# Exotic transition-metal compounds for hydrogen generator and battery electrode

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Mott insulators in transition-metal compounds are classified into (i) Mott-Hubbard type insulators where Mott gap $E_G$ is mainly determined by the Coulomb interaction $U$ between the transition-metal $d$ electrons and (ii) charge-transfer type insulators where $E_G$ is determined by the charge-transfer energy $\Delta$ from the ligand $p$ state to the transition-metal $d$ state (Zaanen-Sawatzky-Allen scheme). The rich electronic properties of the Mott insulators are deeply related to the spin-charge-orbital degrees of freedom of transition-metal $d$ states, and their orderings in the Mott insulators can be described by the Kugel-Khomskii mechanism.

In addition, some transition-metal oxides with high valence (such as $Fe^{4+}$, $Co^{4+}$, and $Cu^{3+}$) are characterized by very small (or even negative) charge-transfer energy $\Delta$, where the ligand (oxygen) $p$ holes play important roles. In the present talk, we would like to focus on two transition-metal oxides $MgTi_2O_4$ and $Li_xCoO_2$ where the exotic electronic states are realized due to the Ti 3$d$ orbital degeneracy and the O 2$p$ holes, respectively. As for $MgTi_2O_4$, an interesting interplay between the bulk $Ti^{3+}$ state the surface $Ti^{4+}$ state has been analyzed using photoemission spectroscopy and x-ray absorption spectroscopy. In addition, we have studied hydrogen generation by the $MgTi_2O_4$ surface which seems to be related to the complicated electronic state realized in the interface between the $Ti^{3+}$ and $Ti^{4+}$ regions.

We will discuss potential application of $MgTi_2O_4$ as a hydrogen generator for fuel cells. The O 2$p$ holes in $Li_xCoO_2$ (x=0.99, 0.66, 0.46, 0.25) have been studied using photoemission spectroscopy and x-ray absorption spectroscopy in order to understand the high performance of $Li_xCoO_2$ as a cathode material of Li-ion batteries. We would like to emphasize the importance of the ligand holes and compare $Li_xCoO_2$ with various cathode materials in terms of ligand effect.

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