**Band offset calculations in the wurtzite / zinc blend interfaces for InP systems.**

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**MOTIVATION**

- InP nanowires may crystallize in the wurtzite phase, presenting stacking faults in the zinc blend phase and vice versa [1].
- The band structure mismatching between the phases contributes to the electro-optical properties of the system.
- The nanowires dimensions (radius of the order of \(\mu\text{m}\)) allow the use of bulk models to study the above mentioned stacking faults contributions.

**METHOD**

- We employed “ab initio” calculations as implemented in the WIEN2k package [2] with the mBJ+LDA potential.
- We built a supercell where the wurtzite phase is matched along its “c” axis with the zinc blend phase in the [111] direction.
- Here, we show the results for a cell with 10 wurtzite layers (dominant phase) and 3 zinc blend ones (stacking faults).

**CELL WITH 1 LAYER OF EACH SYMMETRY**

1) Zinc blend
2) Wurtzite

**RESULTS**

![Graph showing projected DOS and energy gap](image)

**DISCUSSION AND COMMENTS**

- Central atoms in the zinc blend region show DOS more similar to the respective bulk system than the wurtzite atoms.
- Despite of this, the supercell energy gap is still significantly far from the calculated one for zinc blend bulk.
- It is clearly necessary to increase the wurtzite layer in order to reproduce a bulk environment for its central atoms (isolated stacking faults).

**NEXT STEPS**

- Supercells with wider wurtzite layers.
- These computationally demanding calculations should be done at CENAPAD – UNICAMP [3].
- To consider the zinc blend as the dominant phase.
- To calculate the band structure and properties of all these systems.

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**BIBLIOGRAPHY**

