PhD: AIMD/DFT-MD of nanometric solid/liquid water interfaces for material design
(for final outputs on new energies, more efficient heterogeneous catalysis, electrolytes/pollutants transport)

Keywords : theoretical and computational chemistry, ab initio molecular dynamics, DFT-MD, AIMD, spectroscopy, condensed matter, interfaces, solid, liquid water, materials

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The PhD work will consist in applying ab initio molecular dynamics simulations AIMD/DFT-MD to the design and characterization of nanometric solid oxide/liquid water interfaces (i.e. structure, dynamics/transport, catalysis, SFG and THz-IR spectroscopies) in the context of new energies (for instance materials design for more efficient electrocatalytic water splitting and O2/H2 production in green/sustainable new energies), in the context of heterogeneous catalysis (for instance for the cracking of pollutants in chemical processes for depollution in the environment), or in the context of geochemistry (typically for the transport of groundwater and pollutants).

The package CP2K is used for the AIMD simulations, codes developed in our group are used for the analyses and the extraction of structural/dynamical/spectroscopic/reactivity properties from the trajectories. For those interested, theoretical developments can be considered and/or development of codes for trajectory analyses (fortran and C languages mainly).

Our group is internationally recognized in AIMD/DFT-MD simulations of solid/liquid and air/liquid interfaces. The following references illustrate some of our recent original works [PNAS 116:1520(2019), J.Chem.Phys. 150:041721(2019), Phys.Chem.Chem.Phys. 20:5190(2018), Minerals 8:305(2018), J.Phys.Chem.Letters 8:3133(2017), J.Phys.Chem.C. 120:14034(2016)]. We have in particular shown how water is organized at the interface with numerous hydrophobic/hydrophilic surfaces, especially revealing two main layers which structures are intrinsically very different from each other, how these layers have a thickness that depends on e.g. the solid/pH conditions/electrolyte concentrations, and that these 2 layers are the only ones probed in non-linear SFG spectroscopy, giving rise to specific signals and recognizable marker bands. We have also shown how disciplined/undisciplined water at the interface with semi-conductors cobalt oxide can influence the final water splitting reactivity.

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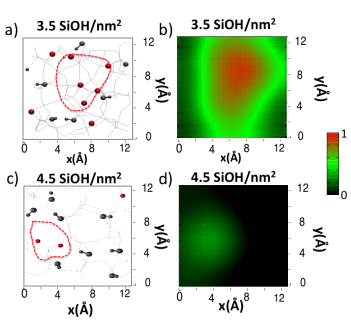
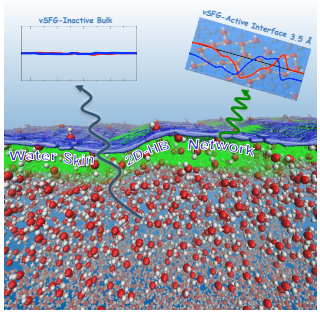
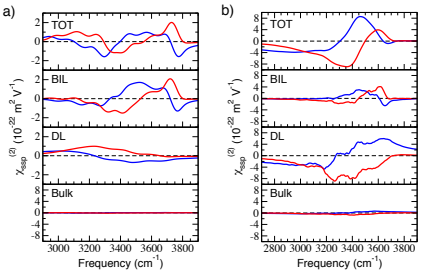
Some illustrations from recent works:



Inhomogeneous patches of hydrophilicity/hydrophobicity at (hydrophilic) SiO_2 silica/liquid water interfaces.
PNAS 116:1520(2019)



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



Deconvolution of SFG signals at silica/water and air/water charged interfaces in terms of BIL (Binding Interfacial Layer), DL (Diffuse Layer) & Bulk contributions, by AIMD/DFT-MD simulations. **PCCP 20:5190(2018)**

PhD: AIMD/DFT-MD of tunable charged/hydrophilic/hydrophobic air/water and solid/water interfaces, in direct relation with interfacial vibrational spectroscopy

