Research Networking Programmes

Short Visit Grant ☒ or Exchange Visit Grant ☐

(please tick the relevant box)

Scientific Report

The scientific report (WORD or PDF file – maximum of eight A4 pages) should be submitted online within one month of the event. It will be published on the ESF website.

***Proposal Title**:* POLYGONA - Understanding POLYtypism in GrOup IV Nanowires from an Ab initio perspective

Application Reference N°: 6361

1) Purpose of the visit

The main aim of project was employing the state-of-the-art ab initio electronic structure simulations - in the framework of Density Functional Theory - to investigate fundamental aspects related to the low dimensionality of novel Ge nanowires polytypes.

The first objective of the work was focused on the investigation of structural properties of different Ge nano-polytypes at fixed diameter. The second one was to analyze the role of quantum confinement, i.e. the reduction of the size of the system on the structural properties. The second part of the project had as main aim the calculation of the electronic structure for all the polytypes considered above in order to understand how different atomic stacking and the quantum confinement can modify the localization and dispersion of electrons in the nanowire.

2) Description of the work carried out during the visit

The main activity of the visit consited in ab initio simulations of the electronic and structural properties of Ge nanowires polytypes. As initial step, we decided to focus only on two geometries of wires, the cubic and the hexagonal one. All the calculations were performed by using the ab initio SIESTA code, implemented in the host group. Due to the huge computational demand, all the simulations have been carried out at the BSC high performance facilities (where the project leader got a CPU time grant in february). After a careful preliminary work to find the optimal convergence parameters of the studied systems, a systematic investigation of their main electronic and structural features

has been performed. The first step of the project has focused on the study of the structural properties in order to find, for each system, which is the geometry of mininum energy and the corresponding ground state properties. This has been carried out by employing total energy DFT calculations with atomic relaxation. Once the all the geometries were obtained, the second step has focused on the investigation of the dependence of the electronic band gap and band structures on the diameter of the wire. After this, an accurate analysis of the results has been carried out.

3) Description of the main results obtained

Calculations concerning the structural properties as function of the diameter of the wire have shown that the variation of the diameter does not affect the cell parameters of the wire. Indeed calculations of the lattice cell parameters in the direction of growth has shown only variations of 0.01 Ang when the diameter of the wire is decreased. This rule has been demonstrated to be valid both for the hexagonal and cubic phases. The study of the electronic structure has demonstrated that the quantum confinement effect has similar effect on the band gap both for the hexagonal and cubic phases. In particular it has been shown, by calculating the energy band gap of structures with diameters from 1 up to 4 nm that the particle-in-a-box model (i.e. the opening of the band gap when the diameter is decreased) is still valid and the phase has not a big influence on that.

4) Future collaboration with host institution (if applicable)

This short visit has offered the possibility to launch a novel and innovative project. During the two weeks of stay of Michele Amato at ICMAB all the necessary input geometries have been prepared and a large amount of preliminary calculations has been launched. Of course, this has been only the first step of such ambitious project, which will last in the next months. Once that the main electronic differences between hexagonal and cubic nanowires phases have been understood, the following work will be focused on the study of the electronic transport in hexagonal/cubic junctions.

5) **Projected publications / articles resulting or to result from the grant *(ESF must be acknowledged in publications resulting from the grantee's work in relation with the grant)***

The project has not yet produced articles as outcomes, however, the writing of one article is envisaged by the end of this year.

6) Other comments (if any)

The continued ESF support for the organization of the visit has been greatly appreciated by all the people involved in this porject.