

Abstract Submitted  
for the MAR11 Meeting of  
The American Physical Society

**Natural interface states in coherent and isovalent III-V heterostructures**<sup>1</sup> VOICU POPESCU<sup>2</sup>, National Renewable Energy Laboratory, Golden, CO, ALEX ZUNGER, National Renewable Energy Laboratory — Interface states occur in semiconductor heterojunctions whenever a significant perturbation is present, caused by interface defects, lattice mismatch, discontinuities in the effective mass or sharp variations in the potential across the interface. We discuss the natural interface states appearing in perfectly coherent and isovalent III-V heterojunctions when a  $\Gamma$ -well and an  $X$ -anti-well coexist in the conduction band. We use empirical pseudopotential calculation to illustrate this type of states for a few III-V heterostructures. For InP/GaP the interface localised states lie energetically in the band-gap and possess, because of their mixed  $\Gamma - X$  character, a strong optical signature. This allows us to provide a different interpretation of the photoemission data existent in the literature for InP/GaP quantum wells and dots. We further discuss the presence of the interface localised states in other III-V heterojunctions, investigating the conditions under which they might be experimentally observed.

<sup>1</sup>Funded by DOE, EFRC for Inverse Design, NREL Subcontract XGC-0-40445-01

<sup>2</sup>Present address: Colorado School of Mines, Golden, CO

Voicu Popescu  
Colorado School of Mines, Golden, CO

Date submitted: 19 Nov 2010

Electronic form version 1.4