Guillaume Fraux

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Research interests

I am a third year PhD student in computational chemistry, working at the interface between physics, chemistry and computer science. I am particularly interested in devising, implementing and studying algorithms used to simulate complex chemical behavior of simple systems and emerging properties.

My PhD subject is the intrusion of liquids in nanoporous materials; the coupling of such intrusion to mechanical properties and deformations; and how to simulate coupled intrusion-deformation using classical methods. I use simulation techniques ranging from *ab initio* dynamics to classical free energy methods and thermodynamic calculations to improve our understanding of the atomistic processes in theses systems.

Research experience

Ongoing	PhD Thesis with F.X. Coudert Asdorption and intrusion in soft porous crystals. Published in [4-10].	*Chimie ParisTech / PSL University*
2015	Master internship with F.X. Coudert Hybrid Monte Carlo simulation in osmotic ensemble	*Chimie ParisTech / PSL University*
2014	Master internship with J. P. K. Doye Heterogeneous nucleation of ice on AgI crystals. Published in [2].	*Chemistry department / Oxford University*
2013	Bachelor internship with R. Vuillemier IR spectra and of CO2 from *ab intio* simulations. Published in [3].	*École Normale Supérieure*
2013	Bachelor internship with J. Fattaccioli Synthesis of small oil droplets coated with a metal. Published in [1].	*École Normale Supérieure*

Peer-reviewed publications

10. G. Fraux, S. Chibani, and F.-X. Coudert. "Modeling of framework materials at multiple scales: current practices and open questions". In: *Phil. Trans. R. Soc. A* **in press** (2019)
9. G. Chaplais, G. Fraux, J.-L. Paillaud, C. Marichal, H. Nouali, A. H. Fuchs, F.-X. Coudert, and J. Patarin. "Impacts of the Imidazolate Linker Substitution (CH3, Cl, or Br) on the Structural and Adsorptive Properties of ZIF-8". In: *The Journal of Physical Chemistry C* 122.47 (Oct. 2018), pp. 26945–26955
8. G. Fraux, A. Boutin, A. H. Fuchs, and F.-X. Coudert. "On the use of the IAST method for gas separation studies in porous materials with gate-opening behavior". In: *Adsorption* 24.3 (Mar. 2018), pp. 233–241
7. L. Scalfi, G. Fraux, A. Boutin, and F.-X. Coudert. "Structure and Dynamics of Water Confined in Imogolite Nanotubes". In: *Langmuir* 34.23 (May 2018), pp. 6748–6756
6. G. Fraux, F.-X. Coudert, A. Boutin, and A. H. Fuchs. "Forced intrusion of water and aqueous solutions in microporous materials: from fundamental thermodynamics to energy storage devices". In: *Chemical Society Reviews* 46.23 (2017), pp. 7421–7437
5. G. Fraux and F.-X. Coudert. "Recent advances in the computational chemistry of soft porous crystals". In: *Chemical Communications* 53.53 (2017), pp. 7211–7221
4. J. D. Evans, G. Fraux, R. Gaillac, D. Kohen, F. Trousselet, J.-M. Vanson, and F.-X. Coudert. "Computational Chemistry Methods for Nanoporous Materials". In: *Chemistry of Materials* 29.1 (Sept. 2016), pp. 199–212
3. M. Basire, F. Mouhat, G. Fraux, A. Bordage, J.-L. Hazemann, M. Louvel, R. Spezia, S. Bonella, and R. Vuilleumier. "Fermi resonance in CO2: Mode assignment and quantum nuclear effects from first principles molecular dynamics". In: *The Journal of Chemical Physics* 146.13 (Apr. 2017), p. 134102
2. G. Fraux and J. P. K. Doye. "Note: Heterogeneous ice nucleation on silver-iodide-like surfaces". In: *The Journal of Chemical Physics* 141.21 (Dec. 2014), p. 216101
1. G. M. Nocera, K. B. M'Barek, D. G. Bazzoli, G. Fraux, M. B.-V. Heijenoort, J. Chokki, S. Georgeault, Y. Chen, and J. Fattaccioli. "Fluorescent microparticles fabricated through chemical coating of O/W emulsion droplets with a thin metallic film". In: *RSC Advances* 4.23 (2014), p. 11564

Oral communication

National conferences

3. **Association Française de l'Adsorption 2018** (Marseille, France, 25/01/2018 – 26/01/2018)
   "Deformation under adsorption in Zeolitic Imidazolate Frameworks"
2. **Groupe Français des Zéolite 2017** (Marne La Vallée, France, 22/04/2017 – 24/04/2017)
   "Co-adsorption in flexible porous materials: Inadequacy of IAST"
1. **Conférence de Physique-Chimie 2016** (Nancy, France, 17/10/2016 – 20/10/2016)
   "Theoretical studies of adsorption in soft porous materials"