Keywords : theoretical and computational chemistry, ab initio molecular dynamics, DFT-MD, AIMD, spectroscopy, condensed matter, interfaces, materials, THz

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The PhD work will consist in applying ab initio molecular dynamics simulations AIMD/DFT-MD to extract structural, dynamical and THz (0-300 cm^{-1}/1-18 THz) vibrational spectroscopic properties of tunable charged/hydrophilic/hydrophobic air/liquid water and solid/liquid water interfaces. One central issue is the calculation of non-linear SFG (Sum Frequency Generation) vibrational spectra, and their interpretation/assignment in terms of structure of water at the interface with the air (air/water interfaces) and at the interface with the solid (solid/water interfaces), in terms of thickness of water being probed experimentally, in terms of chemical reactivity at the interfaces, especially in electrochemical conditions. The work is in strong collaboration with the groups of Profs M. Havenith and P. Petersen at the University of Bochum, Germany, specialists of THz-IR and SFG experiments and developers of unique experiments at interfaces.

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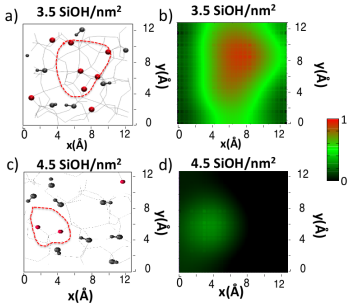

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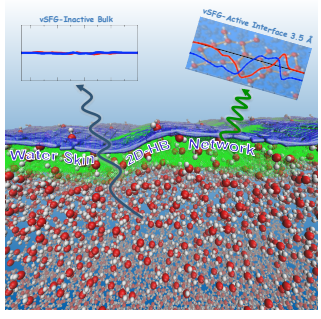
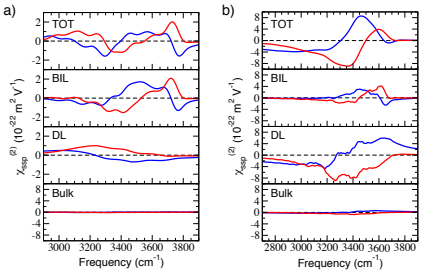


A water 2D-H-Bond-network unraveled at the air/water interface by AIMD/DFT-MD simulations.**J.Phys.Chem.Letters 8:3133(2017)**



Deconvolution of SFG signals at solid or air/water interfaces in terms of BIL (Binding Interfacial Layer), DL (Diffuse Layer) & Bulk contributions. **PCCP 20:5190(2018)**

PhD: Characterization of gas phase biomolecules involved in diseases:
synergy AIMD/DFT-MD and THz vibrational spectroscopy.

Keywords : theoretical and computational chemistry, ab initio molecular dynamics, DFT-MD, AIMD, spectroscopy, gas phase, THz, molecular flexibility, large amplitude motions

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The PhD work will consist in applying ab initio molecular dynamics simulations AIMD/DFT-MD to characterize the structure, dynamics, vibrational spectroscopy in the THz domain (0-300 cm^{-1}/1-18 THz) of biomolecules in the gas phase. The targeted peptidic and glycosidic assemblies are involved in specific recognized diseases, the gas phase medium is crucial in order to reveal the structures free of surrounding environment and free of intermolecular interactions. The aqueous (natural) environment of the biomolecules can be introduced in a controlled way, typically one water molecule at a time, and hence directly measure its influence on the biomolecule structure in a controlled way.

The package CP2K is used for the AIMD simulations, codes developed in our group are used for the analyses and the extraction of structural/dynamical/spectroscopic/reactivity properties from the trajectories. For those interested, theoretical developments can be considered and/or development of codes for trajectory analyses (fortran and C languages mainly).

