nanoribbons are investigated by the first principles calculations. They arise from the cooperative or competitive relations among the significant F-C bond, the finite-size quantum confinement and the edge structure. Fluorine adatoms can create the p-type metals or the narrow-gap semiconductors, depending on whether the π bonding is seriously suppressed by the top-site chemical bonding. There exist five kinds of magnetic configurations, namely, the ferromagnetic and non-magnetic systems with the metallic and semiconducting behaviors, and the anti-ferromagnetic semiconductors. The diverse essential properties are clearly revealed in the spatial charge distribution, the spin density, and the density of states (DOS). Specifically, a lot of structures in DOS could be directly verified by the STS measurements.

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