ab-initio calculations of electronic structure and magnetism of \( \text{O}_2\text{MF}_6 \) (\( M=\text{Sb}, \text{Pt} \)) : 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 \( \text{O}_2\text{MF}_6 \) (\( M=\text{Sb}, \text{Pt} \)), which are composed of two building blocks of strongly correlated electrons: \( \text{O}_2^+ \) dioxygenyls and \( \text{MF}_6^- \) octahedra, by employing the first-principles electronic structure band method. For \( \text{O}_2\text{SbF}_6 \), as a reference system of \( \text{O}_2\text{PtF}_6 \), we have shown that the Coulomb correlation of \( \text{O}(2p) \) electrons drives the Mott insulating state. For \( \text{O}_2\text{PtF}_6 \), we have demonstrated that the Mott insulating state is induced by the combined effects of the Coulomb correlation of \( \text{O}(2p) \) and \( \text{Pt}(5d) \) electrons and the spin-orbit (SO) interaction of \( \text{Pt}(5d) \) states. The role of the SO interaction in forming the Mott insulating state of \( \text{O}_2\text{PtF}_6 \) is similar to the case of \( \text{Sr}_2\text{IrO}_4 \) that is a prototype of a SO induced Mott system with \( J_{\text{eff}} = 1/2 \).