substance: chromium sesquioxide (Cr_2O_3)
property: band structure, energy gap

Cluster calculation; Fig. 1. The O 2p – Cr 3d separation is given as 3 eV. HeII UPS spectrum: Fig. 2. In first order, only one ionization is expected for Cr^{3+} corresponding to $d^3\ ^4A_{2g} \rightarrow d^2\ ^3T_{1g}$. This is shown deconvoluted in Fig. 2, and the O 2p – Cr 3d separation experimentally is far smaller than 3 eV. The skewed O 2p band is composed of two separate transitions, the lower energy one corresponding to the simple O $2p^{-1}$ process and the higher energy one to an O 2p – Cr 3d charge transfer shake up process [80H].

thermal energy gap

$E_{g,th}$	3.2...3.4 eV	T = 1000 ...1400°C	64C, 51H

References:

51H Hauffe, K., Block, J.: Z. Phys. Chem. 198 (1951) 232.
64C Crawford, J. A., Vest, R. W.: J. Appl. Phys. 35 (1964) 2413.
75E Eastman, D. E., Freeouf, J. L.: Phys. Rev. Lett. 34 (1975) 395.
76T Tossell, JA.: J. Electron Spectrosc. Relat. Phenom. 8 (1976)1.
80H Howng, W. Y., Thorn, R. J.: J. Phys. Chem. Solids 41 (1980) 75.

Fig. 1.

Cr_2O_3. SCF-Xα scattered wave valence MO diagrams for (a) a CrO_6^{9-} cluster, (b) CrO_6^{8-} 2p hole state, (c) Cr_6^{8-} $2t_{2g}$ valence hole state [76T]. Arrows indicate spin direction.

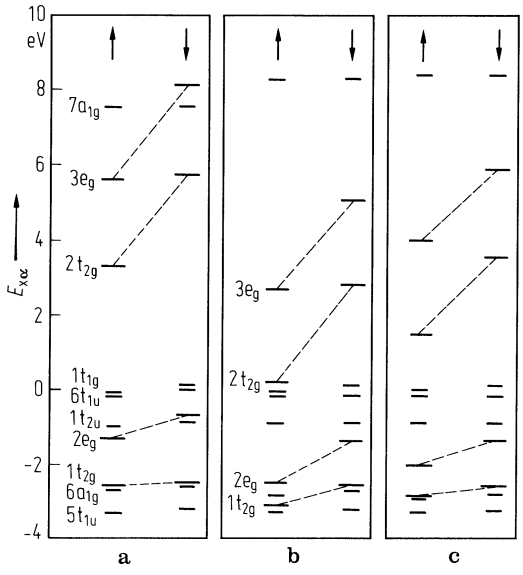

Fig. 2.

Cr_2O_3. He II UPS spectrum (intensity vs. electron binding energy relative to the d-peak) at 40.8 eV photon energy deconvoluted into Cr 3d (dashed line) and O 2p (dashed-dotted line) signals; E_p, E_d are the onsets of the Cr 3d and O 2p photoemission signals and the vertical line is the unbroadened single- state d-ionization [75E].