PhD: Origins of life on the planet Earth : Prebiotic chemistry at air/liquid water interfaces by ab initio molecular dynamics simulations AIMD/DFT-MD

Keywords : theoretical and computational chemistry, ab initio molecular dynamics, DFT-MD, AIMD, spectroscopy, condensed matter, interfaces, air/water, solid/water, peptides, chemical reactivity

PhD Supervisor: Professor Marie-Pierre GAIGEOT
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Research Group 'Theory & Modeling' Laboratory 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 & Université Paris-Saclay – France

The PhD work will consist in applying ab initio molecular dynamics simulations AIMD/DFT-MD to the chemical reactivity at air/liquid water and silica/liquid water interfaces in relation with prebiotic chemistry and the origins of life on the planet Earth, and more specifically in relation with prebiotic chemistry leading to the synthesis of peptides on Earth. 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 language).

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 for the structure, dynamics, spectroscopy of aqueous interfaces [Phys.Chem.Chem.Phys. DOI:/10.1039/c7cp06110b (2018), J.Phys.Chem.Letters 8:3133 (2017), J.Phys.Chem.C. 120 :14034 (2016), J.Phys.Chem.C. 120 :4866 (2016)]. We have especially recently demonstrated for the first time in the literature that water is organized into a 2-Dimensional network of hydrogen bonds at the interface with the air (see illustration at the bottom), and one natural question is whether/how this specific water skin can play a role into prebiotic chemistry.

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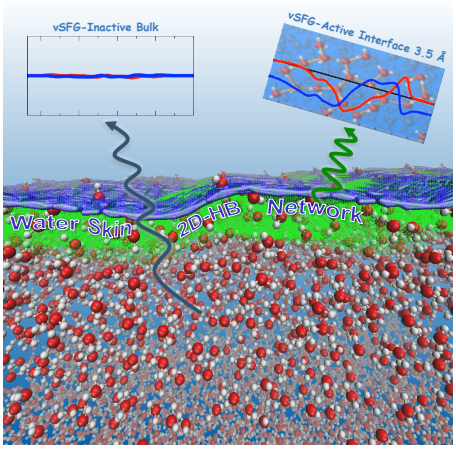

A water 2D-H-Bond-network unraveled at the air/water interface by AIMD/DFT-MD simulations. From our paper J.Phys.Chem. Letters 8 :3133 (2017).

PhD: Ab initio molecular dynamics simulations AIMD/DFT-MD of nanometric solid/liquid water interfaces for energy, material design, heterogeneous catalysis, geochemistry

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 structural characterization of nanometric solid oxide/liquid water interfaces, their dynamics, catalysis and spectroscopy (SFG). Solid oxide/liquid water interfaces are involved in new energies (for instance electrocatalysis and water splitting for H2 production and green/sustainable new energies), in material design and heterogeneous catalysis (for instance design of materials having specific performances for catalysis), in heterogeneous catalysis (for instance for the cracking of pollutants in chemical processes for depollution in the environment), in geochemistry (typically for the transport of groundwater and pollutants), etc. 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 language).

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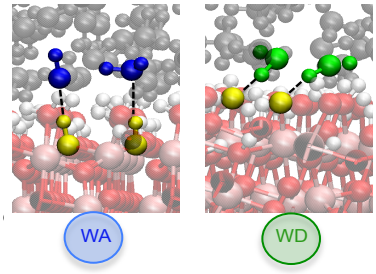
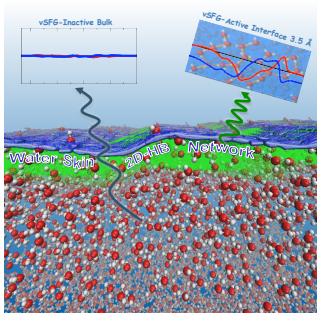
Some illustrations from recent works:



Al_2O_3/liquid water interface, zoom on the water molecules being acceptors (WA)/donors (WD) of H-Bonds to the alumina oxide surface sites. Submitted for publication.