Poster presentations

International conferences

2. **8th Caracterisation of Porous Material** (Delray Beach, Florida, USA, 6/05/2018 – 9/05/2018)
   "Intrusion, Adsorption and Deformations in ZIF-8: Insights from molecular simulation"
1. **6th Biot conference on Poromechanics** (Paris, France, 9/07/2017 – 13/07/2017)
   "Adsorption and intrusion simulation in soft porous materials"

National conferences

2. **Association Française de l'Adsorption 2017** (Paris, France, 30/01/2017 – 31/01/2017)
   "Inadequacy of IAST in flexible porous materials"
1. **Groupe Français des Zéolite 2016** (Montpelier, France, 30/03/2016 – 1/04/2016)
   "Adsorption dans les matériaux poreux flexibles: Quels outils théoriques?"

Teaching experience

Year	Subject	School	Students	Duration
2018-2019	Physical Chemistry Lab	CPES (PSL University)	Bachelor (3rd year)	40h
2018-2019	Thermodynamics	CPES (PSL University)	Bachelor (2nd year)	16h
2017-2018	Physical Chemistry Lab	CPES (PSL University)	Bachelor (3rd year)	24h
2017-2018	Thermodynamics	CPES (PSL University)	Bachelor (2nd year)	16h
2017-2018	General Physics	CPES (PSL University)	Bachelor (1st year)	24h
2017	Theoretical Chem. label	Chimie ParisTech	Master	8h
2016	Theoretical Chem. label	Chimie ParisTech	Master	8h
2016	Dynamol summer school	Chimie ParisTech	Master & PhD	16h
2015	Theoretical Chem. label	Chimie ParisTech	Master	8h
2012–2014	Classe préparatoire	Lycée Ste Geneviève	PCSI/PC*	144h

Year	2012-2013	13-14	14-15	15-16	16-17	17-18	18-19
Total	72h	72h	8h	24h	8h	76h	56h

Education

2016 – now	PhD Thesis in Theoretical Chemistry	*Chimie ParisTech / PSL University – Paris*
2012 – 2016	Diploma of the École Normale Supérieure	*École Normale Supérieure – Paris*
2013 – 2015	Master in Theoretical Chemistry	*École Normale Supérieure / UPMC – Paris*
2012 – 2013	Bachelor in Chemistry	*École Normale Supérieure / UPMC – Paris*
2010 – 2012	Classe préparatoire PCSI/PC*	*Lycée Saint Geneviève – Versailles*

Awards & Honors

Mar. 2016	Poster Prize	*Groupe Français des Zéolite 2016*
Aug. 2011	Gold medal – 28th/290	*43rd International Chemistry Olympiads – Ankara*
Aug. 2010	First prize	*French National Chemistry Olympiads*

Software development

Most of my software development work is done in the open, and you can find all of my public project on GitHub: `http://github.com/Luthaf`. I can work with C++, Python, Rust, Julia, C and Fortran depending on the task. I use modern development practices using version control, continuous testing and static analysis. Here are some highlights of my work related to computational chemistry.

I am the initial author and main contributor to the chemfiles (`http://chemfiles.org`) project. Chemfiles is a polyglot software library providing read and write capabilities for theoretical chemistry file formats, as well as a powerful selection language. The project contains multiple components:

- the chemfiles C++11 core library;
- interfaces to the C++ library in C, Python, Fortran, Julia and Rust;
- the `cfiles` command line tool, providing various analysis algorithms for simulation data: radial distribution function, hydrogen bond autocorrelation, 1D and 1D density profiles, rotational correlations, angles distributions, elastic tensor calculations.

During my PhD, I worked on a lab-private molecular classical simulation engine in C++11, designed to be easy to adapt to new simulation algorithms. I implemented the following features in the engine:

- NVE, NVT and NPT molecular dynamics propagator;
- NVT, NPT, μVT and osmotic ($N_1\mu_2\sigma$T) ensemble Monte Carlo moves;
- Various bonded and non bonded potentials;
- Ewald and Wolf summation methods for electrostatic interactions;

In parallel, I also worked on an open-source molecular simulation engine called lumol (`http://lumol.org`), written in Rust. I implemented most of the features of the private engine in lumol, as well as a few others, such as shared memory parallelism, an input file system and custom simulation output.