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 October 2024 : lead PI of the ANR project MicroSep
- Since January 2024 : in charge of organizing LIPhy's internal seminars
- Since April 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

Scholar My **full publication list** is available from Google Scholar and ORCID.

Grants

2024-2028 **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

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

Presentations

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

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

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