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Dynamical Interplay Between Intrinsic Defects and Impurity Ions in Very Dilute Fe-doped MgO Thin Films YUNG JUI WANG, Northeastern Univ. (NU) and ALS, LBNL, MUKES KAPILASHRAMI, ALS, LBNL, XIN LI, ALS, LBNL and KTH, Royal Institute of Technology (KTH), Sweden, PER-ANDERS GLANS, ALS, LBNL, MEI FANG, KTH, and Fudan University, China, ANASTASIA V. RIAZANOVA, LYUBOV M. BELOVA, K.V. RAO, YI LUO, KTH, B. BARBIELLINI, NU, HSIN LIN, National University of Singapore, Singapore, R.S. MARKIEWICZ, NU, ZAHID HUSSAIN, JINGHUA GUO, ALS, LBNL, A. BANSIL, NU — The nature of intrinsic defects and impurities in the dielectric layer of a typical magneto tunneling junction is of great interest to understand tunneling of spin-polarized currents. In this connection, we have carried out studies of the electronic and magnetic properties of $Mg_{1-x}Fe_xO$. In particular, we have compared results from first principles calculations based on Density Functional Theory with highly accurate experiments. The measurements were performed with a Quantum Interference Device and by using soft x-ray absorption spectroscopy. Our study reveals basic defect units composed a Fe impurity coupled to one or two Mg vacancies. The trimer unit (i.e. Fe with two Mg vacancies) produces a magnetic net spin opposed to the dilute magnetism present in the oxide matrix. These findings could pave a way for engineering dielectric layers with high endurance and optimal tunneling properties by controlling the concentration of impurities and defects in the oxide matrix. Work supported by the US DOE.

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