# Simon Gravelle

Physicist in soft matter
and fluids at interfaces

**LIPhy**
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simongravelle.github.io

## Research experience

**2024-today** CNRS Researcher
Laboratoire Interdisciplinaire de Physique, Université Grenoble Alpes, **Grenoble, France**
*Nanoconfined fluids, soft matter, and molecular simulations*
Team : Statistical Physics and Modeling

**2023-2025** MSCA Fellow
Laboratoire Interdisciplinaire de Physique, Université Grenoble Alpes, **Grenoble, France**
*Hybrid nanoporous materials for fluid mixture separation*
Group leader : CNRS DR Benoit Coasne

**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

## Grants

2023 **Marie Skłodowska-Curie Actions fellowship (MSCA)**
Laboratoire Interdisciplinaire de Physique, Université Grenoble Alpes, Grenoble, France
*Hybrid nanoporous materials for the separation of fluid mixtures*
Total duration of 2 years + approximately 20000 euros research budget

2017 Bourse postdoctorale **FONDECYT-CONICYT**
Universidad Adolfo Ibáñez, Viña del Mar, Chili
*A biomimetic membrane with highly asymmetric water transport properties*
Duration of 3 years + approximately 15000 euros research budget

## Open science projects

[1] **MAICoS** Co-developer of a 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

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

## Interests

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|---|---|
| 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