Abstract Submitted
for the MAR08 Meeting of
The American Physical Society

First-Principles Study on Electronic Structure of TiO_2-Based Dilute Magnetic Semiconductors[1] HIDETOSHI KIZAKI, MASAYUKI TOYODA, KAZUNORI SATO, HIROSHI KATAYAMA-YOSHIDA — We investigate the electronic structure in rutile-TiO_2-based dilute magnetic semiconductors (DMS) within self-interaction- corrected local density approximation (SIC-LDA). These results are compared with those calculated within standard LDA. Although the calculated band-gap energy and energetic position of Ti $3d$ bands are different in the LDA and the SIC-LDA, half-metallic density of states is predicted in transition- metal-doped TiO_2 for both methods. While the LDA calculations predict high-spin state only for Fe-doped one, in the SIC-LDA calculations high-spin state is realized in V-, Cr- and Mn-doped one and low-spin state is realized in Fe- and Co- doped one. However, the absorption and soft x-ray magnetic circular dichroism measurements in $(Ti_{0.97}, Co_{0.03})O_{2-\delta}$ indicate the Co^{2+} high-spin state in the D_{2h}-symmetry crystal field at the Ti site. These experimental results do not agree with our calculated results. We will discuss the origin of the discrepancy between the theoretical predictions and the experimental observations. In addition, we will discuss the ferromagnetism in TiO_2-based DMS.

[1]This work was partially supported by a Grant-in-Aid for Scientific Research in Priority Areas and for specially promoted research

Hidetoshi Kizaki
ISIR, Osaka Univ.

Date submitted: 26 Nov 2007 Electronic form version 1.4