

Research Grants for PhD students from the China Scholarship Council

Information Form (please read the guidelines carefully on the website www-csc.utt.fr)

Supervisor's name : PEDESSEAU Given names : Laurent

Status (prof., assistant prof., ...): Associate Professor

Laboratory : FOTON Institute Website address : <http://foton.cnrs.fr/v2016/?lang=en>

Institution : INSA Rennes Website address : <https://www.insa-rennes.fr/en.html>

Scientific competence of the supervisor:

Laurent Pedesseau whose work is aimed at the understanding of physical processes in the III-V semiconductor nanostructures for silicon photonics, the halide perovskites and novel materials for photovoltaics, and optoelectronic device simulations for optical-communications. His recent scientific interests include: 1) polar surface and interface energies of semiconductors; 2) first principles simulation of mechanical stability, electronic, and optical properties of semiconductors; 3) electronic structure theory from DFT to many-body corrections GW; 4) HPC technology for exotic and highly demanding simulations. He is cited more than 3600 times with a h-factor of 24 (GoogleScholar).

Two major publications in the field proposed for the PhD :

1. M. Grätzel, 'Photoelectrochemical cells', Nature, vol. 414, no. 6861, pp. 338–344, Nov. 2001.
2. S. Hu, et al., 'Amorphous TiO₂ coatings stabilize Si, GaAs, and GaP photoanodes for efficient water oxidation', Science, vol. 344, 6187, 1005, May 2014.

Website address of the personal page : laurent.pedesseau@insa-rennes.fr

Supervisor's email :

Description of the research work proposed for a PhD

Topic # (see list) : V-5

Title : Advanced materials for solar hydrogen production by DFT modeling

Subject :

The production and storage of clean, renewable, and low-cost energy is one of the challenges facing XXIst century science. In this context, the OHM research team (INSA research unit), which has recognized expertise at the highest international level in the mastery and understanding of solar cells and III-V or Si semiconductor materials,[1]–[4] developed in 2018 new III-V materials integrated on the low cost silicon substrate promising high yields of photo-electrodes.[5] The objective is to study the stability of GaP(Sb) surface and also to thoroughly clarify it in terms of pH dependence. First, the extreme cases will be study with surface considered at operating conditions. Our atomistic methodology together with experimental results (RHEED) from MBE will provide the required physical properties. In the second phase, the role of charge accumulation which takes place at the emergence of antiphase boundaries will be also considered. In the third phase, an effective solution with the texturation of the surface by surface energy engineering will be studied.

To this aim, the doctoral student will be able to rely on the advanced technologies of the laboratory, for the realization of samples (molecular beam epitaxy), and for their simulations (DFT), or available in collaboration (STM or XPS).

See Bibliographic references in the PDF file.

Keywords :

Water splitting; Hydrogen; Surfaces and Interfaces of III-V semiconductors on Si; Density Functional Theory; Growth of III-V semiconductors; MBE; Photo-electrodes

Expected collaborations :

Ongoing collaborations: Photoelectrochemical cell for watersplitting (Univ. Coll. London); National High Performance Computing (CINES, Montpellier); Electrical properties (IPR Rennes).

Background required from the applicant :

The applicant should have a master's degree, or an engineering degree, ideally justifying basic knowledge in materials science, physics and semiconductors, and/or in electrochemistry. The applicant should have an interest in the theory (DFT) closely related to experimental work.

Good communication skills in English are required

Existence of a PDF file detailing the proposal ("yes" or "no") : yes

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