**Postdoctoral position at LSI Polytechnique Palaiseau-Saclay**

**Interface Calculations in Silicon for Hexagonal Nanowires Growth**

Employer: CNRS, within a French ANR Contract 'HexaNW'
Salary: according to CNRS scales
Place: Paris-Saclay Campus (LSI, École Polytechnique, C2N, UPS)

Hexagonal diamond (HD) silicon nanowires constitute a good candidate for solar energy production [Rödl et al. 2015, Amato et al. 2016]. Being nanostructures of a highly uncommon phase of a common material, they also constitute interesting systems for fundamental studies.

Such nanowires have recently been obtained in research conditions at the École Polytechnique in Palaiseau [Tang et al. 2017]. The goal is now to understand by which mechanisms the HD phase is stabilised during the growth in order to establish a protocol to reliably reproduce it. One step within this project is to calculate ab initio the structures and energies of various types of surfaces of HD Si using the density functional theory. As for surfaces of cubic diamond Si, possibilities of surface reconstructions will have to be looked for. The structure and energy of the HD Si/metal-catalyst (namely tin) interface will also be studied in the same spirit.

Within the same ANR project, these calculated surface and interface energies will then be used to model the nucleation and growth of these hexagonal silicon nanowires. This part of the work will be carried out at the C2N lab (soon to be relocated in Palaiseau). The candidate selected for the present one-year position will be eligible to it as a possible extension.

Requirements: The candidate should have a good background in Materials Science, Thermodynamics, Crystallography, and Ab initio calculations.

The position can start immediately for one year with a possible extension.

Persons to contact:
Olivier Hardouin Duparc olivier.hardouinduparc@polytechnique.edu (for the first year)
Frank Glas frank.glas@c2n.upsaclay.fr (for the possible extension)
with the following documents:
(1) a personal CV (including a publication list)
(2) a concise research statement outlining research experience and interests
(3) contact information for professional references
(4) a short letter of motivation

[Rödl 2015] C. Rödl, T. Sander, F. Bechstedt, J. Vidal, P. Olsson, S. Laribi and J. F. Guillemoles, *Wurtzite silicon as a potential absorber in photovoltaics: Tailoring the optical absorption by applying strain*, Physical Review B **92**, 045207 (2015)
[Amato 2016] M. Amato, T. Kaewmaraya, A. Zobelli, M. Palummo and R. Rurali, *Crystal phase effects in Si nanowire polytypes and their homojunctions*, Nano Letters **16**, 5694-5700 (2016)
[Tang 2017] J. Tang, J.-L. Maurice, F. Fossard, I. Florea, W. Chen, E. V. Johnson, M. Foldyna, L. Yu and P. Roca i Cabarrocas, *Natural occurrence of the diamond hexagonal structure in silicon nanowires grown by plasma assisted vapour-liquid-solid method*, Nanoscale **9**, 8113-8118 (2017)