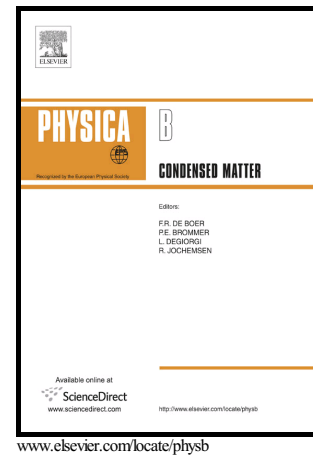


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# First principles calculations of $\text{La}_2\text{O}_3/\text{GaAs}$ interface properties under biaxial strain and hydrostatic pressure

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## Abstract

$\text{La}_2\text{O}_3$  is a potential dielectric material with high permittivity (high- $\kappa$ ) for metal-oxide-semiconductor (MOS) devices. However, band offsets and oxide defects should still be concerned. Smaller band offsets and carrier traps increase leakage current, and degenerate performance of the devices. In this paper, the interface behaviors of  $\text{La}_2\text{O}_3/\text{GaAs}$  under biaxial strain and hydrostatic pressure are investigated, which is performed by first principles calculations based on density functional theory (DFT). Strain engineering is attempted to improve performance of the metal/ $\text{La}_2\text{O}_3/\text{GaAs}$  devices. First of all, we creatively realize band alignment of  $\text{La}_2\text{O}_3/\text{GaAs}$  interface under biaxial strain and hydrostatic pressure. The proper biaxial tensile strain can effectively increase valence band offsets (VBO) and conduction band off-

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