Simon Gravelle

Physicist in soft matter and fluids at interfaces LIPhy (UGA & CNRS)

Grenoble, France
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Current research position

2024-today CNRS Researcher

Université Grenoble Alpes, CNRS, LIPhy, **Grenoble, France** *Nanoconfined fluids, soft matter, and molecular simulations*

Team: Statistical Physics and Modeling

• starting fall of 2024 : lead PI of the ANR JCJC 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

Université 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.

Grants

2024 **JCJC project** (ANR)

Laboratoire Interdisciplinaire de Physique, Université Grenoble Alpes, Grenoble, France Polymères microporeux pour la séparation de mixtures fluides : connecter les échelles moléculaire et macroscopiques (Microsep)

Duration of 4 years, research budget of 330000 €

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

Duration of 2 years, research budget of 24000 €

2017 Postdoctoral fellowship **FONDECYT-CONICYT**

Universidad Adolfo Ibáñez, Viña del Mar, Chili

A biomimetic membrane with highly asymmetric water transport properties

Duration of 3 years, research budget of 15000 €

Open science projects

[1] **MAICoS** Co-developer of software allowing the analysis of the struc-

ture 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** FAIR¹ 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 Molecular dynamics moléculaire 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

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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 <i>Hydrodynamics of graphene suspensions : liquid exfoliation of multilayer graphene (poster)</i>
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 <i>Optimizing water permeability through the hourglass shape of aquaporins : From hydro-dynamics to single-file transport</i>
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 hydro- dynamics 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

University of Stuttgart, Stuttgart, Allemagne 2021-23 Design and supervision of practical assignments for Master's students 128 h in total, 2 students per group Institut universitaire de technologie (IUT) de Lyon, Lyon, France 2013-15 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