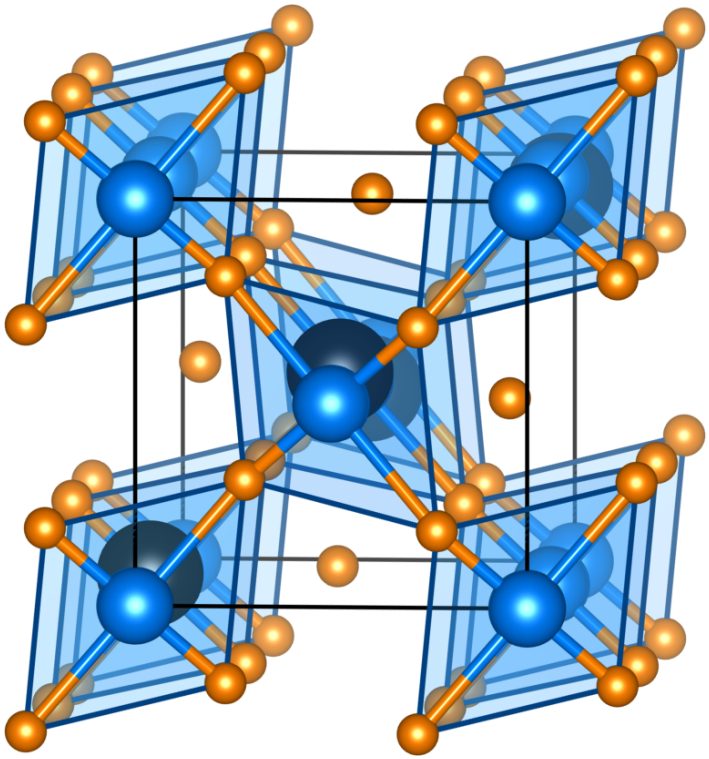
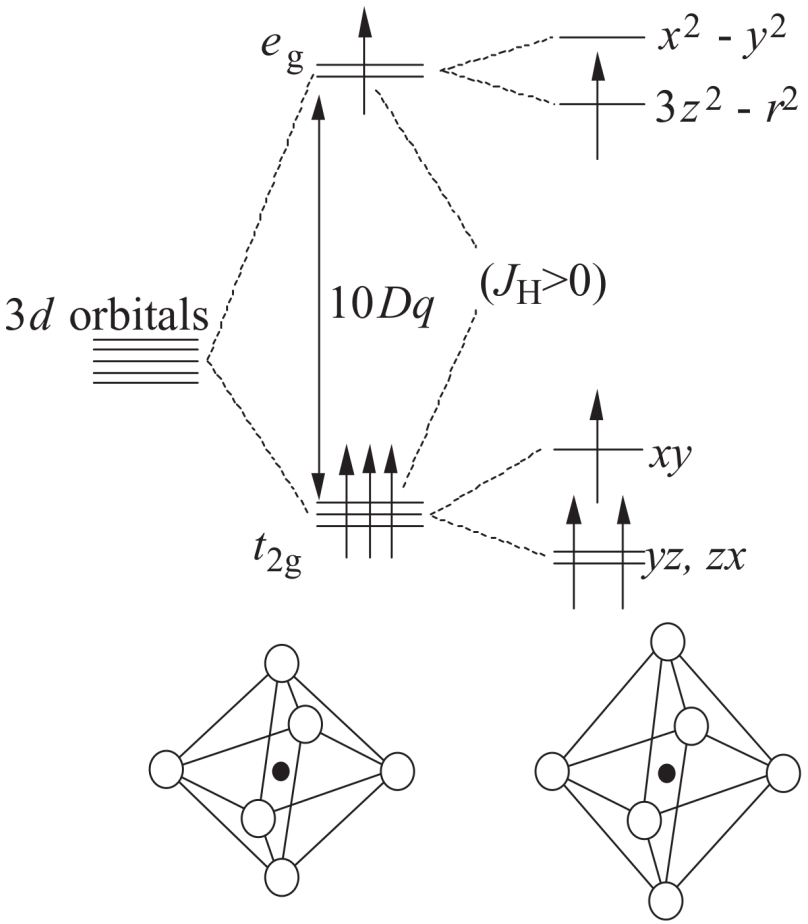
Correlations and the Hubbard model: $LaMnO_3$

