

# Computational modeling of interaction insights of microorganisms and organic species with porous semiconductor frameworks

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## Summary

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*The PhD project is part of research and development activities focused on creating nanofiltration systems using mesoporous materials. Certain defective states that appear on the surface semiconductor frameworks can contribute to the adsorption of contaminants and thus increase the efficiency of electron transfer processes upon illumination. We will characterize novel materials in terms of their electronic structure, entire defect chemistry, and interactions with microorganisms and organic contaminants. This will allow us to suggest materials for experimental validation only when their defect chemistry is suitable for solar-driven nanofiltration systems.*

Research field:	Chemistry and biotechnology
Supervisors:	Dr. Svetlana Polivtseva Marijn van Huis Mihhail Klopov
Availability:	This position is available.
Offered by:	School of Science Department of Chemistry and Biotechnology
Application deadline:	Applications are accepted between October 01, 2024 00:00 and October 25, 2024 23:59 (Europe/Zurich)

## Description

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The research project will use a joint experimental-computational approach to investigate light-matter interactions within photo-triggered processes such as disinfection and decontamination. We will combine knowledge from experiments and ab initio calculations to gain insight into defective states of semiconductor frameworks with distinct microstructural features. We will model adsorption and electron transfer processes between selected semiconductor frameworks and contaminants, revealing intermediates capable of participating in chemical reactions using quantum chemical and molecular mechanics/dynamics methods.

### Requirements for the applicant:

- MSc. in Materials Science, Physics, Chemistry, Mathematics or similar
- Experience with programming languages (C, Fortran, Python, etc.)
- Clear interest in Density Functional Theory (DFT) and Molecular Dynamics (MD) simulations
- Experience in probing molecule interaction with materials based on DFT
- Excellent written and verbal communication skills in English
- Inventive and with an independent attitude
- Out-of-the-box thinking



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