The central issue in the theoretical simulations is to calculate the THz spectra of the biomolecules and hence assign the experimental spectra through the vibrational fingerprints and marker bands. The theoretical work is done in synergy simulations/experiments. The experiments are performed by the group of Dr A.M. Rijs, at the Radboud University, Nijmegen, The Netherlands, within the FELIX Free Electron laser facility. Dr Rijs is pioneer in THz gas phase spectroscopy, our collaboration dates several years. See our recent papers for more details: 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), and 2 Faraday Discussions for 'Advances in ion spectroscopy: From astrophysics to biology', DOI: 10.1039/C8FD00211H (2019) & DOI: 10.1039/C8FD00208H (2019)

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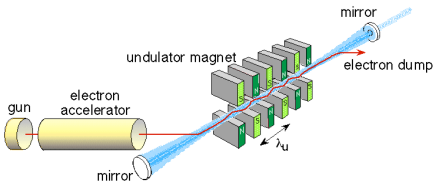
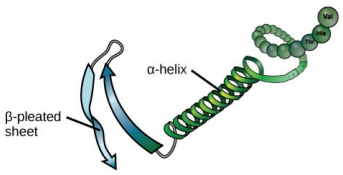
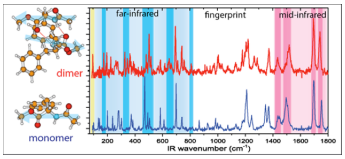




Combining IR-UV ion dip gas phase experiments and AIMD/DFT-MD simulations, structures of biomolecules are unveiled through their spectroscopic fingerprints.



PhD: Graph Theory and Machine Learning in Theoretical and Computational Chemistry

Keywords : theoretical and computational chemistry, ab initio & classical molecular dynamics, DFT-MD, AIMD, FF-MD, graph theory, machine learning, artificial intelligence

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The PhD work will consist in developing and implementing methods from theoretical informatics, i.e. Graph Theory, Machine Learning, Artificial Intelligence, within the domain of Theoretical and Computational Chemistry, and more specifically in relationship with ab initio AIMD/DFT-MD and classical FF-MD molecular dynamics simulations performed in our research group. These dynamics are achieved on (bio)molecules and clusters in the gas phase, on liquids, on solid/water and air/water interfaces, in order to characterize structures, dynamics/transport, chemical reactivity, and vibrational spectroscopies.

This bi-disciplinary PhD research work has one or several of the objectives described below. This is a research conducted in close collaboration in between the group of Prof M.P. Gaigeot at the Laboratory LAMBE at the University of Evry-University Paris Saclay and the group of Prof D. Barth at the Laboratory DAVID at the University of Versailles Saint Quentin-University Paris Saclay. Proposed research:

- Graph Theory and automatic recognition of molecular structures sampled over molecular dynamics simulations, development of a method that can be applied and transferred in between all states of matter, i.e. gas phase, liquids, interfaces. This is a follow-up research from our works presented in J.Chem.Phys. 149:184102(2018) for gas phase molecules, hence extending the methodology to condensed matter. See also our paper J.Mol.Struct.1165:71(2018) for a proof-of-principle at the air/liquid water interface.
- Graph Theory and vibrational spectroscopy, applying graph properties to extract vibrational modes in AIMD/DFT-MD simulations. One proof-of-principle has been published in our paper Faraday Discussions 'Advances in ion spectroscopy: From astrophysics to biology', DOI: 10.1039/C8FD00211H (2019)
- Machine Learning to develop new force fields for classical FF-MD molecular dynamics simulations, capable to treat on the same foot the following properties: structures, dynamics, transport, chemical reactivity, vibrational spectroscopies.

This is a bi-disciplinary PhD. The recruited person will either 1) have a Master degree in theoretical physical-chemistry, already with/or acquiring an expertise during the PhD in AIMD/DFT-MD and FF-MD molecular dynamics simulations and acquiring the expertise in Graph Theory/Machine Learning, or 2) have a Master degree in theoretical informatics, acquiring an expertise during the PhD in AIMD/DFT-MD and FF-MD molecular dynamics simulations. The PhD has a large component in developments and coding, typically in C/C++/python languages.

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