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Half-metallic Armchair Graphene Nanoribbon FUMIYUKI ISHII, KEISUKE SAWADA, MINEO SAITO, Kanazawa University — Among a variety of applications of graphenes, spintronics applications are considered to be hopeful. For an example, spin transport has been experimentally observed by using graphene layers [1]. There are two types of shaped edge in graphene nanoribbon (GNR), one of them is armchair GNR (AGNR) and the other is zigzag GNR (ZGNR). Armchair edges are often observed compared with the zigzag edges [2]. However, the AGNR is believed to have the nonmagnetic structure whereas the magnetic properties in ZGNR attracted much attention. In this study, we perform first-principles density functional calculation on dehydrogenated AGNR. Surprisingly, we find that dehydrogenated AGNR has magnetic states in the case of carrier doping. Magnetic state of the carrier-induced AGNR has ferromagnetic chains at the two edges having the same directions of the magnetic moments. We conclude that the carrier-doped AGNR is half-metallic. [1] M. Ohishi et al., Jpn. J. Appl. Phys. 46, L605 (2007). [2] Y. Kobayashi et al., Phys. Rev. B 71, 193406 (2005).

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