substance: FeO ($Fe_{1-x}O$)
property: band structure

Band structure calculations; [72M, 78K]. Results co mpared to photoe mission data [75E]: Fig. 1. Substantial overlap between the d-orbital energies and the O 2p band is evident. A local cluster calculation on FeO_6^{10-} has also been reported [76T] (see Fig. 2). The qualitative conclusions are si milar to the later band calculation [78K] with the $t_{2g}\uparrow$ (Γ'_{25}) lying below the O 2p valence band edge.

References:

72M Mattheiss, L. F.: Phys. Rev. B5 (1972) 290.
72S Slater, J. C., Johnson, K. H.: Phys. Rev. B5 (1972) 844.
75E Eastman, D. E., Freeouf, J. L.: Phys. Rev. Lett. 34 (1975) 395.
76T Tossell, J. A.: J. Electron Spectrosc. Relat. Phenom. 8 (1976)1.
78K Kunz, A. B., Surratt, G. T.: Solid State Commun. 25 (1978) 9.

Fig. 1.

FeO. Band structure showing (a) Hartree-Fock data, (b) self-consistent calculation with correlation, (c) non-self consistent calculation, (d) experimental density of states from photoemission spectroscopy data [75E].

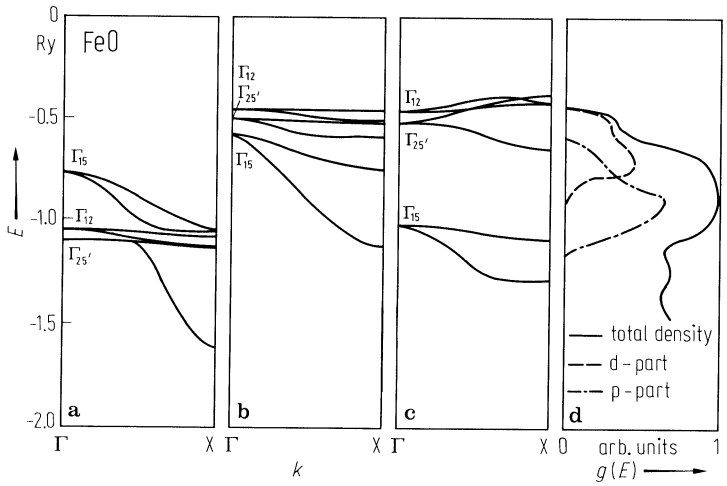

Fig. 2.

FeO. One-electron unrestricted Xα cluster calculation on FeO_6^{10-} [76T]. Shown are the electronic levels of an FeO_6^{10-} cluster and the free-atom energy levels. $E_{x\alpha}$: orbital energy. For discussion of cluster method, see [72S].