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Canted Antiferromagnetism in Electron-Doped CaMnO₃ under Epitaxial Strain HIROMASA OHNISHI, SHOJI ISHIBASHI, National Institute of Advanced Industrial and Science Technology (AIST), KIYOYUKI TERAKURA, Japan Advanced Institute of Science and Technology (JAIST) — CaMnO₃ (CMO) is a G-type antiferromagnetic (G-AFM) insulator at low temperature. A small amount of electron doping to CMO induces electronic and magnetic state change to a weak ferromagnetic (FM) metal. The recent experiment in thin-film [1] has revealed that the metallic character by electron-doping is sensitive to the strain exerted by the substrate. In this study, we clarify the electron-doping effect for CMO with the existence of epitaxial strain from substrates, by first-principles electronic structure calculation with noncollinear version of local spin density approximation. We show that a metallic character with a weak FM component is brought by the spin-canting from the G-AFM spin alignment (cG-AFM) by the double exchange effect. The canting angle becomes larger with increase of doping-amount and c/a, where c and a represent in-plane and out-of-plane lattice constants, respectively. We also show that a magnetic state change from cG-AFM state to C-AFM one takes place by further enhancement of compressive strain. We analyze our results by comparing with the experimental results.

[1] P.-H. Xiang et al., Adv. Mater. 23, 5822 (2011).

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