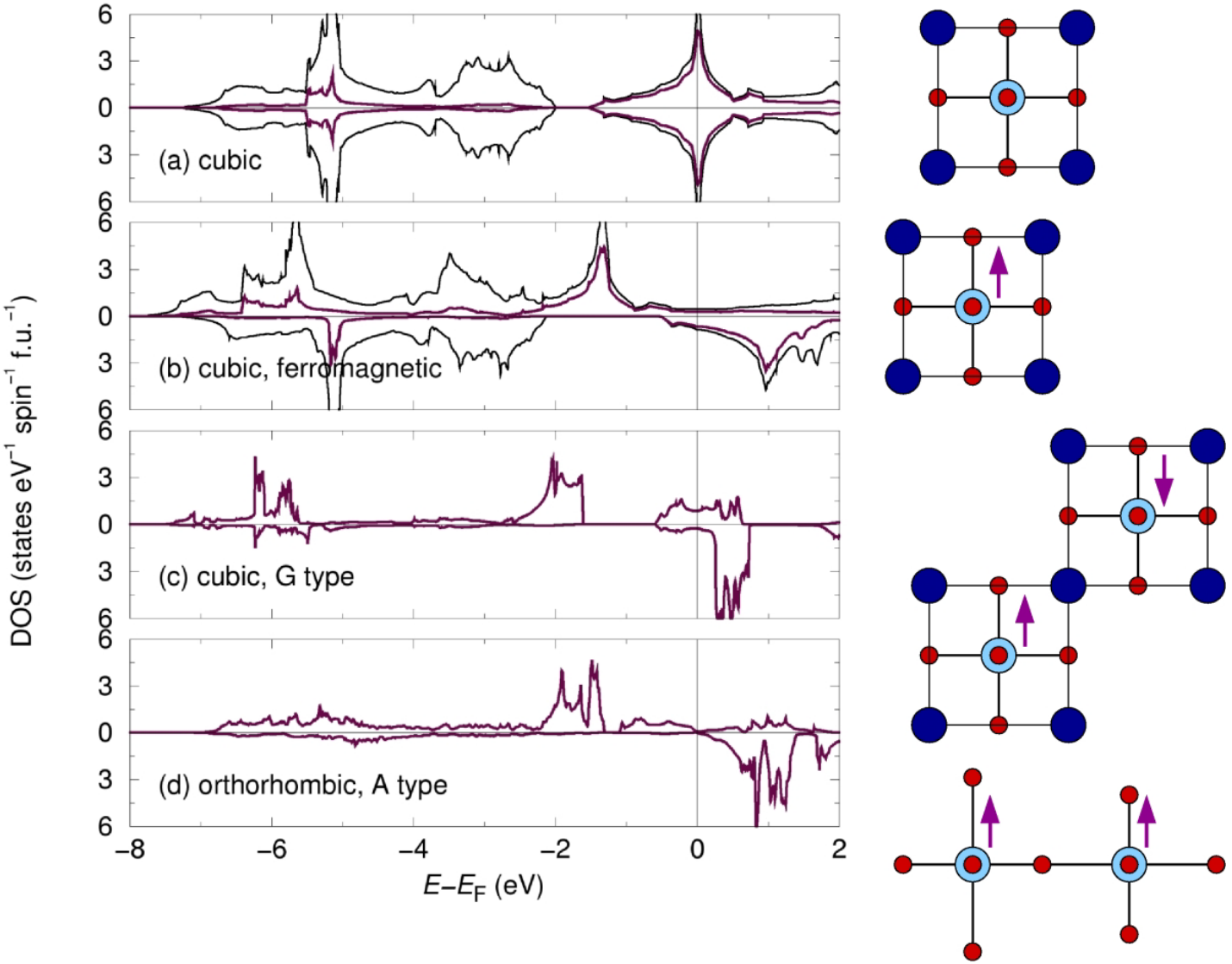




Jahn-Teller distorted orthorhombic perovskite (space group *Pnma*)

