Simon Gravelle

Physicist in soft matter
and fluids at interfaces

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Current research position

2024-today   **CNRS Researcher**
Univ. Grenoble Alpes, CNRS, LIPhy, Grenoble, France
Nanoconfined fluids, soft matter, and molecular simulations
Team : Statistical Physics and Modeling (PSM)
- Starting Feb. 2025 : co-investigator of the ANR MIAM-CO2 (Elise Lorenceau),
- Starting Feb. 2025 : lead PI of the ANR project MicroSep,
- Since Jan. 2024 : in charge of organizing LIPhy's internal seminars,
- Since Apr. 2024 : co-supervision of Pablo Grisanti, PhD candidate.

2023-2025   **MSCA Fellow**
Univ. Grenoble Alpes, CNRS, LIPhy, Grenoble, France
Hybrid nanoporous materials for fluid mixture separation
Group leader : CNRS DR Benoit Coasne

Past research experiences

2021-2023   Postdoctoral Researcher
Institute for Computational Physics, Universität Stuttgart, **Stuttgart, Allemagne**
NMR properties of water at the interfaces of porous salt crusts
NMR dynamics of hydrophilic gels and polymers
Group leaders : Pr. Christian Holm and Assistant Pr. Alexander Schlaich

2019-2021   Postdoctoral Researcher
Queen Mary University of London, **Londres, Royaume-Uni**
Adsorption of two-dimensional nanoparticles at fluid interfaces
Viscosity of graphene nanoparticle suspensions under shear
Group leader : Pr. Lorenzo Botto

2016-2019   Postdoctoral Researcher (FONDECYT)
Universidad Adolfo Ibáñez, **Viña del Mar, Chili**
Bio-inspired water capture systems by desert plants
Modeling microtube dynamics in plant cells
Group leaders : Pr. Jacques Dumais

2012-2015   Doctorant
Institut Lumière Matière, Université Claude Bernard Lyon 1, **Lyon, France**
Fluidic transport in bio-inspired nano-channels
Charge fluctuations and reversible ion adsorption in synthetic nanopores
Supervisors : Pr. Lydéric Bocquet, CNRS DR Christophe Ybert and Pr. Laurent Joly

Publication list

Grants

2025-2029 **ANR MicroSep** (JCJC)
Laboratoire Interdisciplinaire de Physique, Université Grenoble Alpes, Grenoble, France
Polymères microporeux pour la séparation de mixtures fluides : connecter les échelles moléculaire et macroscopiques
Total budget of 330000 €

2023-2025 **Marie Skłodowska-Curie Actions fellowship** (MSCA)
Laboratoire Interdisciplinaire de Physique, Université Grenoble Alpes, Grenoble, France
Hybrid nanoporous materials for the separation of fluid mixtures
Full salary + research budget of 24000 €

2017-2019 **Postdoctoral fellowship** (FONDECYT-CONICYT)
Universidad Adolfo Ibáñez, Viña del Mar, Chili
A biomimetic membrane with highly asymmetric water transport properties
Full salary + research budget of 15000 €

Open science projects

[1] **MAICoS**
Co-developer of software allowing the analysis of the structure of confined and interfacial fluid systems from molecular simulations
https://maicos-analysis.org

[2] **NMRforMD**
Developer of a code allowing the analysis of relaxation T_1 and T_2 from molecular simulations
https://nmrformd.readthedocs.io

[3] **Compte Github**
FAIR[1] sharing of scripts and simulation data
Systematic sharing of research data maximizes the visibility of my work and ensures the re-productivity of results
https://github.com/simongravelle

[4] **LAMMPS tutorials**
Molecular simulation tutorials
The development of this site, which gathers about 2000 visitors per month, has increased my visibility and has even led to the launch of several collaborations
https://lammpstutorials.github.io

Expertise

Simulation moléculaire	Molecular dynamics
	Monte Carlo approach
	Free energy method (*Umbrella sampling*)
Other	Finite element method
	NMR relaxation time measurements
Experimental	Fluorescence correlation spectroscopy (FCS)
	Membrane characterization
Code	Python, Octave - data analysis and software development
	html/css/rST - online content sharing
	Git - collaborative work

Interests

Fields	Nanofluidics, Soft matter, Fluid at interfaces, Biomimetics, Statistical physics
Phénomènes	Fluid transport, Adsorption, Collective effects, Input effects, Nuclear magnetic relaxation
Other	Outreach, Open science, Tutoring, Video production

