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ab-initio calculations of electronic structure and magnetism of O2MF6 (M=Sb, Pt) : Coulomb correlation and spin-orbit interaction effects in 2p and 5d electrons MINJAE KIM, B. I. MIN, Department of Physics, Pohang University of Science and Technology — We have investigated electronic structures and magnetic properties of O_2MF_6 (M=Sb, Pt), which are composed of two building blocks of strongly correlated electrons: O_2^+ dioxygenyls and MF_6^- octahedra, by employing the first-principles electronic structure band method. For O_2SbF_6, as a reference system of O_2PtF_6, we have shown that the Coulomb correlation of O($2p$) electrons drives the Mott insulating state. For O_2PtF_6, we have demonstrated that the Mott insulating state is induced by the combined effects of the Coulomb correlation of O($2p$) and Pt($5d$) electrons and the spin-orbit (SO) interaction of Pt($5d$) states. The role of the SO interaction in forming the Mott insulating state of O_2PtF_6 is similar to the case of Sr_2IrO_4 that is a prototype of a SO induced Mott system with $J_{eff} = 1/2$.

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