Guillaume Fraux

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Research interests

I am a Postdoctoral researcher 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.

Research experience

Ongoing **Postdoctoral researcher with Michele Ceriotti** *EPFL, Switzerland*
Molecular descriptors for machine learning – interactive exploration of material databases [13-17]

2016-2019 **PhD student with François-Xavier Coudert** *Chimie ParisTech, PSL Université, France*
Simulation of adsorption and intrusion coupling to deformation in soft porous crystals. *Ab initio* and classical molecular simulations, implementation of molecular simulation engines [4-12].

2015 **Master internship with François-Xavier Coudert** *Chimie ParisTech, PSL Université, France*
Hybrid Monte Carlo in osmotic ensemble for adsorption simulation

2014 **Master internship with Jonathan P.K. Doye** *Oxford University, UK*
Heterogeneous nucleation of ice on AgI crystals though classical molecular dynamics [2].

2013 **Bachelor internship with Rodolphe Vuillemier** *École Normale Supérieure de Paris, France*
IR and Raman spectra of CO2 from *ab intio* simulations [3].

2013 **Bachelor internship with Jacques Fattaccioli** *École Normale Supérieure de Paris, France*
Synthesis of small oil droplets coated with a metal [1].

Education

2016 – 2019 **Ph.D. in Theoretical Chemistry** *Chimie ParisTech, PSL Université, Paris*
Molecular simulation of fluid adsorption in flexible nanoporous materials at multiple scales

2012 – 2016 **Diploma of the École Normale Supérieure** *École Normale Supérieure, Paris*
Major in Chemistry, minors in numerical physics, statistical learning and material science

2013 – 2015 **Master in Chemistry** *École Normale Supérieure, Sorbonne Université, Paris*
Major in Physical, Analitical and Theoretical Chemistry, with honors (*mention très bien*)

2012 – 2013 **Bachelor in Science and Technologies** *École Normale Supérieure, Sorbonne Université, Paris*
Major in Chemistry, with honors (*mention très bien*)

2010 – 2012 **Classe préparatoire PCSI/PC*** *Lycée Saint Geneviève, Versailles*
2 year preparation for French competitive exams, majors in Physics, Chemistry and Math. Admitted to École Normale Supérieure in Paris.

Peer-reviewed publications

17. Félix Musil, Max Veit, Alexander Goscinski, Guillaume Fraux, Michael J. Willatt, Markus Stricker, Till Junge, and Michele Ceriotti. "Efficient implementation of atom-density representations". *The Journal of Chemical Physics* (Mar. 2021) DOI: 10.1063/5.0044689

16. Alexander Goscinski, Guillaume Fraux, Giulio Imbalzano, and Michele Ceriotti. "The role of feature space in atomistic learning". *Machine Learning: Science and Technology* (Jan. 2021) DOI: 10.1088/2632-2153/abdaf7

15. Benjamin Helfrecht, Rose K Cersonsky, Guillaume Fraux, and Michele Ceriotti. "Structure-property maps with Kernel Principal Covariates Regression". *Machine Learning: Science and Technology* (July 2020) DOI: 10.1088/2632-2153/aba9ef

14. Jonathan Fine, Matthew Muhoberac, Guillaume Fraux, and Gaurav Chopra. "DUBS: A Framework for Developing Directory of Useful Benchmarking Sets for Virtual Screening". *Journal of Chemical Information and Modeling* (Aug. 2020) DOI: 10.1021/acs.jcim.0c00122

13. Guillaume Fraux, Rose Cersonsky, and Michele Ceriotti. "Chemiscope: interactive structure-property explorer for materials and molecules". *Journal of Open Source Software* (July 2020) DOI: 10.21105/joss.02117

12. Guillaume Fraux, Anne Boutin, Alain H. Fuchs, and François-Xavier Coudert. "Structure, Dynamics, and Thermodynamics of Intruded Electrolytes in ZIF-8". *The Journal of Physical Chemistry C* (May 2019) DOI: 10.1021/acs.jpcc.9b02718

11. Guillaume Fraux, Siwar Chibani, and François-Xavier Coudert. "Modeling of framework materials at multiple scales: current practices and open questions". *Philosophical Transactions of the Royal Society A: Mathematical, Physical and Engineering Sciences* (May 2019) DOI: 10.1098/rsta.2018.0220

10. Johannes P. Dürholt, Guillaume Fraux, François-Xavier Coudert, and Rochus Schmid. "Ab Initio Derived Force Fields for Zeolitic Imidazolate Frameworks: MOF-FF for ZIFs". *Journal of Chemical Theory and Computation* (Mar. 2019) DOI: 10.1021/acs.jctc.8b01041

9. Gérald Chaplais, Guillaume Fraux, Jean-Louis Paillaud, Claire Marichal, Habiba Nouali, Alain H. Fuchs, François-Xavier Coudert, and Joël Patarin. "Impacts of the Imidazolate Linker Substitution (CH3, Cl, or Br) on the Structural and Adsorptive Properties of ZIF-8". *The Journal of Physical Chemistry C* (Oct. 2018) DOI: 10.1021/acs.jpcc.8b08706

8. Guillaume Fraux, Anne Boutin, Alain H. Fuchs, and François-Xavier Coudert. "On the use of the IAST method for gas separation studies in porous materials with gate-opening behavior". *Adsorption* (Mar. 2018) DOI: 10.1007/s10450-018-9942-5

