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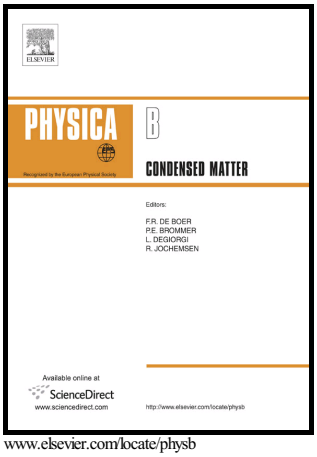

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First principles calculations of La_2O_3/GaAs interface properties under biaxial strain and hydrostatic pressure

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Abstract

La_2O_3 is a potential dielectric material with high permittivity (high-κ) 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 La_2O_3/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/La_2O_3/GaAs devices. First of all, we creatively realize band alignment of La_2O_3/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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