SUMMARY ABSTRACT: ANALYSIS OF CHEMICAL BONDING IN TIC TIN AND TIO USING S. (U) CALIFORNIA UNIV LOS ANGELES DEPT OF CHEMISTRY AND BIOCHEMISTRY S KIM ET AL.

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SUMMARY ABSTRACT: ANALYSIS OF CHEMICAL BONDING IN TiC, TiN, AND TiO
USING SECOND-PRINCIPLES BAND STRUCTURES FROM PHOTOEMISSION DATA

by

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This investigation was motivated in part by the observation that the empirical pseudopotential calculations of the TiC electronic structure produced valence electron densities that disagree severely with those obtained from first-principles calculations. The intent of this study was to see if the mixed-basis band structure interpolation scheme (MBBSIS) could be used to obtain reliable band structures and charge densities for more complex systems, such as TiC, TiN, and TiO.
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