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Ph.D. Position

Advanced materials for solar hydrogen production by DFT modeling

The FOTON Institute – INSA Rennes is offering a 36-months Ph.D. position in the area of renewable energy. This thesis will focus on the exploration of new or advanced materials for solar hydrogen production. More specifically, their bulk properties, surfaces, and interfaces properties by Density Functional Theory

Starting date: between 1 September 2021 and 1 November 2021

Supervisors:

- MCF (HDR), Laurent PEDESSEAU: https://cv.archives-ouvertes.fr/laurent-pedesseau
- PR, Charles CORNET: https://cv.archives-ouvertes.fr/charles-cornet

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

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

Project description:

The production and storage of clean, renewable, and low-cost energy is one of the challenges facing XXIst century science. The photo-electrolysis of water promises the direct conversion of solar energy into hydrogen, which can be reused for the production of heat or electricity on demand. 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 with either H-terminated or O-terminated depending of the reduction or oxidation respectively. 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 aimed and the best way to passivate these textured surfaces will be studied to keep these semiconducting surfaces safe from harm. Finally, the theoretical study will focus on aligned the band edges of GaP(Sb) at the interface with liquid water at 300K by using DFT calculations, molecular dynamics simulations and also a computational hydrogen electrode.

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).

Qualifications

Candidates should have a master degree and PhD 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 an interest in interacting with experimentalist. The applicant should have an interest in the theory (DFT) closely related to experimental work. Good communication skills in English are required.

Partnership

The project will continue the work initiated in collaboration with the Chemistry Department of UCL (London) and will also benefit from all existing collaborations for the structural and optical characterization of materials at national or international level. It is obviously very uncertain to establish a mobility program in view of the current sanitary condition. However, the Ph.D. student will interact with national, European, or international laboratories such as EPFL for methodology, or Rice University (US) to target surface and interface defects on the topic of water cracking. The PhD work will be also supported by projects funded at the national level (French ANRs projects) and international level (H2020 European projects, other international funding).

About the FOTON Institute (CNRS, UMR6082) and National High Performance Computing (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.

CINES hosts advanced equipment including the supercomputer by GENCI (Grand National Equipment for Supercomputing), which appears to date from the first European machines. The computational power made available to the research comunity 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 experience, 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 CINES can be found at: https://www.cines.fr/en/

Further information-Contact

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Candidature

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

- Cover letter
- Detailed CV
- Copy of M.Sc. degree or equivalent
- Grade transcripts
- List of publications, if applicable
- two letters of recommendation

[1] H. Tsai *et al.*, 'High-efficiency two-dimensional Ruddlesden–Popper perovskite solar cells', *Nature*, vol. 536, p. 312, Jul. 2016.
[2] J.-C. Blancon *et al.*, 'Extremely efficient internal exciton dissociation through edge states in layered 2D perovskites', *Science*, vol. 355, no. 6331, pp. 1288–1292, Mar. 2017.
[3] D.-T. Nguyen *et al.*, 'Quantitative experimental assessment of hot carrier-enhanced solar cells at room temperature', *Nature Energy*, vol. 3, no. 3, pp. 236–242, Mar. 2018.
[4] I. Lucci *et al.*, 'Universal description of III-V/Si epitaxial growth processes', *Phys. Rev. Materials*, vol. 2, no. 6, p. 060401(R), Jun. 2018.
[5] I. Lucci *et al.*, 'A Stress-Free and Textured GaP Template on Silicon for Solar Water Splitting', *Advanced Functional Materials*, p. 1801585, May 2018.
[6] M. Grätzel, 'Photoelectrochemical cells', *Nature*, vol. 414, no. 6861, pp. 338–344, Nov. 2001.
[7] S. Hu, M. R. Shaner, J. A. Beardslee, M. Lichterman, B. S. Brunschwig, and N. S. Lewis, 'Amorphous TiO2 coatings stabilize Si, GaAs, and GaP photoanodes for efficient water oxidation', *Science*, vol. 344, no. 6187, pp. 1005–1009, May 2014.