seshadri@mrl.ucsb.edu

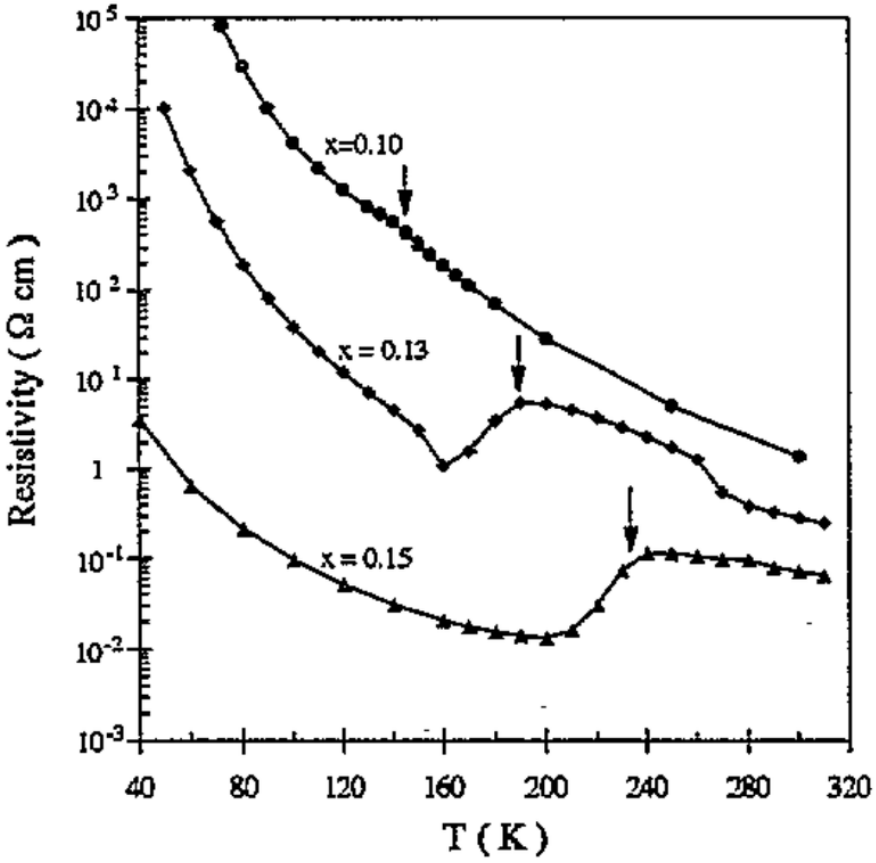
Correlations and the Hubbard model: $LaMnO_3$

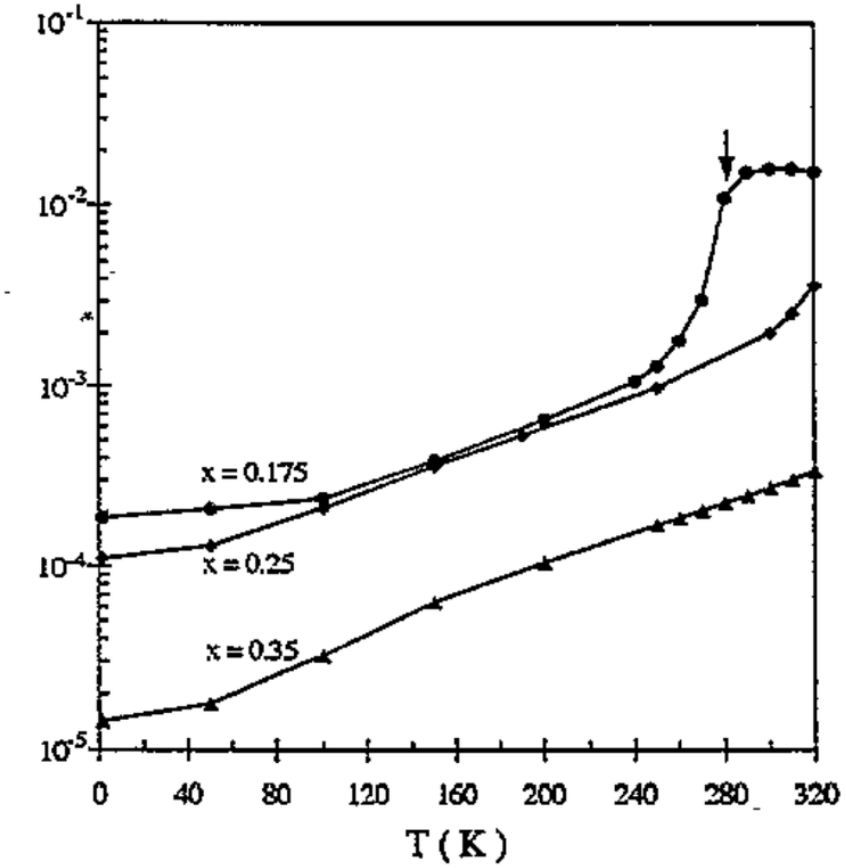


Structure and magnetism do not explain the insulating behavior.

