

Abstract Submitted
for the MAR07 Meeting of
The American Physical Society

Electronic Structure Calculations of Si, SiC, Si₃N₄ and SiO₂¹

RYAN JACOB, A.R. CHOURASIA, Department of Physics, Texas A&M University-Commerce — The band structure of Si, SiC, Si₃N₄ and SiO₂ have been studied using a DFT computational approach implemented in CRYSTAL98. The Becke exchange has been employed. Two types of correlations have been explored: Perdew, Wang, and Lee, Yang, Parr. The atomic basis sets with a polarization function 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 electronic polarizability and the Auger parameter determined previously from x-ray photoelectron spectroscopy will be presented.

¹Work supported by Research Corporation and Faculty Enhancement Research Grant, TAMU-C

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Date submitted: 08 Nov 2006

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