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Electronic structure and magnetic anisotropy of $Sm_2Fe_{17}N_x$[1] HISAZUMI AKAI, ISSP, University of Tokyo, MASAKO OGURA, Dept. Physics, Osaka University — Electronic structure and magnetic properties of $Sm_2Fe_{17}N_x$ are studies on the basis of the first-principles electronic structure calculation in the framework of the density functional theory within the local density and coherent potential approximations. The magnetic anisotropy of the system as a function of nitrogen concentration x is discussed by taking account not only of the crystal field effects but also of the effects of the f-electron transfer from Sm to the neighboring sites. Also discussed is the magnetic transition temperature that is estimated by mapping the system into a Heisenberg model. The results show the crystalline magnetic anisotropy changes its direction from in-plane to uniaxial ones as x increases. It takes the maximum value near $x \sim 2.8$ and then decreases slightly towards $x = 3$. The mechanism for these behaviors is discussed in the light of the results of detailed calculations on the bonding properties between Sm and its neighboring N.

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Hisazumi Akai
ISSP, University of Tokyo

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