Submitted: 22 May 2013
Accepted: 12 June 2013
Published Online: 18 July 2013

All-out band structure and band offset *ab initio* predictions for AlN/GaN and AlP/GaP interfaces

Journal of Applied Physics **114**, 033709 (2013); https://doi.org/10.1063/1.4812493

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ABSTRACT

We studied the electronic properties of the AlP/GaP and AlN/GaN interfaces and their cubic constituents. The work is developed using approximate quasiparticle approach LDA-1/2 method. First, we provide a detailed calculation of bulk AlN, AlP, GaN, and GaP. In addition to accurate results for fundamental band gap, we also obtained accurate electronic transition levels along valence and conduction bands profiles, compared to experiments and theoretical results using GW and hybrid functionals methods. For the conduction (valence) band offset we obtained 0.27 eV (0.43 eV) for AlP/GaP and 1.47 eV (0.36 eV) for AlN/GaN interfaces, in good agreement with experimental results.

ACKNOWLEDGMENTS

Acknowledges the LCCA-Laboratory of Advanced Scientific Computation of the University of São Paulo for computational support and FAPESP and CNPq for financial support.

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