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The electronic structure and properties of negative charge transfer gap and mixed valent Oxides

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In high oxidation state oxides like the trivalent Nickel oxides, tetravalent Co and Fe oxides as well as the parent superconductors BaBiO₃ and SrBiO₃ the cation electron affinity in the formal valence could end up larger than the O²⁻ ionization potential leading to a so called negative charge transfer gap. If the charge transfer energy is strongly negative, then we should really adopt starting electronic configurations such as Ni²⁺ rather than 3⁺ or Bi³⁺ rather than 4⁺ with compensation holes in the O 2p valence band for charge neutrality. This leads to very different electronic structures and descriptions of the physical properties and the interpretation of spectroscopies than when starting from the formal oxidation state picture. We demonstrate that with this in mind we can very well explain many of the properties and phases of the Nickelates and the Ba(Sr)Bi O₃ perovskite oxides as well as their spectroscopic properties. We discuss the general problem of treating such systems resulting in inverted crystal field [pictures and low spin rather than high spin states even for modest crystal fields. We also use a cluster exact diagonalization calculation to show that the x ray spectroscopy results now agree very well with experiment which has been a problem for decades. In the intermediate range of negative charge transfer gap systems we have to deal with mix valent starting points for which SmB₆ is a typical example but also may include 3d transition metal compounds. We describe how these systems often termed as Kondo Lattice problems can be described in terms of mixed valent in momentum space when they are in their coherent low temperature state. Mixed valent in moment space we argue requires a strongly momentum dependent self energy in the description of the quasi particle spectral functions.