seshadri@mrl.ucsb.edu

Correlations and the Hubbard model: $LaMnO_3$



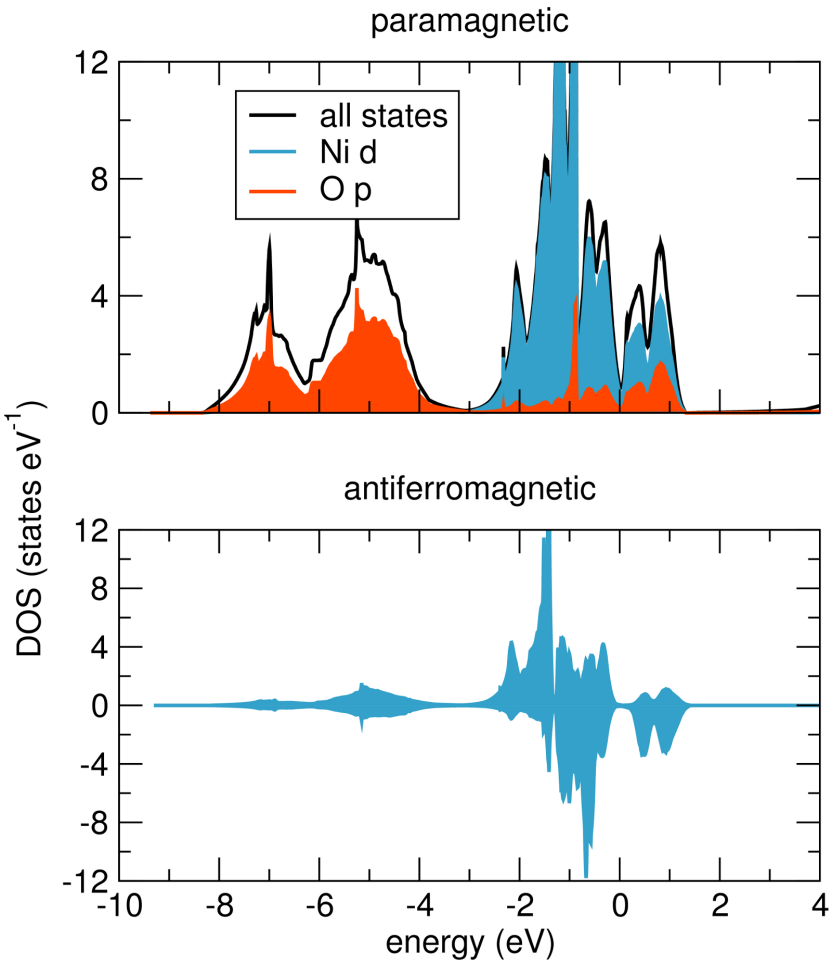


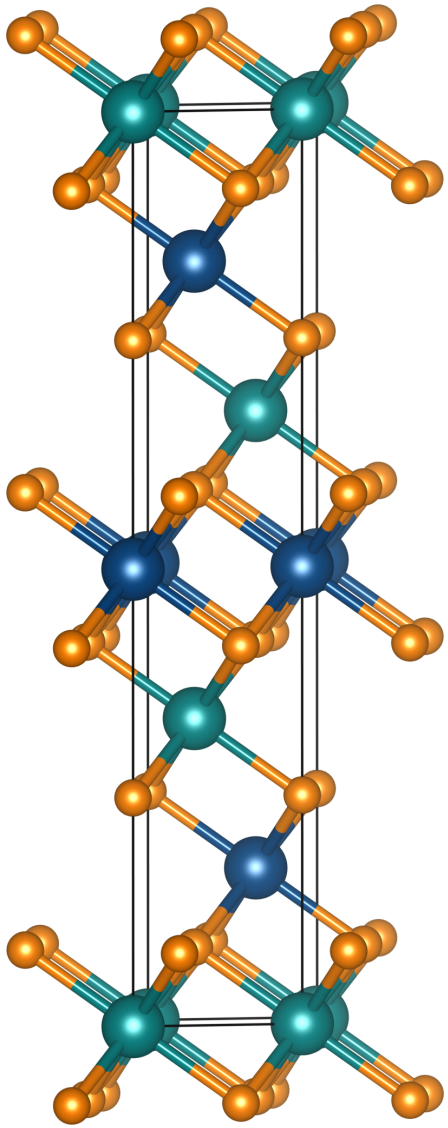
Electrical resistivity behavior in $La_{1-x}Sr_xMnO_3$

Anane, Dupast, Dang, Renard, Veillet, de Leon Guevare, Millot, Pinsard, Revcolevschi, *J. Phys.: Condens. Matter* **7** (1995) 7015-7021.

