SHORT CURRICULUM VITAE
Dr. Sophie Sacquin-Mora

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Research Interests

After an initial training and PhD in Chemical Physics, I joined the *Laboratoire de Biochimie Théorique* (LBT) in october 2006. The LBT is a CNRS unit where the structure, mechanics, dynamics and interactions of biological macromolecules are studied by developing and applying algorithms for molecular simulations.

Here, I started developing modeling tools to investigate proteins biological function. Proteins are a central feature of the cellular machinery and constitue an increasingly important target for drug design. My goal is to develop new simulation approaches that can help build a bridge between the available structural data for proteins and their activity in the cell. A long term perspective of my fundamental research work is the development of new drugs that can specifically target proteins involved in a given disease.

My projects are mainly focused on coarse-grain models for investigating protein mechanics (which is tightly related to their biological activity) and protein interactions within large biomolecular assemblies or with solid surfaces. These coarse-grain simulations are usually coupled with more classic all-atom Molecular Dynamics simulations, bioinformatics or experimental approaches in order to obtain complementary information regarding protein function on the atomic level.

Research positions

Oct. 2021
Promoted to Research Director (DR2 CNRS, CID 51) Laboratoire de Biochimie Théorique, Paris
Sept. 2020-July 2021 Guest researcher in the research group of Pr. Mroginski, TU Berlin, Germany
Oct. 2010-Sept. 2021
Senior research scientist CNRS (section13) Laboratoire de Biochimie Théorique, Paris
Oct. 2006-Oct. 2010
Junior research scientist CNRS (section13) Laboratoire de Biochimie Théorique, Paris

Post-Doctoral positions

Sept. 2005-Sept. 2006
INSERM postdoc, DECRYPTHON program, advisor : Pr. Alessandra Carbone
Analytical Genomics team, INSERM U511, Paris, France
Nov. 2004-August 2005
Research and Teaching assistant (ATER), advisor : Pr. Daniel Borgis
Physics Department, Université d'Évry Val d'Essonne, France
Nov. 2003-Oct. 2004
CNRS Postdoc, advisor : Richard Lavery
Laboratoire de Biochimie Théorique, CNRS UPR9080, Paris, France

Education

Dec. 2011 Habilitation à Diriger les Recherches (HDR) U. Paris 7-Denis Diderot, France
Sept. 2000-Oct.2003 Joint french-german PhD in Physical Chemistry
Fluides Nanoconfinés dans des Systèmes de Basse Symétrie : Simulations et Théorie
supervised by Pr. Alain Fuchs (Laboratoire de Chimie Physique, CNRS UMR8000, Orsay)
and Pr. Martin Schoen (Stranski Lab. für Physikalische und Theoretische Chemie, TU Berlin)
2000 Agrégation de Sciences Physiques option Chimie.
1999 M. Sc. research in Molecular Physical-Chemistry U. Paris XI, Orsay, France

Prizes, Awards and Fellowships

1997-2001 Scholarship, École Normale Supérieure, Paris, France
2006 Postdoctoral grant from the Keystone Symposia
Multi-Protein Complexes Involved in Cell Regulation
2020 Research grant from the *Deutscher Akademiker Austauschdienst*

Major research grants (2019-2024)

2024-2028 ANR SIMPA (566k€) *Selective sugar-protein interactions*
2021-2025 ANR MAGNETAU (639k€) *Dynamics of the microtubule-tau interaction*
2021-2025 ANR SuperET (510k€) *Superoxide production by transmembrane electron transfer*
2017-2021 ANR ENZYMOR (496k€) *Orienting enzymes on electrochemical surfaces*
2012-2014 Labex DYNAMO (760k€) *Energy transduction in membranes*
since 2009- Regular user of the national HPC facilities (GENCI)

