

DRF: Thesis SL-DRF-19-0532

## RESEARCH FIELD

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Solid state physics, surfaces and interfaces / Physique de l'état condensé, chimie et nanosciences

## TITLE

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Theoretical study of the physical and optical properties of some titanium oxide surfaces for gas sensing applications

## ABSTRACT

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The international community under the auspices of the United Nation Framework Convention on Climate Change (UNFCCC) is engaged in developing the policy to reduce greenhouse gases (GHGs) emission and minimize the risks of climate change. Consequently, it is very important to develop a low power, high performance sensor suitable to monitor the GHGs for proper mitigation. A common and existing method for sensing the concentration of gases is by using semiconducting metal oxides like SnO<sub>2</sub>, ZnO, and TiO<sub>2</sub>. Some models emphasize the importance of charge transfer in the sensing mechanism, but an study from first principles, including the electronic coupling with phonons, is necessary to understand quantitatively the adsorption process and the consequent optical response of the system.

The optical response and electron-phonon coupling will be investigated with methods based on the time-dependent density functional theory on which the host team has developed an expertise. Numerical simulations will be performed with the Quantum ESPRESSO package. Part of the project may consist of theoretical and numerical implementations. The Ph.D. subject requires the candidate to be highly motivated by modelling, computing and programming.

## LOCATION

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Institut rayonnement et matière de Saclay

Laboratoire des Solides Irradiés

Laboratoire des Solides Irradiés

Place: Saclay

Start date of the thesis: 01/10/2019

## CONTACT PERSON

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## UNIVERSITY / GRADUATE SCHOOL

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Ecole Polytechnique

Interfaces: Approches interdisciplinaires / fondements; applications et innovation

## FIND OUT MORE

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<https://www.polytechnique.edu/annuaire/fr/users/nathalie.vast>

<https://portail.polytechnique.edu/lsi/fr/recherche/theorie-de-la-science-des-materiaux>

## THESIS SUPERVISOR

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