

## Opened Ph.D. Position

### Advanced DFT modeling of surfaces and interfaces for the monolithic integration of III-V semiconductors on Si

The FOTON Institute – INSA Rennes is offering a 36-months Ph.D position funded by a national project - ANR (NUAGES) in the field of Physics and more precisely dealing with the description at the atomic scale of surfaces and interfaces in III-V and Si materials. This thesis will support state-of-the-art atomically-resolved Transmission Electron Microscopy (TEM) with in-situ epitaxial growth observations to be performed within the ANR project "NUAGES".

**Starting date:** 1<sup>st</sup> October 2022.

#### **Supervisors:**

-MCF (HDR), Laurent PEDESSEAU: <https://cv.archives-ouvertes.fr/laurent-pedesseau>

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**Research team:** Optoelectronics, Heteroepitaxy and Materials (OHM), at INSA–Rennes

**Keywords:** Materials science, Condensed matter physics, Density Functional Theory, Surfaces and Interfaces of III-V semiconductors on Si, Growth of III-V semiconductors, MBE.

#### **Project description:**

Integrating III-V compound semiconductors on (001) Si substrates is a long-standing challenge, which has driven many researches for the past 40 years. This integration is a route to decrease significantly the fabrication cost of many devices since the standard Si industrial processes offer the advantages of a cheaper and larger substrate. In addition, a large portfolio of passive photonic devices and their matured fabrication technology are available on the Si platform. This gives greater flexibility to design photonics integrated circuits (PICs) as compared to the pure III-V technologies and opens a number of possibilities for e.g. lasers, photovoltaic energy production, or energy storage via solar hydrogen production.

The ANR NUAGES project will aim at imaging directly (in real-time, in situ) and clarify the nucleation and crystal growth of III-V semiconductors on Si substrates at the atomic scale. To account for the experimental observations, a theoretical support is expected through Density Functional Theory (DFT) at the atomic scale. The theoretical activity of the ANR NUAGES is thus to determine the absolute III-V surface, and interface energies for various III-V configurations. In addition, special attention will be paid to the description of crystal defects properties (Antiphase

boundaries, dislocations). Based on the results obtained by DFT, the student will help to interpret the experimental data and will propose realistic scenario for nucleation.

To this aim, the doctoral student will mostly conduct DFT simulations, but he will also rely on the advanced technologies available at the laboratory, for the realization of samples (molecular beam epitaxy), or available in collaboration with the consortium (in situ & real-time TEM, STEM, XRD).

## Qualifications

Candidates should have a master degree in materials science or solid-state physics or physics, preferably including documented qualifications in the areas of semiconductor, insulator, or material. The candidate should have a real interest in interacting with experimentalist. The applicant should have an interest in the theory (DFT) closely related to experimental work especially TEM/STEM. Good communication skills in English are required.

## Partnership

The NUAGES project is funded at the national level by the Agence Nationale de la Recherche (ANR), and is leaded by the **C2N** (Centre de Nanosciences et de Nanotechnologies, CNRS/Université Paris-Saclay) together with **IES** (Institut d'Electronique et des Systèmes, Université de Montpellier/CNRS) and **FOTON** (see below). The Ph.D. student will interact constantly with these three teams, which are well recognized in the field.

## About the FOTON Institute (CNRS, UMR6082) and National High Performance Computing (TGCC, CINES)

The **FOTON Institute** is a research unit of the French National Centre for Scientific Research (CNRS) associated to University of Rennes 1 and the National Institute for Applied Sciences (INSA) of Rennes. FOTON Institute is composed of three research teams: the "Optoelectronics, Heteroepitaxy and Materials" (OHM) team, the "laser Dynamics, microwave photonics, Polarimetry, terahertz, imaging" team located in Rennes, and the "Photonic Systems" team located in Lannion. The two cities are located approximatively 170 km apart, in the province of Brittany, Western France. The OHM research team has an established reputation in the area of advanced materials for photovoltaics, photonics or energy conversion applications.

**The successful candidate will carry out research in Rennes, France.**

More information about FOTON can be found at: <http://foton.cnrs.fr>.

**TGCC and CINES** host advanced equipment including the supercomputer by GENCI (Grand National Equipment for Supercomputing), a European leader in high-performance computing. The computational power made available to the research community gives researchers the opportunity to address big scientific challenges. Extreme simulations of complex physical situations, which were not realizable until recently, in various domains as fluid mechanics, physics, chemistry, biology,

climatology, astrophysics, environment etc...are now possible. Numerical simulation has become a method for research at the same level as analysis and experiments, and therefore, the community of users of supercomputing capabilities increases and is renewed every year. A supercomputer ranked at world level with a peak performance of 3.5Pflops. More information about TGCC and CINES can be found at: <http://www-hpc.cea.fr/en/complexe/tgcc.htm> and <https://www.cines.fr/en/>

## Further information-Contact

Further information may be obtained by contacting:

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## Candidature

Please submit your application at your earliest convenience by e-mail to: [laurent.pedesseau@insa-rennes.fr](mailto:laurent.pedesseau@insa-rennes.fr). Your application should include:

- Cover letter
- Detailed CV
- Copy of M.Sc. degree or equivalent
- Grade transcripts
- English test (TOEIC, TOEFL) (except for native)
- List of publications, if applicable
- two letters of recommendation