Institutional responsibilities

2018-2022 Head of the French Network for Theoretical Chemistry (RFCT, GDR3333)
Recruitment committees for Associate Professor positions
2024 U. Évry, **2021** U. Lyon1, **2020** U. Gustave Eiffel, **2018** UTC Compiegne
2021-2025 Nominated member of the **Comité National pour la Recherche Scientifique** (CoNRS), section 13, Physical Chemistry
Elected member for the interdisciplinary section 51 (modeling for life sciences)
2012-2016 Elected member of the **Comité National pour la Recherche Scientifique** (CoNRS), section 13 (`http://www.cnrs.fr/comitenational/english/UK_acc.htm`)
Member of Ph.D. Committees 2015-2024 : Member of 21 Ph.D committees and 4 HDR committees.
Reviewing grant proposals
2019 Isite-NExT, Investissement d'Avenir
2018 Programma per Giovanni Ricercatori-Rota Levi Montalcini
2016 AIC call INRA, **2014** Émergence, Sorbonne Université
Editorial board Frontiers in Molecular Biosciences

Selection of recent peer reviewed publications (10 out of 49 in total)

1. *A Perspective on the Prospective Use of AI in Protein Structure Prediction*
R. Versini, ..., S. Sacquin-Mora and A. Taly*, J. Chem. Info. Model, **64**, 26-41 (2024)
2. *It takes tau to tango : Investigating the fuzzy interaction between the R2-repeat domain and tubulin C-terminal tails*, J. Marien, C. Prévost, and S Sacquin-Mora*
Biochemistry, **62**, 2492-2502 (2023), on BioRxiv, doi : https ://doi.org/10.1101/2023.02.09.527845

3. *Modeling the dynamics of protein-protein interfaces, how and why?*
   E. Karaca, C. Prévost and S. Sacquin-Mora*, Molecules, **27**, 1841 (2022)
4. *Between two walls : Modeling the adsorption behavior of β-glucosidase on bare and SAM-functionalised gold surfaces*, N. Bourassin, F. Barbault, M. Baaden and S. Sacquin-Mora*, Langmuir, **38**, 1313-1323 (2022), on BioRxiv, doi : https ://doi.org/10.1101/2021.07.02.450859
5. *When order meets disorder : Modeling and function of the protein interface in fuzzy complexes*
   S. Sacquin-Mora and C. Prévost*, Biomolecules, **11**, 1529 (2021)
6. *Moving pictures : Reassessing docking experiments with a dynamic view of protein interfaces*
   C. Prévost and S. Sacquin-Mora*, Proteins, **89**, 1315-1323 (2021)
   on BioRxiv, doi : https ://doi.org/10.1101/2020.12.08.415885
7. *Implicit modeling of the impact of adsorption on solid surfaces for protein mechanics and activity with a coarse-grain representation*
   N. Bourassin, É. Lojou, M. Baaden and S. Sacquin-Mora*, J. Phys. Chem. B, **124**, 8516 (2020), on BioRxiv, doi : https ://doi.org/10.1101/2020.03.30.015537
8. *Coarse-grain simulations on NMR conformational ensembles highlight non catalytic functional residues in proteins*, S. Sacquin-Mora*, J. R. Soc. Interface, **16**, 20190075 (2019)
   on BioRxiv, doi : https ://doi.org/10.1101/532507
9. *Hidden partners : Predicting binding sites for proteins with multiple interaction partners*
   N. Lagarde, A. Carbone and S. Sacquin-Mora*, Proteins, **86**, 723-737 (2018)
   on BioRxiv, doi : https ://doi.org/10.1101/244913
10. *Mobility and core-protein binding patterns of disordered C-terminal tails in β-tubulin isotypes*
    Y. Laurin, J. Eyer, C. Robert, C. Prévost and S. Sacquin-Mora*, Biochemistry, **56**, 1746-1756 (2017)

Selection of conferences and talks

May 2024 Invited talk, ISQBP 2024 President's meeting, Athens, Greece
Investigating the dynamics of protein-protein interfaces in well structured and fuzzy complexes

March 2023 Invited talk, Atelier thématique *Bioélectrochimie aux Frontières*, Marseille, France
Modelling redox enzymes on solid surfaces : Lessons from multiscale approaches

June 2022 Invited talk, Journées Plénières du GdR EMIE, Dunkerque, France
Multiscale modelling approaches for the protein-solid interface

