



## PhD Thesis Offer in Theoretical Modelling and Computational Simulation

(4-years FPI contract within the NanoSENS4env Project)

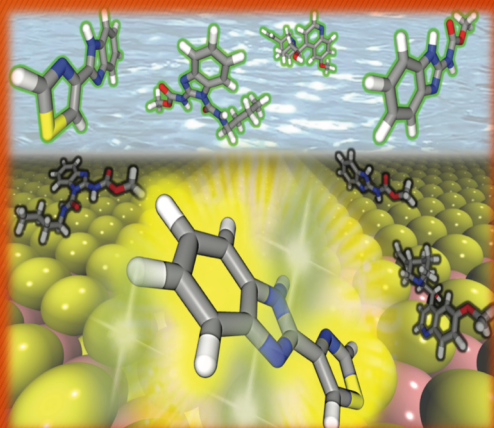
### Fundamentals of the Interaction of Emerging Contaminants with Low Dimensionality Materials

The **ESISNA** group is seeking a highly motivated student to join the **NanoSENS4env** project, which focuses on investigating the interaction of emerging contaminants (ECs) with advanced nanomaterials. This **4-year scholarship** is designed for the candidate to complete a **PhD thesis** in computational simulation.

#### Project and Specific Tasks

- **Atomistic and quantum simulations:** Structural and electronic characterization of nanomaterials and catalytic platforms.
- **Catalytic process modeling:** Simulation of reaction pathways and contaminant degradation mechanisms.
- **UHV Simulations:** Study of EC interactions on MOF layers and other 2D materials.
- **Development of computational AI tools.**

Apply within  
the 2024 FPI  
program!!!



#### Additional Opportunities

- Synergistic collaboration with experimental scientists.
- Training in scientific writing and attendance at international conferences.
- Networking with leading groups in nanomaterials and environmental remediation.
- Experience in advanced bibliographic research and international exposure.

#### Requirements

- Bachelor's degree in Physics, Chemistry, Materials Science, or related fields.
- Experience in computational simulation is valued.
- Intermediate/advanced level of English.



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