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Authors

Kowalczyk, S.P.
Ley, L.
McFeely, F.R.
et al.

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S. P. Kowalczyk, L. Ley, F. R. McFeely, and D. A. Shirley

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COMMENT ON "ELECTRONIC STRUCTURE OF TRANSITION METALS III. d-BAND RESONANCE AND REGGE POLE THEORY"*

S. P. Kowalczyk, L. Ley,† F. R. McFeely, and D. A. Shirley

Department of Chemistry and
Lawrence Berkeley Laboratory
University of California
Berkeley, California 94720

ABSTRACT: X-Ray photoemission measurements of the d-band width of the 3d transition metals are shown to exhibit a linear relationship with "chemical valence" as predicted by Animalu's calculations using a reformulated version of Ziman's resonance model.

In a series of papers Animalu[1-3] has developed a transition-metal model potential (TMMP) method, based on the pseudopotential approximation, to discuss the electronic structure of the transition metals. In the third paper of that series (referred to here as III), Ziman's resonance model of s-d hybridization[4] is reformulated. The basic result of III is the prediction of systematic variation of d-bandwidth with chemical valence in the 3d, 4d, and 5d series.

In III, the ultraviolet photoemission (UPS) results of Eastman and Grobman[5] and Smith and Traum[6] were employed as an experimental test of the TMMP method. As stated in III, the results are strictly valid only for the first half of the 3d, 4d, and 5d series, so comparison with the UPS data on Rh, Pd, and Ag[6] is not a very good test of the model. An even more fundamental objection to such a comparison is that, in ultraviolet photoemission studies, final-state modulation effects can strongly distort the apparent density of states.[7-9] The experiments of refs. 5 and 6 were done in the range of photon energies $4 \leqslant h\nu \leqslant 11.6$ eV.

A more valid comparison would be to use the bandwidth Δ obtained by x-ray photoemission spectroscopy, for which final-state modulation is negligible. In Fig. 1, we plot Δ for Sc through Mn, as obtained from our XPS ($h\nu$ = 1486.6 eV) results,[8] versus the squared "chemical valence" Z^2. For Δ we have used the total observed bandwidth as in most cases the d-bandwidth is a somewhat ambiguous quantity to separate out of the measured spectrum. Also plotted in Fig. 1 is Δ vs. Z^2 as predicted in III. Both theory and experiment exhibit a linear dependence, with the experimental line being higher and possessing a slightly different

slope. Possible causes of the upward shift of the experimental results include experimental resolution (0.55 eV), many-body effects (relaxation) and lifetime broadening. The experimental density of states were compared in detail in ref. 8 to the band-theoretic results and were found to be generally in good agreement. Thus the correlation of our results with III lends support to the Ziman resonance model as given in III.

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FOOTNOTES AND REFERENCES

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†Present address: Max Planck Institute fur Festkorperforschung, Stuttgart, Germany.

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FIGURE CAPTION

Fig. 1. Plot of Δ (d-band width) for the transition metals obtained from x-ray photoemission studies (ref. 8) and Z^2 (the square of the "chemical valence"). The dots (·) represent values obtained from Table I of ref. 8 and squares (□) were obtained from Fig. 4 of III.

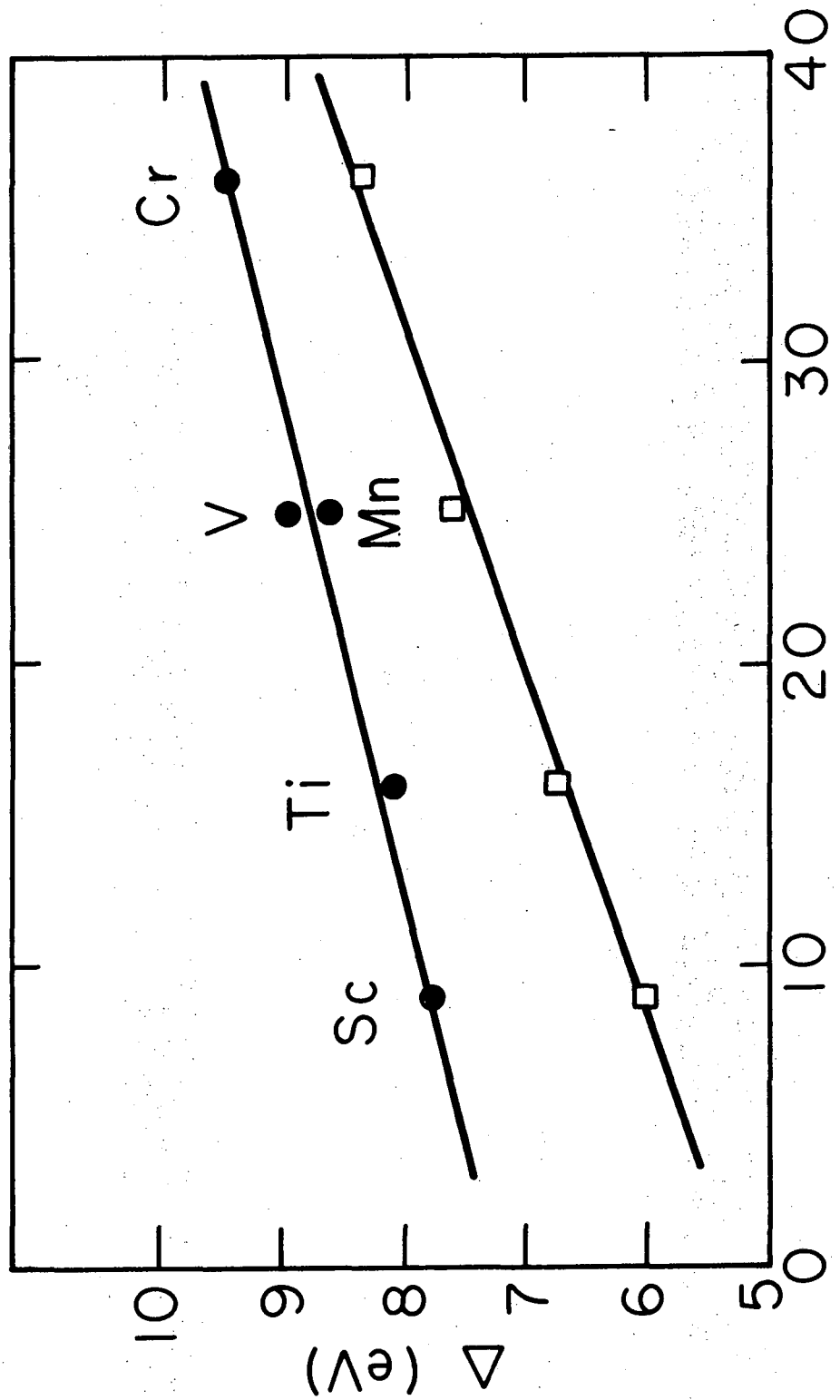

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Fig. 1

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