June 2021 Contributed talk, ISQBP 2021 President's meeting, Online-Strasbourg, France
Moving pictures : Reassessing docking experiments with a dynamic view of protein interfaces

Feb. 2020 Invited talk, TMS 149th Annual Meeting and Exhibition, San Diego, USA
Enzymes Grafted on Electrodes for Biofuel Cells : Lessons from Multiscale Modeling Approaches

April 2019 Invited talk, CECAM 50th anniversary symposium, IDRIS Orsay, France
50 years of modeling life

Sept. 2018 Contributed talk, CECAM workshop on Normal Modes Analysis, Paris, France
Mechanical variations in proteins with large-scale motions highlight the formation of structural locks

June 2018 Invited talk, École thématique DynaMoPPI, Nantes, France
Great interactions and hidden partners : Lessons from protein blind docking on protein binding sites and function.

June 2017 Invited talk, Gordon Research Conference : Computational Aspects - Biomolecular NMR
Sunday River USA, *Protein Mechanics as a Bridge Between Structure and Function, a Coarse-Grain Approach.*

Organization of scientific meetings (2017-2024)

Oct. 2022 **CECAM Workshop, Immobilizing peptides and proteins**, Paris, France, 40 participants
May 2019 **CECAM Workshop, Biomolecular mechanismes at functionalized soid interfaces**, Paris, France, 40 participants
Oct. 2017 **CECAM Workshop, Disordered protein segments : revisiting the structure-function paradigm**, Paris, France, 50 participants
April 2017 **Understanding Protein Interactions : from Molecules to Organisms**, Lyon, France, 100 participants

Supervision of junior researchers (2015-2024)

June 2022- June 2024 – Burcu Aykac Fas Postdoc (LABEX DYNAMO/CoFund)
Multiscale approaches to investigate the conformational landscape of flexible protein assemblies : Deciphering the NADPH oxidase complex (1 paper publisehd)
Jan. 2022- – Jules Marien Master Thesis and PhD Thesis (U. Paris-Cité)
Modeling the impact of phosphorylation on the tau/tubulin interaction (1 paper published)
Jan. 2017-July 2021 – Nicolas Bourassin Master Thesis and PhD Thesis (U. de Paris)
Modeling enzymes orientation on electrode surfaces for green energy production
(3 papers published)
Sept. 2016-Sept. 2017 – Nathalie Lagarde Postdoc (ANR project MAPPING)
Prediction of binding sites for proteins with multiple interaction partners (1 paper published)
July 2014-Dec.2015 – Lydie Vamparys-Laurent Postdoc (ANR project MAPPING)
Binding incorrect partners to understand protein recognition and function (1 paper published)
Oct. 2013-Sept.2016 – Yoann Laurin PhD Thesis (U. Paris 7-LABEX DYNAMO)
Investigating the structural variability and binding modes of the glioma targeting NFL-TBS.40-63 peptide on tubulin (2 papers published)

Teaching activities (2017-2023)

2012-2023 *Kinetics and Thermodynamics* Lecturer in chemistry, Université de Paris, France
Since 2015- *Multiscale modelling for biological systems* Theoretical Chemistry label.

Selection of general public communications

2021-2022 *Protéines, un voyage au centre de la cellule*; *Protéines 2, le carnaval du vivant*
Ed. EDP Sciences, two popularization books about proteins (in french).
Since 2019 *Top of the Prots* : `https://topoftheprots.com`
A popularization blog about proteins (in french)
July 2018 *Making gender equality more than theoretical*
Comment published in Chemistry World regarding gender balance in scientific events
`https://tinyurl.com/ChemWorldSacquin`
Oct. 2017 Biochemistry expert for the general scientific journal *Pour la Science* : `https://tinyurl.com/PLScalamar`
March 2017 Highlight of the project regarding the anti-cancerous NFL-TBS.40-63 peptide on the GENCI website for the *Semaine du cerveau* : `http://www.genci.fr/fr/node/834` .
Sept. 2016 The ProPHet program for investigating protein mechanics is available online on the RPBS webserver : `http://mobyle.rpbs.univ-paris-diderot.fr/cgi-bin/portal.py#forms::ProPHet`