seshadri@mrl.ucsb.edu

Correlations and the Hubbard model: NiO

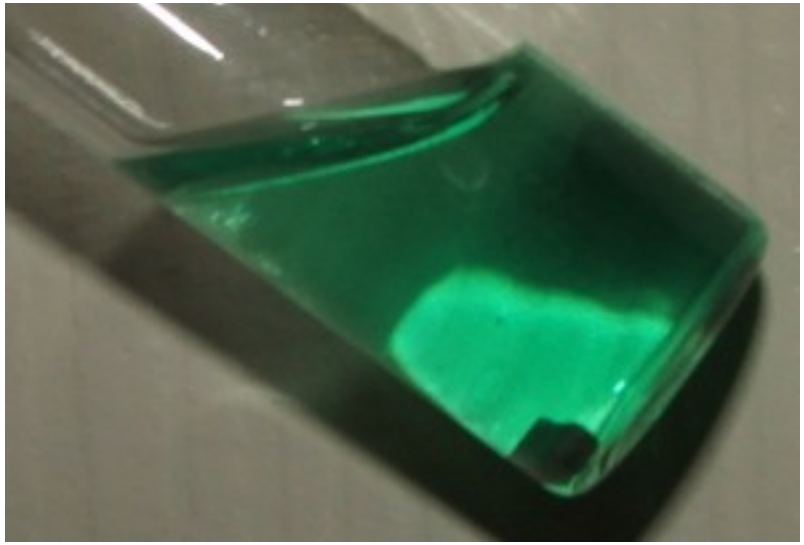


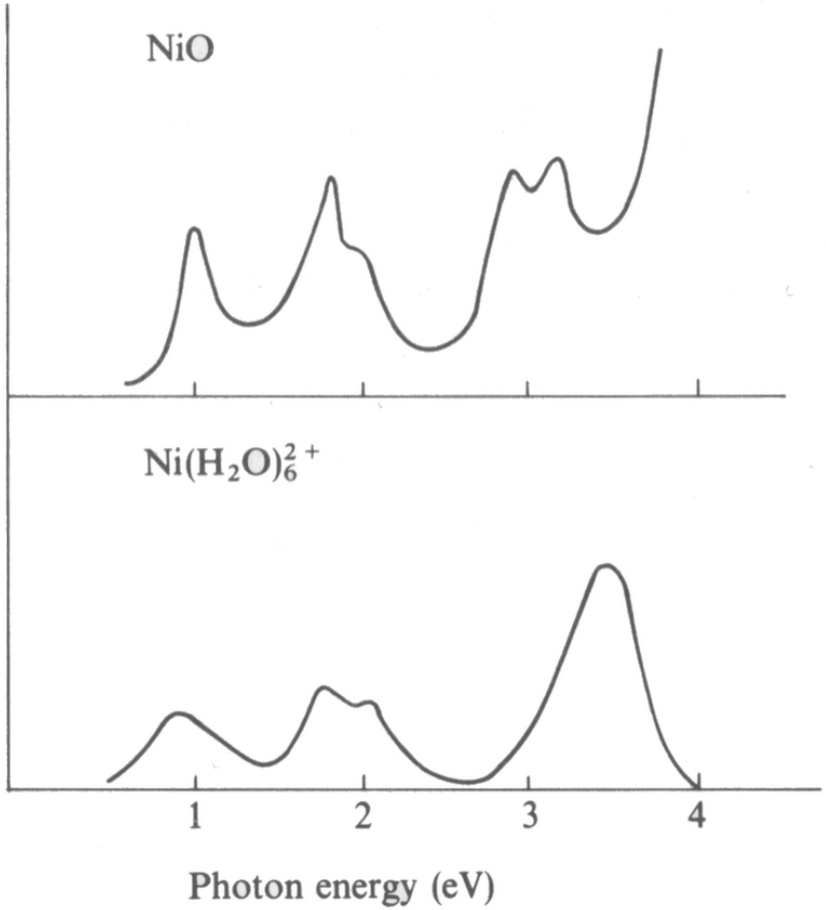


NiO displays the color of isolated Ni^{2+} in solution, with similar spectra.

