Abstract Submitted
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Density of States of Silicon, Silicon Dioxide, Silicon Nitride and Silicon Carbide[1] HONG DONG, A.R. CHOURASIA, Department of Physics, TAMU-Commerce, S.D. DESHPANDE, Department of Physics, Amravati University, India — The density of states of Si, SiC, Si_3N_4 and SiO_2 have been studied using a DFT computational approach implemented in CRYSTAL06. This code employs linear combinations of Gaussian type functions to represent single particle wave functions. The Becke exchange and Lee, Yang and Parr correlation have been employed. The atomic basis sets with a polarization function have been optimized for each configuration in these materials. The unit cell parameters have also been optimized. The density of states in the valence and conduction bands have been computed in each case. The projected density of states of the constituents has also been computed. The band gap has been calculated for these materials. These values are 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.

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