Unquenched $e_g^1$ orbital moment in the Mott insulating antiferromagnet $\text{KO}_4\text{OsO}_4$\textsuperscript{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 $e_g$ manifold of $\text{KO}_4\text{OsO}_4$, 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 $\text{KO}_4\text{OsO}_4$ (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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