Master M2 Internship:

Applications of the DFT-MD DFT-based molecular dynamics method to modeling oxide/liquid water interfaces or air/liquid water interfaces

Keywords : theoretical and computational chemistry, DFT-MD, AIMD, spectroscopy, condensed matter

Host contact: Professor Marie-Pierre GAIGEOT
Email: mgaigeot@univ-evry.fr, see also http://mpgaigeot-research.fr/
Group Theory and Modeling: Laboratoire LAMBE UMR 8587, Laboratoire Analyse et Modélisation pour la Biologie et l'Environnement, Université d'Evry val d'Essonne, Blvd F. Mitterrand, Bat Maupertuis, 91025 EVRY - PARIS, Université Paris-Saclay, France

Project: Learn and apply the principles of AIMD/DFT-MD simulations for characterizing the structure, dynamics, chemical reactivity and vibrational spectroscopy of heterogeneous condensed matter molecular systems at finite temperature. Here we are specifically interested in modeling the interface between an oxide and liquid water, or between the air and liquid water. These heterogeneous interfaces can also contain electrolytes/organic molecules. The CP2K DFT-MD package is used for the simulations, while codes developed in the group are applied to extract structural, dynamical and spectroscopic information from the trajectories. We will not only extract structural properties from the dynamics but also the non linear SFG (Sum Frequency Generation) vibrational signatures of the interfaces, and thus directly interpret experimental data. The interfaces of interest are of importance to geochemistry, heterogeneous catalysis, atmospheric aerosols. The monthly salary is regulated by French University laws, ≈550€/month.

The interested student will join the group on one of the following current projects:

- AIMD/DFT-MD simulations of silica oxide/liquid water interfaces. Silica oxides are known to be of crystalline/amorphous character and have various degrees of hydrophilicity/hydrophobicity. We will here characterize how liquid water is organized at the interface with various silica oxides (cristals, amorphous) and evaluate how this structure evolves depending on the hydrophilicity/hydrophobicity of the solid surface. Simulations will be performed for neat and charged electrolytic interfaces. These investigations follow our recent papers: J.Phys.Chem.C. 120:14034 (2016) ; J.Phys.Chem.C. 119:27354 (2016) ; J.Chem.Theory.Comput. 8:1037 (2012) ;

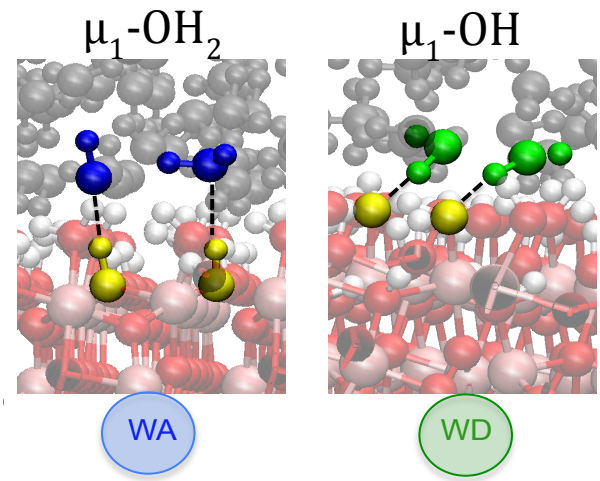
- AIMD/DFT-MD simulations of the air/liquid water interface containing electrolytes. This investigation follows our very recent paper J.Phys.Chem.Letters 8:3133 (2017) on the neat air/water interface where we have demonstrated the existence of a 2-Dimensional H-Bond network formed by the water molecules at the interface with the air. We investigate here whether/how ions/electrolytes accommodate within this network.

The 'Theory and Modeling' hosting group is composed of 7 permanent researchers (University and CNRS), 5 PhD students, 2 Post-Docs, 1 Informatics Engineer, 2-3 foreign visitors join/year. The group is internationally recognized, funded on several ANR and LABEX projects, amongst which currently 1 bilateral France-Germany ANR-DFG, 1 national ANR with the IFPEN company. The University of Evry is member of the new University Paris-Saclay, and our group is a member of the Chemistry department of University Paris-Saclay.

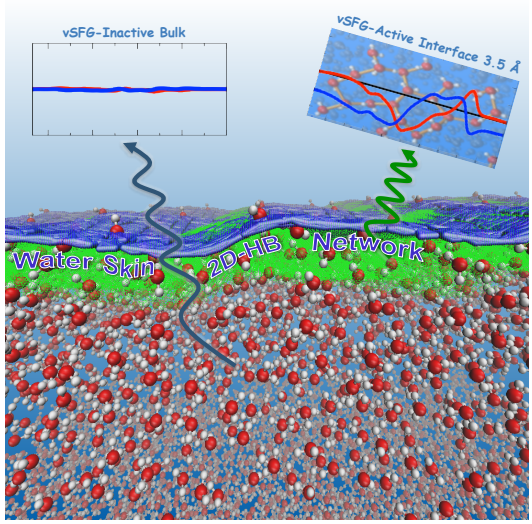
The intern will be able to get a PhD funding from the Doctoral School 2MIB from University Paris-Saclay.

Evry is located 45 minutes from central Paris, through RER D train connections. The University is 2 minutes walk from the RER station Evry-Courcouronnes.
Please see http://www.univ-evry.fr/fr/nous_contacter/plan_d_acces.html for more practical details.

Illustrations from very recent research projects:



Al_2O_3 oxyde/liquid water interface, zooms on the water molecules being acceptor (WA)/donor (WD) of H-Bonds to the surface sites (WA, left/WD, right)



The 2Dimensional H-Bond network formed by water molecules at the interface with the air, revealed by AIMD/DFT-MD simulations. Extracted from our recent paper J.Phys.Chem.Letters 8 :3133 (2017).