Guillaume Fraux

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Research interest

I am a second year PhD student working on 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 am using Hybrid Monte-Carlo simulations in the Osmotic ensemble to overcome the limitations of both Monte-Carlo and Molecular Dynamics in the simulation of flexible open systems.

Peer-reviewed publications

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: *Chem. Soc. Rev.* 23.46 (2017), pp. 7421–7437
5. G. Fraux and F.-X. Coudert. "Recent Advances in the Computational Chemistry of Soft Porous Crystals". In: *Chemical Communication* 53 (2017), pp. 7211–7221
4. M. Basire, F. Mouhat, G. Fraux, A. Bordage, J.-L. Hazemann, M. Louvel, R. Spezia, S. Bonella, and R. Vuilleumier. "Fermi Resonance in CO_2 : Mode Assignment and Quantum Nuclear Effects from First Principles Molecular Dynamics". In: *The Journal of Chemical Physics* 146.13 (Apr. 7, 2017), p. 134102
3. 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 (Jan. 10, 2017), pp. 199–212
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. 7, 2014), p. 216101
1. G. M. Nocera, K. Ben M'Barek, D. G. Bazzoli, G. Fraux, M. Bontems-Van 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

Teaching experience

Year	Course name	School	Role	Duration	Students level
2017-2018	Thermodynamics	CPES	TA	16h	Bachelor
2017-2018	General Physics	CPES	TA	48h	Bachelor
2017	Theoretical Chem. label	Chimie ParisTech	TA	8h	Master
2016	Introduction to molecular simulation	ENS Ulm	TA	8h	BcS
2016	Theoretical Chem. label	Chimie ParisTech	TA	8h	Master
2016	Dynamol summer school	Chimie ParisTech	TA	16h	Master & PhD
2015	Theoretical Chem. label	Chimie ParisTech	TA	8h	Master
2012–2014	Classe préparatoire	Lycée Ste Geneviève	Oral exam	144h	PCSI/PC* (BcS)

Year	2012	2013	2014	2015	2016	2017	2018
Total	36h	72h	36h	8h	32h	40h	32h

Oral communication

National conferences

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

Poster presentations

International conferences

1. **6th Biot conference on Poromechanics** (Paris, 9/07/2017 – 13/07/2017)
   "Adsorption and intrusion simulation in soft porous materials"

National conferences

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

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*

Education

2015 – now	PhD Thesis in Theoretical Chemistry	*Chimie ParisTech – 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*
2010	Bacalaureat Scientifique (A-Level)	

Software development

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 analysis algorithms for simulation data.