Master M2 Internship:
Applications of the AIMD/DFT-MD molecular dynamics method to
vibrational spectroscopy in the TeraHertz (THz) domain

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

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Project Learn and apply the principles of AIMD/DFT-MD simulations for characterizing the structure, dynamics, chemical reactivity and vibrational spectroscopy of gas phase or condensed matter molecular systems at finite temperature. Our expertise is in the modeling of gas phase molecules and clusters, as well as liquid water, as well as solid/liquid water and air/liquid water heterogeneous interfaces. 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. For students interested, codes developments can be done, as well as theoretical developments around the THz spectroscopy signal. 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 gas phase peptides assemblies in order to extract their vibrational spectra in the TeraHertz (THz) domain, i.e. 0-300 cm^{-1}/1-18 THz. This is a project within a long-standing collaboration with the experimental group of Dr A.M. Rijs at the Radbout University of Nijmegen/The Netherlands. The focus is to characterize the structure(s) of peptides assemblies and relate the structure(s) to the vibrational THz signatures. See our recent papers: S. Jaeqx, J. OOmens, A. Cimas, M.P. Gaigeot, A. Rijs, Angewandte Chemie Int. 53 :3663 (2014) ; J. Mahé, D.J. Bakker, S. Jaeqx, A.M. Rijs, M.P. Gaigeot, Phys. Chem. Chem. Phys. 19 :13778 (2017).

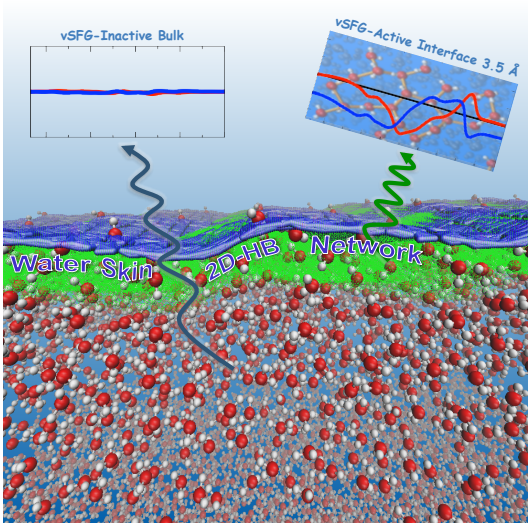
- AIMD/DFT-MD simulations of alcohols immersed in liquid water in order to calculate and interpret vibrational spectra in the TeraHertz (THz) domain, i.e. 0-300 cm^{-1}/1-18 THz. Collaborative project with the experimental group of Prof M. Havenith at the University of Bochum. Our focus is to characterize the structure of water around the hydrophobic alcohols and relate the structure to the vibrational THz signatures.

- AIMD/DFT-MD simulations of the air/liquid water interface containing electrolytes in order to calculate and interpret vibrational spectra in the TeraHertz (THz) domain, i.e. 0-300 cm^{-1}/1-18 THz. These interfaces are of relevance in atmospheric chemistry of aerosols. This project follows our very recent paper J.Phys.Chem.Letters 8:3133 (2017) on the neat air/liquid 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, and whether there are direct signatures of the structures in the THz domain.

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.



A 2D H-Bond network at the air/liquid water interface unravelled by AIMD/DFT-MD simulations. Extracted from our J.Phys.Chem.Letters 8 :3133 (2017).