seshadri@mrl.ucsb.edu

Correlations and the Hubbard model: NiO



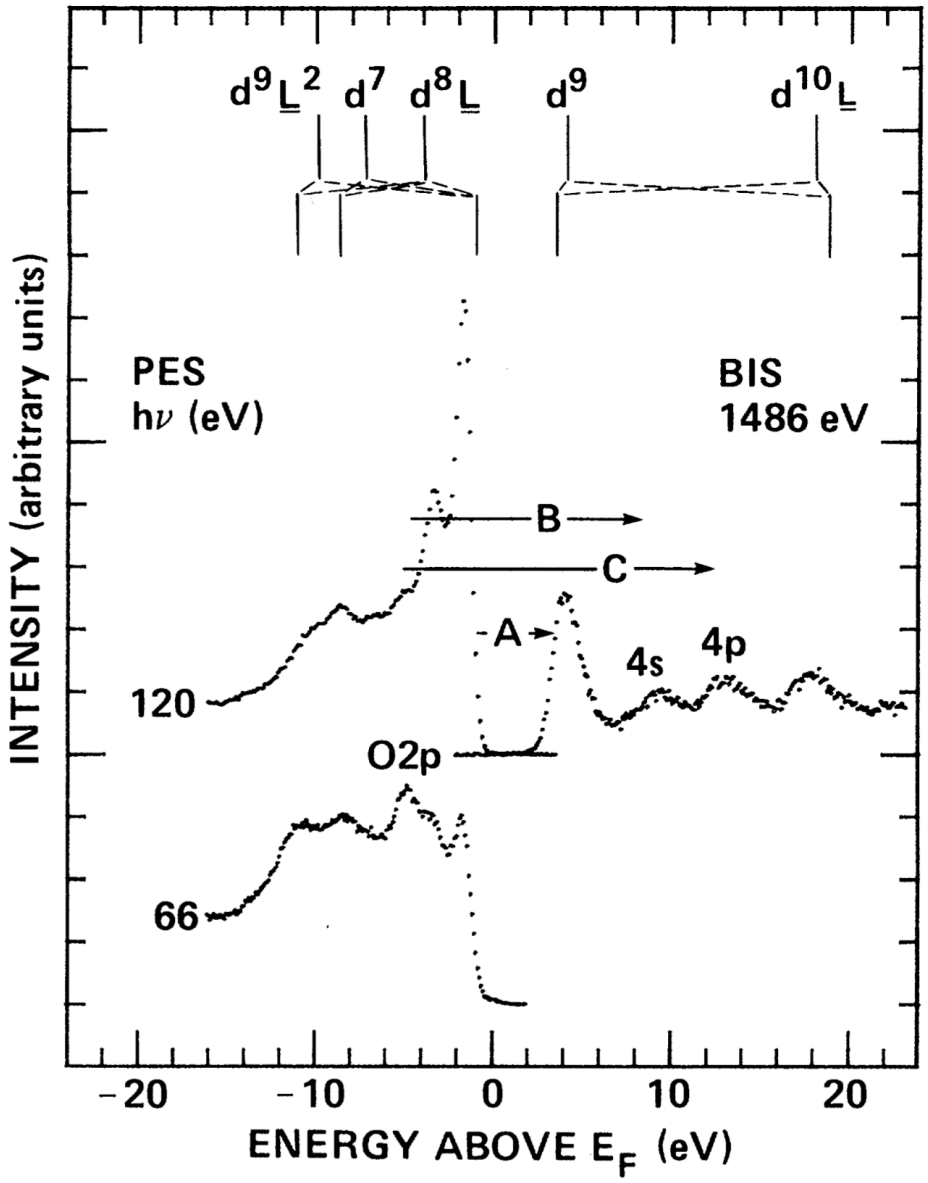


From the Cox text, page 151

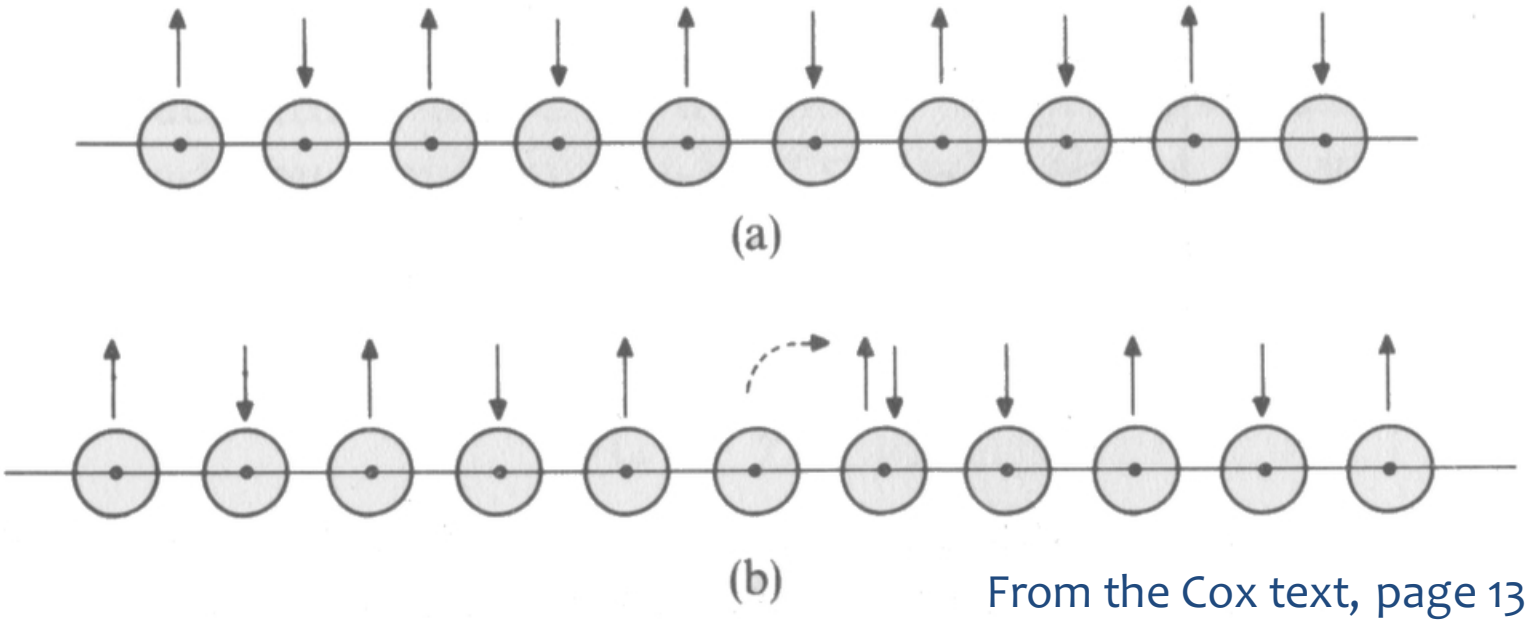
NiO displays the color of isolated Ni^{2+} in solution, with similar spectra.

