

The explicit role of O 2p states in high oxidation state transition metal Oxides

G.A.Sawatzky

University of British Columbia

For late 3d transition metal oxide with formally high oxidation states like Cu^{3+} , Ni^{3+} , Co^{4+} , Fe^{4+} , $5+$, Mn^{4+} the charge transfer energy for transferring electrons from O to the transition metal may be negative resulting in a formally more correct starting point in which the oxidation state is lowered and holes in the O 2p orbitals are introduced. In this talk we present experimental evidence for this in a number of systems of present day importance and discuss the consequences in terms of magnetic properties and issues such as potential charge disproportionation. We use x ray spectroscopies and model cluster like calculations to demonstrate the importance of considering the hole occupation of the O 2p states explicitly and discuss some popular materials like the Cuprates, Nickelates, and Cobaltates from this rather different starting point. For example in this relatively new approach we can explain the "effective" charge disproportionation observed with only very small actual charge motion as well as the charge and magnetic super lattice structure in the insulating rare earth Nickelates. I also address the importance of the octahedral rotations in determining the phase diagram for the Nickelates as present by Torrance. I will present arguments that actually these ideas are rather generally applicable to a very wide range of systems of compounds involving high cation oxidation states.