Ecole Doctorale des Sciences Fondamentales

Title of the thesis: First principles calculations providing insight into properties and reactions of III-V and III-N semi-conductor nanowires grown in our research group.

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Summary :

The host research group is the Surfaces and Interfaces group of Institut Pascal that has projects in common with the Cristal Growth Group.

The candidate will carry out theoretical work whilst benefiting from the scientific background mostly comprising experimentalists who grow or characterise III-V semiconductors, in particular nanowires.

Recently, several publications have studied core-sheath nanowires using Density Functional theory (DFT) adapted to periodic systems (1).

The aim of this study is to adapt and develop *ab initio* Perdew Burke Ernzehof functional (PBE) plane-wave calculations to the GaAs and GaN defect-free wires grown in the institute (i.e. at known optimal geometry).

This choice of PBE is justified by its accuracy for solid state lattice parameters and band structure (2). The software used by the candidate will be the ABINIT DFT/plane wave code, along with a graphic interface, such as Diamond for input and for illustrative output.

Several model supercells for the GaAs zinc-blende structure wires have already been tested, in the course of research for a Master's thesis.

Deposition of a GaN layer at the surface of the GaAs nano-wires is an integral part of this study. In spite of a 25% lattice mis-match, this has been shown to proceed in our group, notably on planar surfaces of GaAs. The result is also defect free, and some element of explanation was provided during previous DFT work in our group (3).

The ABINIT code is well-suited to parallel computers in regional (CRRI) and national (IDRIS) centers.

References:

1 Electronic and structural properties of InAs/InP core/shell nanowires: A first principles study. Cláudia L. dos Santos and Paulo Piquini. J. Appl. Phys. 111, 054315 (2012); doi: 10.1063/1.3692440

2 Density-functional calculations for III-V nitrides using the local-density approximation and the generalized gradient approximation. C. Stampfl* and C. G. Van de Walle Xerox Palo Alto Research Center, 3333 Coyote Hill Road, Palo Alto, California 94304, PRB 59 (8) 1999

3 Thesis in second year, H. Mehdi, Institut Pascal