seshadri@mrl.ucsb.edu

Correlations and the Hubbard model: NiO, spectroscopic studies



seshadri@mrl.ucsb.edu



From the Cox text, page 135

Consider a chain of orbitals, each with one electron. To hop an electron, an orbital has to be ionized at cost *I*, which is compensated a little by the electron affinity *A*.

$U = I - A$

For H atoms, $I = 13.6$ eV and $A = 0.8$ eV, meaning $U = 12.8$ eV. However, this does not account for some screening (due to the dielectric not being vacuum).

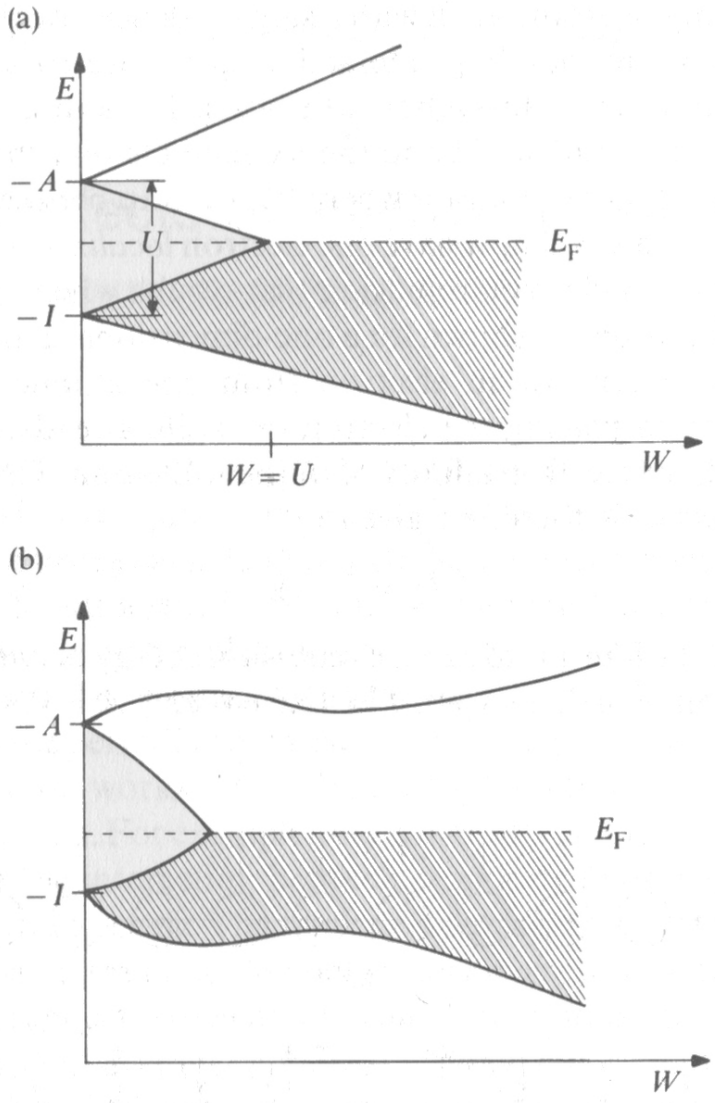
seshadri@mrl.ucsb.edu

$$H = -t \sum_{<i,j>,\sigma} (c^{\dagger}_{i,\sigma} c_{j,\sigma} + c^{\dagger}_{j,\sigma} c_{i,\sigma}) + U \sum_{i=1}^{N} n_{i\uparrow} n_{i\downarrow}$$

