

Laura Scalfi

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🗣 Bilingual in French and Italian, fluent in English

Academic research in Computational, Theoretical and Physical Chemistry

Research interests: interfacial physical-chemistry, statistical mechanics & enhanced sampling
molecular simulations & intensive scientific computation (HPC)

Post-doctoral project.....

- **Non-Markovian Memory-Based Modelling of Chemical Reactions** **R. Netz**
Freie Universität Berlin, AG Netz, Berlin *September 2021–now*

Doctoral thesis.....

- **Influence of the metallicity of a surface on the properties of fluids at interfaces** **B. Rotenberg**
Sorbonne Université, Laboratoire PHENIX, Paris *May 2018–August 2021*

Research internships.....

- **Free energy studies for the discharge mechanism of a lithium battery** **D. Limmer**
University of California Berkeley – Limmer Group *October 2017–March 2018*
- **Water absorption in imogolite nanotubes** **A. Boutin, F.-X. Coudert**
Ecole Normale Supérieure, Lab. PASTEUR et Institut de Recherche de Chimie Paris *February–June 2017*
- **FOB Surface Hopping for charge transport in organic semiconductors** **J. Blumberger, A. Carof**
University College London, Blumberger Group *March–July 2016*

Awards.....

- **Ph.D. prize of the Physical Chemistry Division (DCP)** of the French Chemical Society (SCF) *2022*
- **Young Talents France L'Oréal-UNESCO For Women in Science Prize** *2021*
- Co-beneficiary of the **Atos-Joseph Fourier Prize 2021**: "special prize" for the code *MetalWalls* *2021*
- French selection for the 45th International Chemistry Olympiads: ranked 8th over 24 *2013*
- Girls Scientific and Technical Vocation Prize *2012*
- 28th French National Chemistry Olympiads : ranked 16th over 42 *2012*

Selected publications.....

- C. Ayaz, L. Scalfi, B. A. Dalton, and R. R. Netz, Generalized Langevin equation with a nonlinear potential of mean force and nonlinear memory friction from a hybrid projection scheme, *PRE* (2022)
- L. Scalfi and B. Rotenberg, Microscopic origin of the effect of substrate metallicity on interfacial free energies, *PNAS*, 118 (50) (2021).
- A. Serva, L. Scalfi, B. Rotenberg, M. Salanne, Effect of the metallicity on the capacitance of gold - aqueous sodium chloride interfaces, *JCP*, 155 (4), 044703 (2021).
- L. Scalfi, M. Salanne, B. Rotenberg, Molecular Simulation of Electrode-Solution Interfaces, *Annu. Rev. Phys. Chem.*, 72 (2021).
- L. Scalfi, T. Dufils, K. Reeves, B. Rotenberg, M. Salanne, A semiclassical Thomas-Fermi model to tune the metallicity of electrodes in molecular simulations, *JCP*, 153 (17), 174704 (2020).
- A. Marin-Laflièche, M. Haefele, L. Scalfi, A. Coretti *et al.*, MetalWalls: A molecular dynamics software dedicated to the modelling of electrochemical systems, *JOSS*, 5 (53), 2373 (2020).
- L. Scalfi, D. Limmer, A. Coretti, S. Bonella, P. Madden, M. Salanne, B. Rotenberg, Charge fluctuations from molecular simulations in the constant-potential ensemble, *PCCP*, 22, 10480 (2020).

Participation to research projects.....

- Co-applications for HPC Computer time allocations
 - HLRN (Allemagne): 4.100.000 hCPU 2021–2022
 - CINES (France): 3.500.000 hCPU 2019–2020
- Doctoral funding (*Allocation Spécifique Normaliens*) September 2018–August 2021

Education in Physical and Theoretical Chemistry

- **Doctorate in Physical Chemistry and Analytical Chemistry** 2018–2021
Sorbonne Université, ED 388, Paris
- **Ecole Normale Supérieure Diploma in Chemistry** **Master equivalent**
Chemistry major and supplementary classes in biology and computer science
Paris Sciences et Lettres University / Ecole Normale Supérieure, Paris 2014–2018
- **Master of Analytical, Physical and Theoretical Chemistry** **with highest honors**
Université Pierre et Marie Curie / Ecole Normale Supérieure, Paris 2015–2017
- **Bachelor of Chemistry** **with highest honors**
Université Pierre et Marie Curie / Ecole Normale Supérieure, Paris 2014–2015
- **'Classes préparatoires aux Grandes Ecoles' in Mathematics, Physics and Chemistry**
Lycée du Parc, Lyon 2012–2014
- **Scientific Baccalauréat Général** **with highest honors**
Lycée Français Stendhal, Milan (Italy) 2012

Teaching activities

- **Teaching assistant** at Sorbonne Université 2018–2021
Lab sessions & scientific computing classes - 64h/year
- **High school science outreach** actions 2020–2021
 - Coding Sisters: tutoring of young girls to learn them how to code 2021–2023
 - Déclics 2020 & 21: dialogues between researchers and high-school students about the construction of knowledge
- **Supervision of master interns** at the laboratory PHENIX and AG Netz 2020–2022
- **Exam Manager** at the 51st International Chemistry Olympiads in Paris 2018–2019
Testing and writing of exams, corrections and discussions with mentors from ~ 80 countries
- **Oral examiner in chemistry** *Lycée Chaptal, Paris – 60h* 2016–2017
- **Teaching and supervision of lab sessions** for the French National Chemistry Olympiads 2014–2016