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Electronic Investigation on Fe intercalated hard magnet $Fe_{0.25}TaS_2$ K.-T. KO, c-CCMR & Dept. Physics POSTECH, J.-Y. KIM, Pohang Accelerator Laboratory, POSTECH, J.-H. PARK, c-CCMR & Dept. Physics, POSTECH, KYOO KIM, B.-I. MIN, Dept. Physics, POSTECH, SUNG BAEK KIM, l-FEM & Dept. Physics, POSTECH, S-W. CHEONG, R-CEM & Dept. Physics and Astronomy, Rutgers University — The electronic structure of $Fe_{0.25}TaS_2$ was investigated by using the x-ray absorption spectroscopy (XAS) at Fe $L_{2,3}$-edge and density functional theory (DFT) calculation. The x-ray magnetic circular dichroism (XMCD) revealed that the intercalated Fe^{2+} has extremely large orbital magnetic moment, consistently with a large magnetic coercive in this system. Additionally, the orbital states were determined from the polarization dependent XAS, in which the lowest orbital state is identified to have strong in-plane characters. The detailed XAS results were analyzed in terms of the theoretical cluster model calculations. We also found that the observed orbital occupation as well as the spin and orbital magnetic moments agree well with the predictions of the DFT calculations including on-site Coulomb interaction (U) and spin-orbit coupling (S.O.). Finally, we discuss the orbital anisotropy including local electronic structure and the giant magnetocrystalline anisotropy of $Fe_{0.25}TaS_2$.

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