

Abstract Submitted
for the MAR09 Meeting of
The American Physical Society

Electronic Structure of Aluminum compounds¹ A.R. CHOURASIA, Dept. of Physics, Texas A&M Univ-Commerce, HONG DONG, S.D. DESHPANDE, Aurangabad University, India — The valence and conduction bands of aluminum and aluminum compounds (AlB, AlN, and Al₂O₃) have been studied using a DFT computational approach implemented in CRYSTAL06. The Becke exchange with the LYP correlation has been employed. The atomic basis sets with diffuse and polarization functions have been optimized for each configuration in these materials. The density of states in the valence and conduction bands has been computed in each case. The projected density of states of the constituents has also been computed. The band gap and the dielectric constant have been calculated for these materials. These values have been compared with the available experimental data. The correlation between the partial density of states and the chemical bonding will be presented.

¹Work supported by Research Corporation and Organized Research, TAMU-Commerce.

A. R. Chourasia
Dept. of Physics, Texas A&M Univ-Commerce

Date submitted: 28 Nov 2008

Electronic form version 1.4