substance: hematite (α-Fe_2O_3)
property: band structure

No extended band structure calculation reported. Xα-cluster calculation: Fig. 1 (see [74T, 73T, 76T]). From this, the topmost O 2p level is $1t_{1g\downarrow}$ and Fe d–$t_{2g\uparrow}$ levels lie well below the O 2p edge. The highest occupied level is the Fe d–$e_{g\uparrow}$.

References:

73T Tossell, J. A., Vaughan, D. J., Johnson, K. H.: Nature (London) 244 (1973) 42.
74T Tossell, J. A., Vaughan, D. J., Johnson, K. H.: Am. Mineral. 59 (1974) 319.
76T Tossell, J. A.: J. Electron Spectrosc. Relat. Phenom. 8 (1976)1.

Fig. 1.

Fe_2O_3. Xα-cluster calculation on FeO_6^{9-}. Energy for Fe, O and the spin up and down states of the cluster [74T].