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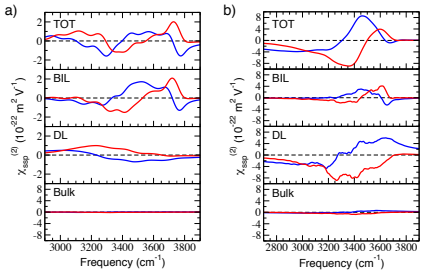

Deconvolution of SFG signals at silica/water and air/water charged interfaces in terms of BIL (Binding Interfacial Layer), DL (Diffuse Layer) & Bulk contributions, by AIMD/DFT-MD simulations. From our paper PCCP DOI :10.1039/c7cp06110b (2018)

PhD: Ab initio molecular dynamics simulations AIMD/DFT-MD of air/water and solid/water interfaces, in 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 charged 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 group of Prof M. Havenith from the University of Bochum, Germany, specialist of THz experiments and developer of unique experiments at interfaces. 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 language).

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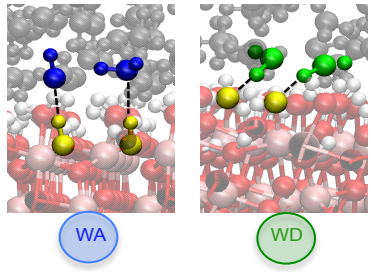

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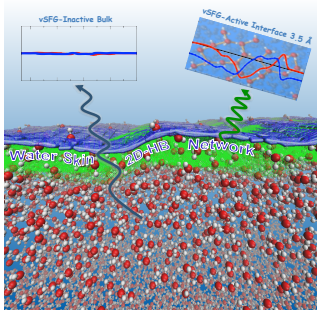

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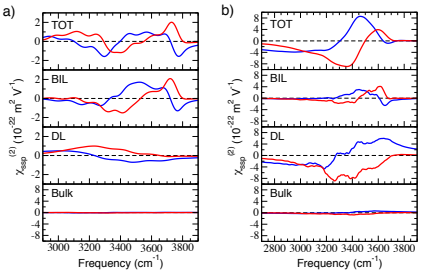

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PhD: Structure of gas phase biomolecules involved in neurodegenerative diseases.
Synergy ab initio molecular dynamics simulations AIMD/DFT-MD and THz vibrational spectroscopy.

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 peptidic assemblies characterized in the work are involved in neurodegenerative diseases. The gas phase medium is crucial in order to reveal the structures free of surrounding environment and free of intermolecular interactions, i.e. free of any external perturbation. 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 language).

The central issue in the theoretical simulations is to calculate the THz spectra of the biomolecules and hence compare and interpret the experimental spectra in terms of structure and underlying vibrational motions. Vibrational fingerprints and marker bands are analyzed and revealed. The theoretical work is done in synergy simulations/experiments. The experiments are performed by the group of Dr A.M. Rijs, at the Radbout 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).

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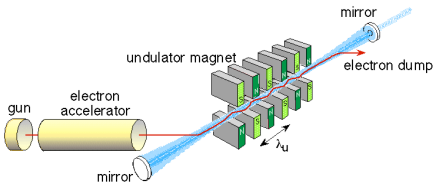

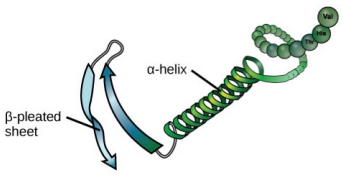

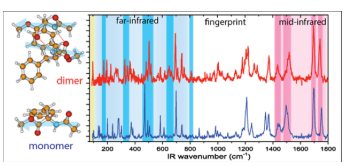

Combining IR-UV ion dip gas phase experiments and AIMD/DFT-MD simulations, structures of biomolecules are unveiled through their spectroscopic fingerprints.