Mobility of NEXT/NanoX tenured Scientists

Name	**BENOIT Magali**
Position	DR2
NEXT/NanoX affiliation	CEMES SINanO
Host laboratory	Dept. of Chemistry and Courant Institute of Mathematical Sciences New York University 100 Washington Square East New York, NY 10003
Country of host lab.	USA
Inviting contact	Prof. Mark E. Tuckerman (mark.tuckerman@nyu.edu)
Dates of stay	From 08/03/2020 to 22/03/2020

Brief Description of the host lab

The Department of Chemistry at New York University (NYU) develops research that covers the disciplines of chemistry, including organic, inorganic, physical and theoretical/informatics chemistry. In addition, laboratories established in these traditional fields are addressing problems at the interface of biology and materials science. The department benefits greatly from a highly interdisciplinary and collaborative environment, including strong interactions with other NYU units, at NYU's global sites within the vast scientific community in New York, and around the world.

Research project during the stay

Descriptive Title Application of Machine Learning methods to the study of the Ag+ ions release by Ag nanoparticles implanted in silica

Very recently, Prof. M. E. Tuckerman of New York University and his collaborators proposed a method to solve the DFT equations using a machine learning (ML) apporach, by directly learning the potential-density and density-energy maps[1]. They demonstrated the effectiveness of their approach on model systems and molecules and achieved the first molecular dynamics with electron density learned by ML on malonaldehyde and were able to capture the intramolecular proton transfer process.

The purpose of the stay in Prof. M.E. Tuckerman's group is to learn this new method of ML and to apply it to the problems that interest me and for which I already have databases obtained by DFT. In particular, I am interested in the process of the Ag+ ions release by silver nanoparticles that are implanted in a silica matrix. These devices are developed with the aim of achieving a controlled release of Ag+ ions into an aqueous medium, which allows them to be used as bactericidal devices, for example[2]. However, a detailed understanding of the processes of detachment and diffusion of Ag+ ions from nanoparticles when they are buried in silica is essential to achieve this control. Our first studies by atomic modelling showed the importance of treating these systems with an electronic structure calculation because covalent bonds are formed spontaneously at the interfaces between nanoparticles and silica[3]. To go further, we want to model a complete nanoparticle surrounded by silica as well as the diffusion of Ag+ ions in amorphous silica, which is very computer time consuming. For these reasons, a machine learning approach such as that proposed by M.E. Tuckerman would be perfectly suited to our problem.

[1] F. Brockherde et al, Nature Communications 8, 872 (2017)
[2] A. Pugliara et al, Science of The Total Environment 565, 863 (2016)
[3] H. Balout et al, ACS Appl. Nano Mater. 2(8), 5179 (2019)