The group "Theory and Modeling" at the University of Evry UEVE-Paris Saclay (LAMBE, UMR CNRS 8587) is currently seeking candidates for a PhD position. Deadline for applications is 17th April 2017, for starting date 1st Oct 2017. Funding is by the Doctoral School Paris-Saclay 2MIB, recruitment by competitive examination through presentation and interview by a jury. The opened position is under the supervision of Prof Marie-Pierre Gaigeot, http://www.mpgaigeot-research.fr/ & mgaigeot@univ-evry.fr

Activities in the group "Theory and Modeling" are in the scientific domain of Theoretical and Computational Chemistry, the group is internationally recognized for its expertise in ab initio molecular dynamics simulations (AIMD: DFT-MD, MP2-MD, semi empirical-MD, QM-MM-MD), with original research activities in the gas phase, liquid phase and at interfaces between solids and liquids & between liquids and air. 4 ANR funding are currently active in the group, 2 of them in collaborative works with the USA, 1 with Germany, and 1 with IFPEN petroleum company.

2017 Opened PhD position : Ab initio molecular dynamics for vibrational spectroscopies in the TeraHertz (THz)

Tera-Hertz (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 [Angewandte Chemie 126 :3737 (2014) ; Int. Rev. Phys. Chem. 34 :1 (2015)], liquids [J. Am. Chem. Soc. 136 :12800 (2014)], and interfaces (air/water, solid/water) [J. Phys. Chem. C. 33 :18665 (2016)]. Low-frequency modes directly probe large amplitude motions, such as intermolecular librations, molecular translations & rotations, collective motions involving for instance an ensemble of water molecules in the condensed phase or several torsional motions along a flexible peptide or protein backbone. These motions are not detected *directly* in other spectral domains, although they provide direct information on molecular structures and the environment.

The group 'Theory and Modeling' of Laboratory LAMBE UMR 8587 is expert in ab initio molecular dynamics simulations (AIMD, DFT-MD) applied in particular to vibrational spectroscopy calculations (non harmonic spectra) [40 papers published since 2006, including 2 book chapters in 2015 & 2016, 1 review paper in 2010]. In collaboration with our colleague experimentalist Dr A.M. Rijs and her group in The Netherlands, we have demonstrated that these simulations allow assign gas phase peptide conformations, without ambiguity, using the THz vibrational signatures.

The PhD subject will be applications of AIMD/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 and structural assemblies of molecules. 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, du laboratoire FELIX, 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) ; other papers are submitted and under review in 2016 et 2017]

- 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.

Practical details. The PhD funding is by the Doctoral School 2MIB, the recruitment follows a competitive examination through presentation and interview by a jury.
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 opportunity 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.
See http://www.univ-evry.fr/fr/nous_contacter/plan_d_acces.html for more details.

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. For the 2MIB funding, competition is high, and applications with high marks are only retained.

Applications. Please send an email to Prof Marie-Pierre Gaigeot, mgaigeot@univ-evry.fr including a detailed CV and letter of motivation. Supporting letters will also be necessary.
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.