7. Laura Scalfi, Guillaume Fraux, Anne Boutin, and François-Xavier Coudert. "Structure and Dynamics of Water Confined in Imogolite Nanotubes". *Langmuir* (May 2018) DOI: 10.1021/acs.langmuir.8b01115

6. Guillaume Fraux, François-Xavier Coudert, Anne Boutin, and Alain H. Fuchs. "Forced intrusion of water and aqueous solutions in microporous materials: from fundamental thermodynamics to energy storage devices". *Chemical Society Reviews* (2017) DOI: 10.1039/c7cs00478h

5. Guillaume Fraux and François-Xavier Coudert. "Recent advances in the computational chemistry of soft porous crystals". *Chemical Communications* (2017) DOI: 10.1039/c7cc03306k

4. Jack D. Evans, Guillaume Fraux, Romain Gaillac, Daniela Kohen, Fabien Trousselet, Jean-Mathieu Vanson, and François-Xavier Coudert. "Computational Chemistry Methods for Nanoporous Materials". *Chemistry of Materials* (Sept. 2016) DOI: 10.1021/acs.chemmater.6b02994

3. Marie Basire, Félix Mouhat, Guillaume Fraux, Amélie Bordage, Jean-Louis Hazemann, Marion Louvel, Riccardo Spezia, Sara Bonella, and Rodolphe Vuilleumier. "Fermi resonance in CO2: Mode assignment and quantum nuclear effects from first principles molecular dynamics". *The Journal of Chemical Physics* (Apr. 2017) DOI: 10.1063/1.4979199

2. Guillaume Fraux and Jonathan P. K. Doye. "Note: Heterogeneous ice nucleation on silver-iodide-like surfaces". *The Journal of Chemical Physics* (Dec. 2014) DOI: 10.1063/1.4902382

1. Giovanni Marco Nocera, Kalthoum Ben M'Barek, Dario Giovanni Bazzoli, Guillaume Fraux, Morgane Bontems-Van Heijenoort, Jeannette Chokki, Sonia Georgeault, Yong Chen, and Jacques Fattaccioli. "Fluorescent microparticles fabricated through chemical coating of O/W emulsion droplets with a thin metallic film". *RSC Advances* (2014) DOI: 10.1039/c3ra47063f

Oral communications

International conferences

3. **13th Fundamentals of Adsorption** (Cairns, Australia, 26/05/2019 – 31/05/2019)
   "Peeking inside the pores: structure of adsorbed phases in ZIF-8 and its cousins."

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** (Montpellier, France, 30/03/2016 – 1/04/2016)
   "Adsorption dans les matériaux poreux flexibles: Quels outils théoriques?"

Supervised and mentored research students

2020	**Ella Rajaonson**	*Master Student*	Creating a dataset for training universal reactive forcefield
2019	**Alexander Goscinski**	*PhD Student*	Comparing features generated by different molecular descriptors [16]
2017	**Laura Scalfi**	*Master Student*	Simulation of water adsorption in imogolites [7]

Teaching experience

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

Awards & Honors

2016	Three year PhD fellowship	*Allocation Spécifique Normalien*
2016	Poster Prize	*Groupe Français des Zéolite 2016*
2011	Gold medal – 28th/290	*43rd International Chemistry Olympiads – Ankara*
2010	First prize	*French National Chemistry Olympiads*

Professional skills

Languages	French (native), English (proficient), Spanish (intermediate)
Scientific software	CP2K, CRYSTAL14, LAMMPS, COLVARS, Mathematica, VMD
Communication	LaTeX, Apple Office / Libre Office, Website design (HTML/CSS/JS)
Programming	C++11, Python3, Rust, TypeScript/JavaScript, Fortran, Bash, C, Julia, Lua
Development tools	GNU/Linux, git, valgrind, lldb, CMake, documentation (sphinx, doxygen, rustdoc), unit testing, continuous integration, code linter (clang-tidy, cargo-clippy, eslint), packaging (pip, conda, cargo, debian/apt, rhel/yum, macOS/brew)

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. Here are some highlights of my work related to computational chemistry.

`chemiscope` **Interactive structure/property explorer for materials and molecules**

http://chemiscope.org

Chemiscope is an online interactive explorer for databases of molecules and materials. It presents a map containing structural descriptors and physical properties of compounds in the database together with the atomistic structure of the compounds. It allow users to explore, understand and rationalize structure/property relationships within the database.

`chemfiles` **Read and write the file formats of computational chemistry**

http://chemfiles.org

Chemfiles is a software library providing read and write capabilities for the file formats used in computational chemistry. The goal of this project is to enable interoperability between simulation, visualization and analysis software. It also provides an advanced atomic selection language to facilitate the implementation of analysis algorithms.

`cfiles` **Trajectory analysis and management**

http://github.com/chemfiles/cfiles

A command line tool based on chemfiles, which implements multiple trajectory analysis algorithms: radial distribution functions, hydrogen bonds networks, rotational correlations, elastic tensor computation, *etc.*

`lumol` **Universal extensible molecular simulation engine**

http://lumol.org

Lumol is a classical molecular simulation engine, designed to be easy to adapt to new simulation algorithms. It already provides molecular dynamics simulations in NVE, NVT and NPT ensembles; Metropolis Monte Carlo simulations in NVT and NPT ensemble. Various bonded and non-bonded interaction potentials are available, as well as Ewald and Wolf summation methods for electrostatic interactions computation.