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Unquenched e_g^1 orbital moment in the Mott insulating antiferromagnet $KOsO_4$[1] KWAN-WOO LEE, YOUNG-JOON SONG, KYO-HOON AHN, Department of Applied Physics, Graduate School, Korea Univ, Sejong, Korea, WARREN E. PICKETT, Department of Physics, Univ. of California, Davis, CA, USA — In condensed matter physics, spin-orbit coupling (SOC) has many important consequences, including some recent hot topics such as topological insulators, unconventional metal-insulator transitions, so-called relativistic Mott insulators, large orbital moments, and of course magnetic anisotropy. Whereas SOC in a t_{2g} manifold has been intensively discussed recently, SOC in an e_g manifold has rarely been considered due to the conventional (usually correct) wisdom that an orbital moment is completely quenched in the e_g subshell. In this presentation, using correlated band theory including SOC, we will address effects of SOC in an e_g^1 of $KOsO_4$, which contains OsO_4 tetrahedra such that the e_g subshell is partially occupied. In contrast to the conventional wisdom, our results show very definite magnetocrystalline anisotropy and unquenched orbital moments of substantial size in $KOsO_4$ (half that of the Os spin moment). We have analyzed and interpreted the origin of the orbital moment on the basis of a small crystal splitting and symmetry breaking (crystalline, and additionally due to SOC itself).

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