

Abstract Submitted
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Influence of Shallow Core Level Hybridization on the Electronic Structure of Metal Oxides¹ R.G. EGDELL, Inorganic Chemistry Lab., Oxford University, P-A GLANS, T. LEARMONTH, K.E. SMITH, Physics Dept., Boston University, J. GUO, Advanced Light Source, LBNL, C. MCGUINNESS, A. WALSH, G. WATSON, Trinity College Dublin. — The influence of shallow core level hybridization on the electronic structure of HgO, ZnO, CdO, and In₂O₃ has been investigated using high-resolution soft x-ray emission and absorption spectroscopies.^{a,b} Synchrotron radiation excited O K_α emission spectra provide a direct measure of the O 2*p* partial density of states and shallow core level hybridization, and reveal significant mixing of O 2*p* and shallow-core metal *d* states. The extent of shallow core hybridisation with the O 2*p* levels is much more pronounced in HgO than in ZnO or CdO and shows an inverse correlation with the binding energy of the core state. Bandstructure calculations confirm the importance of mixing between Hg 5*d* and O 2*p* states in HgO. However the assumption that direct intra-atomic mixing between Hg 6*s* and Hg 5*d* orbitals determines the linear stereochemistry in HgO is shown to be incorrect.^b

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