

Density functional theory in practice: electronic structure of Ga_2O_3 and band boundary character in Al_2O_3 matrix

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Understanding how local chemistry and structure influence electronic properties is fundamental to designing next-generation optoelectronic and sensor materials. In this talk, we demonstrate how first-principles Density Functional Theory (DFT) can be used to analyze the electronic structure of a gallium oxide (Ga_2O_3) region embedded in an aluminum oxide (Al_2O_3) host matrix, a model system motivated by potential ultraviolet photodetector and solar-blind applications. Beginning with a chemically embedded Ga-rich supercell derived from an Al_2O_3 lattice, we perform self-consistent DFT calculations to obtain the ground-state electronic density, total and projected densities of states (DOS/PDOS), and real-space charge densities associated with band edges. Our results reveal a clear insulating band gap of approximately 4.1 eV (PBE), with the valence band maximum dominated by O-2p states and the conduction band minimum by Ga-p states. Orbital decomposition shows deep Ga-d states within the valence manifold and characteristic antibonding features above the gap. Charge-density visualizations confirm that the highest occupied states localize primarily on oxygen, while the lowest unoccupied states localize on gallium sites. These findings provide a coherent picture of band-edge physics in embedded oxide systems and establish a baseline for future studies of chemically confined quantum dots and UV-active materials.

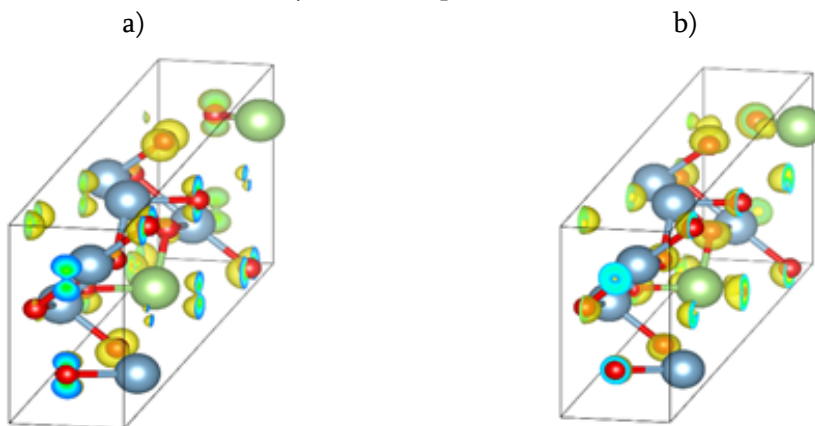


Figure 1: Isosurface representation of the Kohn–Sham charge density corresponding to the highest occupied state of (VBM) (a) and lowest occupied state of (CBM) (b). In (a) the density is strongly localized on oxygen atoms (red balls) while in (b) it is primarily localized on gallium atoms (green-balls).