PhD position opened : Ab initio molecular dynamics simulations for vibrational spectroscopies in the Terahertz (THz)

The group of Prof Marie-Pierre Gaigeot in Evry-Paris is expert in DFT-based molecular dynamics simulations (DFT-MD, AIMD) applied to vibrational spectroscopy calculations (non harmonic spectra) [40 papers published since 2006, including 2 book chapters in 2015 & 2016, 1 review paper in 2010]. Terahertz (THz) vibrational spectroscopy has emerged in the past few years as a new tool for probing conformational structures and dynamics in the low frequency spectrum of gas phase (bio)molecules and clusters, liquids, and interfaces (air/water, solid/water). Low-frequency modes directly probe large amplitude motions, such as intermolecular librations, molecular translations & rotations, collective motions, that are not detected *directly* in other spectral domains, although they provide direct information on molecular structures and the environment.

The PhD subject will be concerned with applications of DFT-MD simulations for the calculations of vibrational spectra in the THz domain, for the systems described below, systematically involving collaborations with international colleague experimentalists. By associating theory and experiments, we are able to precisely characterize molecular structures responsible for the spectroscopic signatures. The systems of interest for the PhD are listed below (the PhD student will choose 1 or several systems):
- Peptides in the gas phase, in collaboration with the experimental team of Dr A.M. Rijs, from FELIX lab, Radbout University, The Netherlands. This continues our ongoing collaboration. See for instance our recent papers [Angewandte Chemie 126 :3737 (2014) ; Phys Chem Chem Phys 17 :25905 (2015)].
- Water clusters containing salts, in collaboration with the experimental team of Prof K. Asmis, Leipzig University, Germany. This is a newly started collaboration in 2016.
- Alcohols dissolved in liquid water, in collaboration with the experimental team of Prof M. Havenith, Ruhr University of Bochum, Germany. This is a newly started collaboration in 2016.

Candidate profile. We welcome candidates with background in Chemistry, Physics, Chemical-Physics, Master courses with a large component in theory and simulations, knowledge of one coding language would be welcome.

Practical details. The PhD funding is by the Doctoral School 2MIB, the recruitment follows a competitive examination through presentation and interview by a jury. Applications with high marks are only retained.
The PhD student will have his/her own personal computer(s) in the lab, and will use GENCI national supercomputers for the simulations. The PhD will be strongly involved in the collaborations with our colleague experimentalists, and will in particular be able to make experiments with them. The PhD will have ample opportunities to present his/her work at national and international conferences.
Evry is located 45 minutes from central Paris by RER D line. The University is 2 minutes walk from the train station Evry-Courcouronnes. The University of Evry is part of the University Paris-Saclay. See http://www.univ-evry.fr/fr/nous_contacter/plan_d_acces.html for details.

Applications. Please send an email to Prof Marie-Pierre Gaigeot, mgaigeot@univ-evry.fr including a detailed CV, letter of motivation, and copies of marks for Master years and before. Supporting letters will also be necessary afterwards. Deadline for online application is 15th April 2017, for starting date 1st Oct 2017.
Also see website: http://www.mpgaigeot-research.fr/
Final applications will go online through the ADUM website : www.adum.fr, and please go to the 2MIB Doctoral school website for detailed explanations on how to submit your application on the ADUM platform.