

# Simon Gravelle

Physicist in soft matter  
and fluids at interfaces

LIPhy, UGA, CNRS

Grenoble, France

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[simongravelle.github.io](https://simongravelle.github.io)

## 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 January 2025 : co-investigator of the ANR project MIAM-CO2 lead by Elise Lorenceau,
  - Starting January 2025 : 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 microtubule 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 mélanges 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<sup>1</sup> 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://lammptutorials.github.io>

## Expertise

Simulation moléculaire	Molecular dynamics Monte Carlo approach Free energy method ( <i>Umbrella sampling</i> )
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

- 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 Bacculaureate**  
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