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. 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.

Permanent Research positions

Oct. 2010-
Senior research scientist CNRS (section13)
Laboratoire de Biochimie Théorique, UPR9080 (IBPC, Paris).

Oct. 2006-Oct. 2010
Junior research scientist CNRS (section13)
Laboratoire de Biochimie Théorique, UPR9080 (IBPC, 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)
Université 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
Université 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

Major research grants (2013-2018)

2017-2021 ANR ENZYMOR (496k€) *Orienting enzymes on electrochemical surfaces*
2012-2019 Labex DYNAMO (760k€) *Energy transduction in membranes*
2012-2017 ANR Investissements d'avenir Bio-informatique MAPPING (180k€) *Protein interactions*
2010-2014 ANR BIOPAC (127k€) *Biocatalytic enzymes for biofuel cells*

Institutional responsibilities

January 2018 Head of the French Network for Theoretical Chemistry (RFCT, GDR3333)
2018 Recruitment comittee for an Associate Professor position in Université Technique de Compiegne
2016 Recruitment comittee for an Associate Professor position in Université Paris-sud
2014-2017 Secretary for the French Network for Theoretical Chemistry (RFCT, GDR3333)
2012-2016 Elected member of the **Comité National pour la Recherche Scientifique (CoNRS), section 13, Physical-Chemistry, (**`http://www.cnrs.fr/comitenational/english/UK_acc.htm`**)**
Member of Ph.D. Committees 2013-2019 : Member of 7 Ph. D committees and 2 HDR committees.
Reviewing grant proposals
2018 Programma per Giovanni Ricercatori-Rota Levi Montalcini
2016 AIC call INRA, 2014 Émergence, Sorbonne Université

Selection of recent peer reviewed publications (10 out of 37 in total)

1. *Conformational stability adaptation of a double-stranded RNA binding domain to transfer RNA ligand* C. Bou-Nader, P. Barraud, L. Pecqueur, C. Velours, M. Fontecave, C. Tisné, S. Sacquin-Mora, and D. Hamdane*, Biochemistry, **58**, 2463-2473 (2019)
2. *Mechanical changes in proteins undergoing large-scale motions highlight the formation of structural locks* S. Sacquin-Mora*, J. Structural Biology, **203**, 195-204 (2018), available on BioRxiv, doi : https ://doi.org/10.1101/221077.
3. *Hidden partners : Predicting binding sites for proteins with multiple interaction partners* N. Lagarde, A. Carbone and S. Sacquin-Mora*, Proteins, **86**, 723-737 (2018), available on BioRxiv, doi : https ://doi.org/10.1101/244913

4. *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)
5. *Bridging enzymatic structure and function via mechanics : A coarse-grain approach* S. Sacquin-Mora*, G.A. Voth, editor, Methods in Enzymology : Computational Approaches for Studying Enzyme Mechanism Part B,**578**, 227-248 (2016)
6. *Great interactions : How binding incorrect partners can teach us about protein recognition and function* L. Vamparys, B. Laurent, A. Carbone and S. Sacquin-Mora*, Proteins, **84**, 1408-1421 (2016)
7. *Fold and Flexibility : What can protein mechanical properties tell us about their folding nucleus ?* S. Sacquin-Mora*, J. R. Soc. Interface, **12**, 20150876 (2015)
8. *Investigating the structural variability and binding modes of the glioma targeting NFL-TBS.40-63 peptide on tubulin* Y. Laurin, P. Savarin, C. H. Robert, M. Takahashi, J. Eyer, C. Prévost and S. Sacquin-Mora*, Biochemistry, **54**, 3660-3669 (2015)
9. *Fluctuations in the dipole moment of membrane-bound hydrogenase from Aquifex aeolicus account for its adaptability to charged electrodes* F. Oteri, A. Ciaccafava, A. de Poulpiquet, M. Baaden, E. Lojou and S. Sacquin-Mora*, PhysChemChemPhys **16**, 11318-11322 (2014)
10. *Protein-protein interactions in a crowded environment : An analysis via cross-docking simulations and evolutionary information*, A. Lopes, S. Sacquin-Mora, V. Dimitrova, E. Laine, Y. Ponty and A. Carbone*, PLoS Computational Biology **9**, e1003369 (2013).

Selection of conferences and talks

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.*

June 2015 Contributed talk, TheoBio, Cagliary, Italy
Multiscale modeling of the mechanical nucleus in globular proteins

May 2013 Contributed talk, Molecular Perspectives on Protein-Protein Interactions, Pultusk, Poland *High-throughput investigation of protein-protein interactions via cross-docking simulations*

Nov. 2012 Invited talk, Congrès SFBBM-SFB : Mécanismes moléculaires et processus vitaux intégrés, Grenoble, France *Modeling protein mechanics with coarse-grain representations : From structure to function*

Sept. 2011 Invited talk, Workshop, Hands on course on Coarse Grain Methods for Biomolecular Simulations, Institut Pasteur de Montevideo, *Coarse-Grain Models for Protein Mechanics*

Organization of scientific meetings

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

Oct. 2014 Protein-Protein Interactions on the Genomic Scale, Paris, France, 100 participants

Oct. 2011 XVIIème congrès du GGMM,(Groupe de Graphisme et Modélisation Moléculaire), La Rochelle, France, 120 participants

Supervision of junior researchers (2013-2018)

January 2017 – Nicolas Bourassin(1 paper published)
Master Thesis and PhD Thesis (Université Paris 7)
Modeling enzymes orientation on electrode surfaces for green energy production.

Sept. 2016-Sept. 2017 – Nathalie Lagarde(1 paper published)
Postdoc (ANR project MAPPING)
Prediction of binding sites for proteins with multiple interaction partners

July 2014-Dec.2015 – Lydie Vamparys-Laurent(1 paper published)
Postdoc (ANR project MAPPING)
Binding incorrect partners to understand protein recognition and function

Oct. 2013-Sept.2016 – Yoann Laurin(2 papers published)
PhD Thesis (Université Paris 7-LABEX DYNAMO)
Investigating the structural variability and binding modes of the glioma targeting NFL-TBS.40-63 peptide on tubulin

Sept. 2011-Sept. 2013 – Francesco Oteri(2 papers published)
Postdoc (ANR project BIOPAC)
Modeling biocatalytic enzymes for biofuel cells

Teaching activities (2013-2018)

Since 2012- *Kinetics and Thermodynamics*
Lecturer in chemistry, Université Paris 5-Descartes, France

2016 *Protein mechanics*
DynaMol Summer school.

Since 2015- *Multiscale modelling for biological systems*
Theoretical Chemistry label.

General public communications

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`