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Angular-Momentum Resolved Partial Density of States of Rutile TiO2: Theory and Experiment

J.C. Woicik, E.J. Nelson (NIST), L. Kronik, M. Jain, and J.R. Chelikowsky (U. Minn.), D. Heskett (Uni. Rhode Island), L.E. Berman (NSLS), and G.S. Herman (HP)

Beamline(s): X24A

Introduction: We have determined the partial density of valence states of rutile TiO2.

Methods and Materials: We used the method of high-resolution valence photoelectron x-ray standing-wave spectroscopy [1,2,3].

Results: Excellent agreement with *ab initio* local density approximation calculations for the Ti and O partial density of states is found, provided the individual angular-momentum components are corrected for their relative photoionization cross sections. Surprisingly, a large amount of Ti 4p and O 2s hybridization is found in the valence spectra. Additionally, no differences in final-state contributions to the valence binding energies are detected for the Ti and O sites.

Conclusions: These data elucidate the conflicting interpretations of photoemission data for the transition-metal oxides and the necessity to correctly account for the different angular-momentum components of the density of states when comparing theory to experiment.

References:

[1] J.C. Woicik, E.J. Nelson, and P. Pianetta, Phys. Rev. Lett. 84, 773 (2000).
[2] J.C. Woicik, E.J. Nelson, T. Kendelewicz, P. Pianetta, M. Jain, L. Kronik, and J.R. Chelikowsky, Phys. Rev. B 63, R41403 (2001).
[3] J.C. Woicik, E.J. Nelson, D. Heskett, J. Warner, L.E. Berman, B.A. Karlin, I.A. Vartanyants, M.Z. Hasan, T. Kendelewicz, Z.X. Shen, and P. Pianetta, Phys. Rev. B 64, 125115 (2001).