hopping or tight-binding (LCAO) part

double-occupancy cost or on-site repulsion

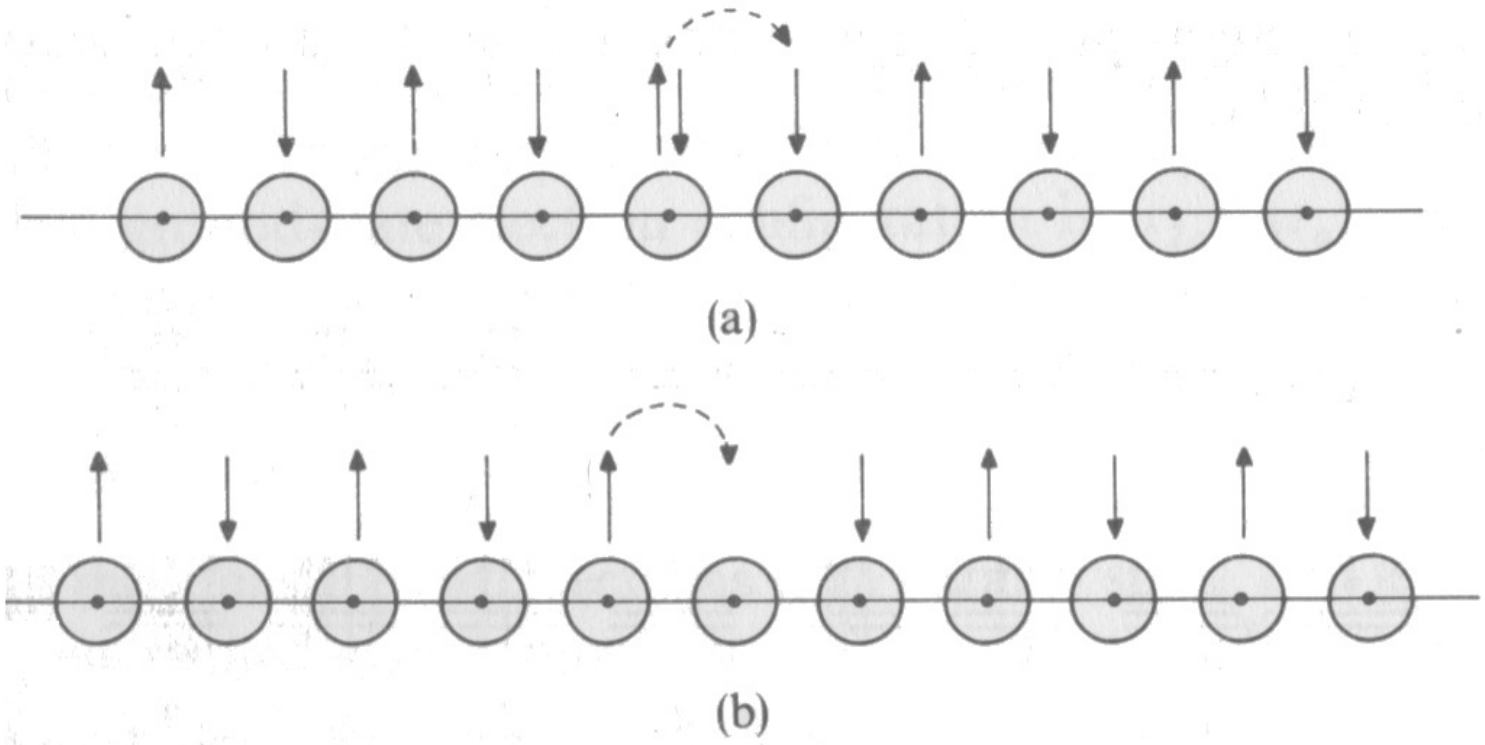
seshadri@mrl.ucsb.edu



As the bandwidth is increased, (or as the atoms approach closer) the gap can close.

From the Cox text, page 137

seshadri@mrl.ucsb.edu



Doping of holes (removal of electrons) as in (b) makes hopping much easier, with the on-site repulsion having been removed.

From the Cox text, page 149

seshadri@mrl.ucsb.edu