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1. FAIR : *Findability, Accessibility, Interoperability, Reusability*

Presentations

11/2024	**Invited seminar**, PHENIX, Paris, France *Probing NMR relaxation in nanoconfined fluids using intermittent molecular dynamics*
02/2024	**Modeling workshop in Cermav**, Grenoble, France *Modelling fluid transport in porous materials : connecting nanoscale and macroscale*
10/2024	**French/German Adsorption Conference**, Strasbourg, France *Separation of water and ethanol mixtures by nanoporous organosilica ; a molecular dynamics study*
10/2023	**Invited seminar**, Kyung Hee University, Korea *Using simulations to design nanoporous materials for the separation of fluids*
09/2023	**Thematic School in Soft Nanosciences**, Grenoble, France *Using molecular simulations to design nanoporous materials for the separation or fluids*
06/2022	**International Society for Porous Media (InterPore),** online *Water confined in salt crusts : insights from molecular simulations*
10/2021	**Invited seminar,** LOMA, Bordeaux, France *Unidirectional water valve in Tillandsia plant*
03/2021	**March meeting of the American Physical Society,** online *Adsorption of graphene-oxide nanoparticles at a water-vapour Interface : a molecular dynamics investigation*
01/2021	**Physics at Veldhoven,** online *Fluid dynamics of a nanographene*
11/2020	**Division of Fluid Dynamics of the American Physical Society,** online *Deviations from Jeffery's theory in the dynamics of atomically-thin sheet-like molecules in shear flow*
01/2020	**Physics at Veldhoven,** Physics at Veldhoven, Eindhoven, Pays-Bas *Hydrodynamics of graphene suspensions : liquid exfoliation of multilayer graphene (poster)*
11/2019	**Division of Fluid Dynamics of the American Physical Society,** Seattle, Washington, États-Unis *Liquid phase exfoliation of graphene : a molecular dynamics investigation*
10/2018	**GdR Liquides aux interfaces,** Bordeaux, France *Design of a unidirectional water valve in Tillandsia*
05/2018	**Séminaire invité,** LIPhy, Grenoble, France *Nanofluidics : a theoretical and numerical investigation of fluid transport in nanochannels*

Presentations (following)

04/2016   **Séminaire invité,** Universidad Adolfo Ibáñez, Viña del Mar, Chili
Optimizing water permeability through the hourglass shape of aquaporins : From hydrodynamics to single-file transport

11/2015   **Soutenance de thèse,** Lyon, France
Nanofluidics : a theoretical and numerical investigation of fluid transport in nanochannels

12/2014   **Computer Simulation of Combined Fluids,** Londres, Royaume-Uni
Optimizing water permeability through the hourglass shape of aquaporins : From hydrodynamics to single-file transport

10/2014   **GdR Liquides aux interfaces,** Bordeaux, France
Pink noise of ionic current, theory and modelisation

07/2014   **Séminaire invité,** ICE group, Londres, Royaume-Uni
Optimizing water permeability through the hourglass shape of aquaporins

11/2013   **Division of Fluid Dynamics of the American Physical Society,** Pittsburgh, Pennsylvanie, États-Unis
Does the hourglass shape of aquaporins optimize water permeability ?

10/2013   **GdR Liquides aux interfaces,** Lyon, France
Optimizing water permeability through the hourglass shape of aquaporins

Education

2012-15   **PhD in Physics**
Université Claude Bernard Lyon 1, Lyon, France

2010-12   **Master of Science in Fundamental Physics**
École Normale Supérieure (ENS) de Lyon, Lyon, France

2007-10   **Bachelor of Physics**
Université de Franche Comté, Besançon, France

2007   **Scientific Baccalaureate**
Lycée Édouard Belin, Vesoul, France

Teaching

Starting 2025   Institut universitaire de technologie (IUT) de Grenoble, Grenoble , France
Practical work in materials science for 1st year students

2021-23   University of Stuttgart, Stuttgart, Allemagne
Design and supervision of practical assignments for Master's students
128 h in total, 2 students per group

2013-15   Institut universitaire de technologie (IUT) de Lyon, Lyon, France
Materials science course for 1st year students
19 h in total, approximately 30 students per class

2012-15   Institut universitaire de technologie (IUT) de Lyon, Lyon , France
Practical work in materials science for 1st year students
185 h in total, approximately 20 students per class

2011-13   Lycée La Martinière Monplaisir, Lyon, France
Preparation and supervision of exams for first year students in "classes préparatoires aux grandes écoles"
2 hours per week, 3 students per session