Master thesis proposal

Machine learning modelling of new bactericidal coatings based on silver nanoparticles

Keywords : machine learning, silver nanoparticles, molecular dynamics, DFT, silica, nano-safe-by-design

SCIENTIFIC DESCRIPTION :

Silver has been known since ancient times for its remarkable antimicrobial properties. The use of silver nanoparticles is a promising strategy for the development of antimicrobial surface coatings, thanks to the release of Ag^+ ions into the environment. This type of device has direct applications in the healthcare sector, the food industry and for various consumer products. In this project, we are developing new 'nano-safe by design' devices in which silver nanoparticles (AgNPs) are incorporated into a silica matrix, allowing the location and duration of Ag^+ ion release into the surrounding environment to be controlled.

To optimize these devices, a detailed understanding of the mechanisms of Ag^+ ion detachment at the AgNP/silica interface is essential. These processes are based on multi-scale phenomena, involving both the atomic structure of the nanoparticle/matrix interface, interactions with chemical species of the environment, and the dissolution dynamics of the particles. To access this information, which is difficult to observe experimentally, numerical studies play an essential complementary role.

This internship aims to study, through molecular dynamics (MD) simulations, the influence of the silica matrix on the AgNPs morphology as a function of their size and temperature in order to identify the surface sites of AgNPs that are reactive with regard to the release of Ag+. Previous studies on the nature of the interface between the surface of AgNPs and the surrounding silica have been conducted using DFT, first in the form of thin films [1], then in the form of small AgNPs (55 and 147 atoms) embedded in a silica matrix [2]. We have shown that the presence of the amorphous silica matrix around the AgNP leads to the formation of covalent bonds between the nanoparticle and the matrix, as well as electron depletion in the AgNP, which becomes cationic. More recently, we have developed a machine learning interaction potential (MLIP) to study the diffusion of Ag^+ ions in silica [3]. In order to better characterize the initial stages of Ag^+ ion detachment, the next step is to model nanoparticles of realistic sizes and at finite temperatures, incorporated into the silica matrix.

This internship offers a unique opportunity to contribute to research on nanomaterials and acquire advanced skills in DFT, molecular modelling and machine learning.

[1] H. Balout, N. Tarrat, J.Puibasset, S. Ispas, C. Bonafos, and M. Benoit, ACS Applied NanoMaterials, 2019, 2, 8, 5179
[2] M. Benoit, J. Puibasset, C. Bonafos and N. Tarrat, Nanoscale, 2022, 14, 7280
[3] S. Trillot, N. Tarrat, N. Combe, P. Benzo, C. Bonafos and M. Benoit, J. Chem. Phys., 2025, 162, 104701.

Techniques/methods in use :

The main tasks to be carried out during the internship will include:

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1. Development of interatomic potentials for the AgNP/silica system: DFT database generation and comparison of several machine learning software programs to generate accurate interatomic potentials (N2P2, VASP-MLFF, MACE, etc.).
2. Molecular dynamics simulations: Performing MD simulations to study the morphology and reactivity of AgNPs within the matrix as a function of different parameters (size, temperature).
3. Analysis of results: Interpreting simulation data to identify sites that are reactive with regard to the detachment of Ag^+ ions.

To carry out these tasks, the candidate will need to learn how to use various modelling software programmes, master high-performance computing and develop data analysis tools in Python.

Applicant skills : The candidate should preferably have a background in solid-state physics and/or chemistry or materials science with knowledge of quantum chemistry and numerical simulation.

Internship supervisor(s) : Magali Benoit, magali.benoit@cemes.fr, and Nathalie Tarrat, nathalie.tarrat@cemes.fr

Internship location : This internship will take place within the 'Surfaces, Interfaces and Nano-Objects' (SINanO) team at the CEMES laboratory in Toulouse. The SINanO team's research focuses on the design, development and study of nano-objects or nanostructures, either isolated or interacting with their environment, throughout their life cycle, in a context where there is a need for new functional nanomaterials with a reduced environmental footprint. It aims to answer fundamental questions about the identification of the basic mechanisms governing local chemical order and structure, which drive electronic, physical and chemical properties, with a particular focus on the role of surfaces and interfaces. Our approach is multidisciplinary (physics, chemistry), sometimes at the interface with other disciplines (biology), with a strong interconnection between theory and experiment, which feed into each other within the team.