2025-2026

Master thesis proposal

Campus Pierre et Marie Curie
Tower 23 – 3rd floor – 23-22
Director: Massimiliano Marangolo

Title: Adsorption of Organic Acids on MgO Surfaces: Experimental and Theoretical Investigations

Keywords: nanopowders, synthesis, adsorption, infra-red spectroscopy, DFT.

Scientific description: The adsorption of Brønsted acids on metal oxide surfaces plays a central role in catalysis, surface chemistry, and geochemical processes. As demonstrated in recent work (Fallacara et al., *Angew. Chem. Int. Ed*. (2024), e202409523) on formic acid adsorption on TiO_2 nanopowders, acid–oxide interactions can lead to unusually strong hydrogen bonding, resulting in pronounced vibrational frequency shifts and unique spectroscopic signatures. Understanding such interactions in detail is essential for unravelling reaction mechanisms at oxide interfaces.

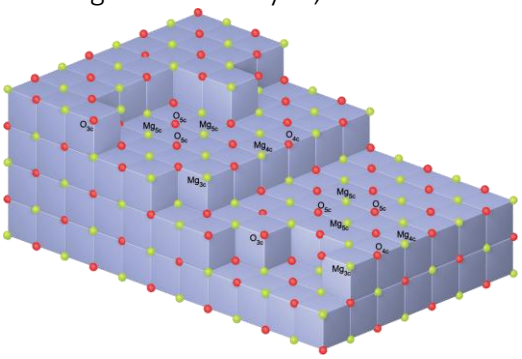
This M2 internship will extend these insights to magnesium oxide (MgO) nanopowders and explore the adsorption of carboxylic acids from formic acid to higher-chain analogues. The project will combine experimental and theoretical approaches:

i) Experimental work will involve controlled adsorption studies of selected acids on MgO nanopowders, probed using in situ infrared spectroscopy under ultrahigh vacuum and variable temperature conditions.

ii) Theoretical work will employ ab initio (within the DFT) molecular dynamics predicting the stability of distinct adsorption configurations and semiclassical nuclear quantum simulations to account for the proton transfer dynamics and for the infrared spectra including temperature and quantum effects. The theoretical work will be in collaboration with Prof. M. Ceotto in Milano University.

The interpretation of the experimental spectra by theoretical simulations enables to establish the vibrational signatures of distinct adsorption geometries with/o hydrogen bonding.

The final outcome of this internship is to establish MgO as a model system for studying acid–oxide interactions and to uncover systematic trends in the adsorption of formic acid to more complex carboxylic acids. Comparative analysis across varying acid chain lengths will highlight how molecular size and polarity influence interaction strength, hydrogen bonding, and stability of adsorbed species. Such findings can provide a broader framework for understanding heterogeneous catalysis, environmental chemistry, and surface modification processes.



Sketch of the MgO(001) surface in nanopowders, illustrating surface point defects such as corners and edges, which are identified as the most reactive sites [Haque et al., JPC C, 122 (2018), 17738.].

Techniques/methods in use: Experimental: synthesis via physical method (evaporation based, metal combustion), TEM and FTIR spectroscopy.

Theory: Density Functional Theory calculations; semi-classical molecular dynamics.
Applicant skills: any experience with the indicated experimental techniques will be considered as an advantage. A knowledge of surface physics and chemistry is a plus.
Industrial partnership: No (specify the company)
Internship supervisor(s) Slavica Stankic: slavica.stankic@insp.jussieu.fr; and Fabio Finocchi: fabio.finocchi@insp.jussieu.fr
Internship location: 4, place Jussieu 75252 Cedex05 Paris. Tower 22, corridor 22-12,5th floor.
Possibility for a Doctoral thesis: can be foreseen (funding Ecole Doctorale ED397).