

ZERNIKE INSTITUTE COLLOQUIUM

Wednesday, October 8th, 2014

16:00h, Lecture Hall: 5111.0080

Coffee and cakes from 15:30h

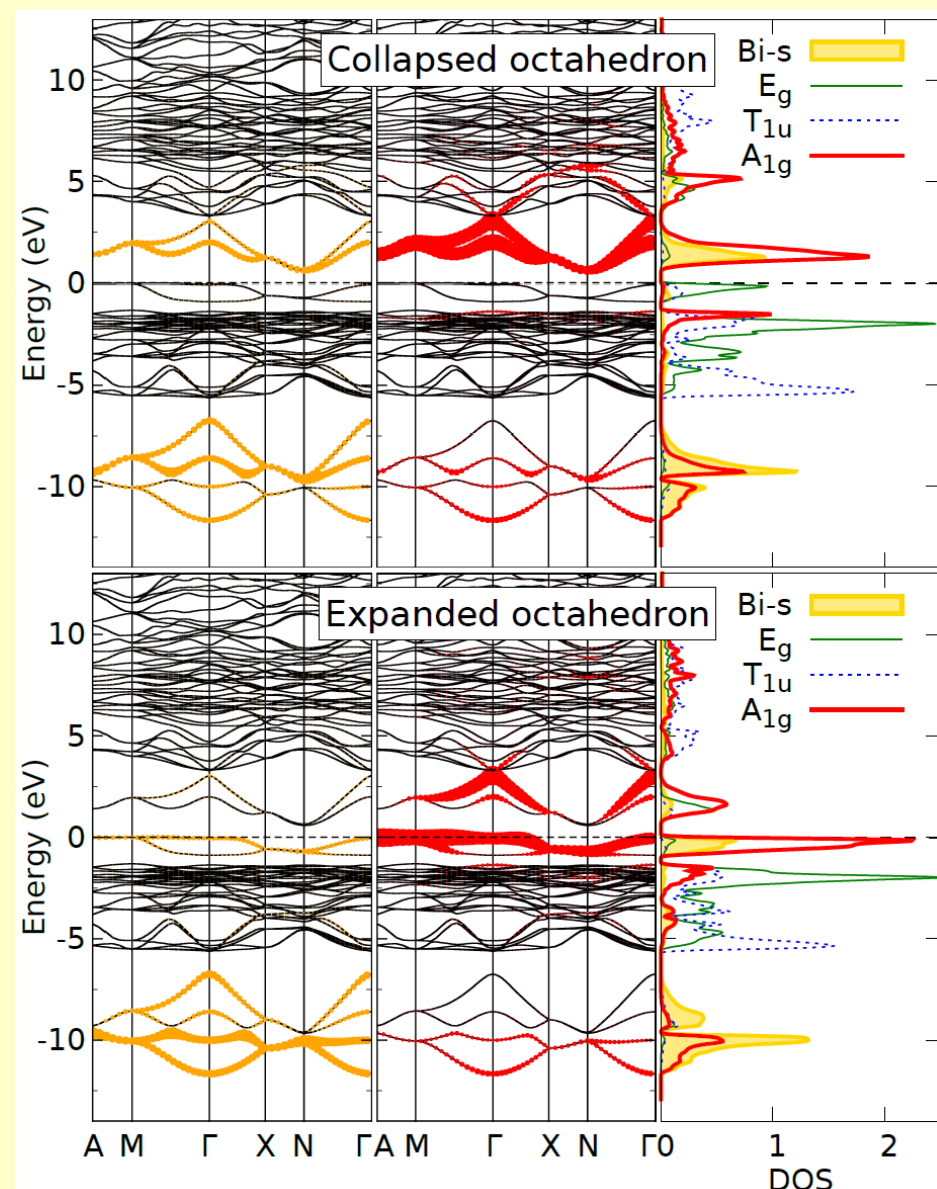
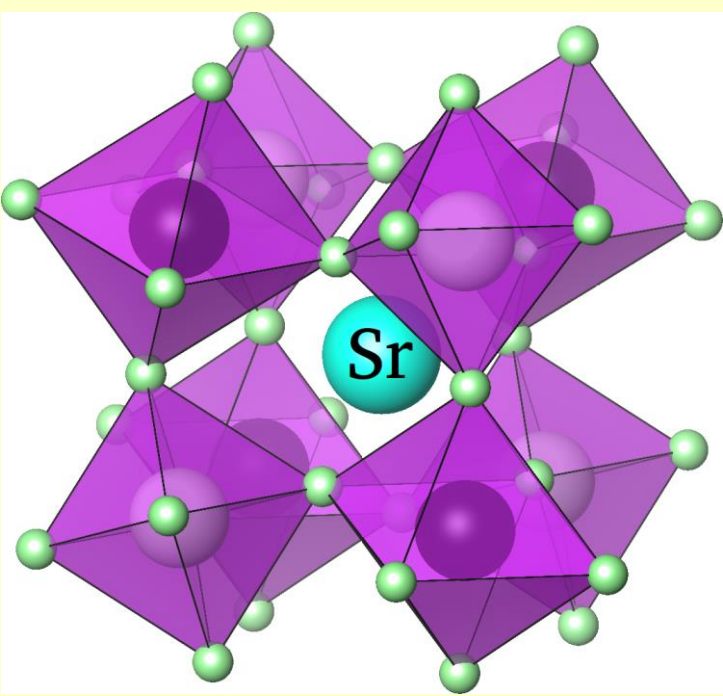
The explicit role of O 2p states in high oxidation state transition metal oxides

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For late 3d transition metal oxide with formally high oxidation states like Cu^{3+} , Ni^{3+} , Co^{4+} , Fe^{4+} , Mn^{4+} , and on a different but it turns out similar note Bi^{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 and variational approaches as well as density functional where applicable (SrBiO_3) to demonstrate the importance of considering the hole occupation of the O 2p states explicitly and discuss some popular materials like the Cuprates, Nickelates, Cobaltates and SrBiO_3 , 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. We demonstrate that the low energy scale charge degrees of freedom are mainly of O 2p hole character with very strong electron phonon coupling forming O Octahedra molecular orbital like states in the low temperature phases. 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 including systems like BaBiO_3 which when doped with K is a fairly high temperature superconductor preceding the cuprate era.



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