substance: MoO_3
property: electronic properties: calculated cluster energies

No band calculation has been reported. An Xα-calculation on an ideal octahedral MoO_6^{6-} cluster gives the following energy levels (given in Ry)

E	– 0.117	orbital:	$4a_{1g}$	(Mo5s)	although the 78B
	– 0.181		$3e_g$	(Mo 4d)	qualitative
	– 0.308		$2t_{2g}$	(Mo 4d)	ordering of
	– 0.374		$1t_{1g}$	(O 2p)	these levels
	– 0.381		$4t_{1u}$	(O 2p)	is very
	– 0.396		$1t_{2u}$	(O 2p)	reasonable
	– 0.432		$3t_{1u}$	(O 2p)	the predicted
	– 0.475		$3a_{1g}$	(O 2p)	bandgap
	– 0.488		$1t_{2g}$	(O2p)	(O(2p)–Mo(4d))
	– 0.495		$2e_g$	(O2p)	is far too low

References:

78B Broclawik, F., Foti, A. E., Smith, V. H.: J. Catal. 51 (1978) 380.