

# Florian E. C. Blanc, PhD

CNRS RESEARCH SCIENTIST IN COMPUTATIONAL MOLECULAR BIOPHYSICS

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## Research interests

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Protein dynamics, molecular machines & motors, integrative MD simulations, free energy calculations, machine learning, statistical mechanics

## Current position

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### CNRS Research Scientist

*Biophysics of Complex Systems team - Institut des Sciences Analytiques*

*Villeurbanne (Lyon), France*

Since October 2024

Permanent independent position.

## Research experience

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### Post-doctoral researcher

*Biophysics of Complex Systems team - Institut des Sciences Analytiques*

*Villeurbanne (Lyon), France*

September 2023 - September 2024

Integrative molecular modelling of bacterial silver-resistance proteins  
Advisors: Olivier Walker, Maggy Hologne

### Post-doctoral researcher

*Department of Theoretical Biophysics - Max-Planck Institute of Biophysics*

*Frankfurt am Main, Germany*

May 2019 - August 2023

Computational study of ATPase molecular machines  
Advisor: Gerhard Hummer

### Post-doctoral researcher

*Molecular Function and Design team - Université de Strasbourg*

*Strasbourg, France*

October 2018 - March 2019

Computational investigations of functional transitions in biological and artificial molecular machines  
Advisor: Marco Cecchini

### PhD candidate

*Molecular Function and Design team - Université de Strasbourg; Structural Motility team - Institut Curie*

*Strasbourg and Paris, France*

September 2014 - September 2018

Exploring chemo-mechanical transduction in the myosin molecular motor through computer simulations  
Advisors: Marco Cecchini, Anne Houdusse

## Collective responsibilities

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### Elected Post-doc representative

Max Planck Institute of Biophysics

Frankfurt-am-Main, Germany

November 2020 - August 2023

## Education

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### PhD in Theoretical and Computational Chemistry

Institut de Sciences et d'Ingénierie Supramoléculaires / Université de Strasbourg / Institut Curie

Strasbourg and Paris, France

September 2014 - September 2018

Highest rating ("exceptional") on all evaluation criteria.

### MSc in Bioinformatics

Université Paris-Diderot

Paris, France

September 2013 - June 2014

With high honours.

### École Normale Supérieure Diploma in Biology (major) and Physics (minor)

École Normale Supérieure (ENS)

Paris, France

September 2010 - June 2014

### Admission to ENS - Biology Department

Nationwide competitive entrance evaluation - rank: 1. Admitted to ENS with the status of paid civil servant (élève-normalien).

July 2010

### Classes Préparatoires BCPST

Preparatory classes for nationwide competitive admission exams to French "Grandes Écoles" - 2-year intensive training in biology, chemistry, physics, Earth sciences and mathematics

Marseille, France

September 2008 - June 2010

### Baccalauréat Scientifique

French High-School diploma, scientific specialization

Toulon, France

With highest honours.

June 2008

## Skills

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**Communication** Oral and written scientific communication

**Languages** French (native), English (fluent), German (A1.2)

**Programming** Python/SciPy, bash, Fortran 90 (basic knowledge), Tcl (basic knowledge)

**Molecular Simulations** Molecular Dynamics, free energy calculations, enhanced sampling, quantum chemistry

**Machine Learning** Generative deep learning, dimensionality reduction, clustering

## Teaching duties

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**Qualification Universitaire** (2020-2028) in Sections 31 (Theoretical, Physical, Analytical Chemistry) and 64 (Biochemistry, Molecular Biology)

### Computational Drug Design

Frankfurt University

Frankfurt-am-Main, Germany

2020-2021 Winter semester

Prepared and gave a 12 hour lecture series on **Advanced Simulation Methods for Drug Design**  
Invited a guest lecturer from the private sector  
Supervised and graded practicals and student presentations

### Temporary teacher (physical and computational chemistry)

Université de Strasbourg

Strasbourg, France

September & November 2017

Taught a 1-week tutorial class on **Mathematical Methods for Chemistry** to first-year physical chemistry undergraduates  
Gave a 2-hour **Statistical Mechanics** lecture in the Chemoinformatics Master program  
Supervised a 4-hour lab session on **Normal Mode Analysis** in the Chemoinformatics Master program

### Temporary teacher (bioinformatics)

Institut Supérieur des Biosciences

Noisy le Grand, France

December 2014 & December 2015

Supervised a 8-hour lab session on **Biomedical Signal Acquisition and Processing**

### Volunteer mentor for high-school students

TalENS (ENS student association for high-school student mentoring)

Paris, France

September 2010 - June 2014

Mentored and taught scientific concepts to high-school students  
Designed transdisciplinary scientific classes

## Publications

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### **Mechanism of Ag<sup>+</sup>-Induced Folding of a Bacterial Peptide from Replica-Exchange Molecular Simulations.**

Blanc, F. E. C.\*; Hologne, M.; Demontrond, M.; Chermette, H.; Walker, O.\* (\* corresponding authors)

ChemRxiv April 18, 2025.

<https://doi.org/10.26434/chemrxiv-2025-pfwmz-v2>

### **Metadynamics Simulations for Rational Ligand Design in the Reversible Inhibition of Human Peroxiredoxin 5.**

Troussicot, L.; Blanc, F. E. C.; Pascal, Y.; Vidal, S.; Lancelin, J.-M.; Guillièrre, F.

bioRxiv April 27, 2025, p 2025.04.25.650576.

<https://doi.org/10.1101/2025.04.25.650576>

### **A weak coupling mechanism for the early steps of the recovery stroke of myosin VI: A free energy simulation and string method analysis**

Florian E.C. Blanc\*, Anne Houdusse, Marco Cecchini\* (\* corresponding authors)

*PLOS Computational Biology*, 2024

<https://dx.plos.org/10.1371/journal.pcbi.1012005>

### **Mechanism of proton-powered c-ring rotation in a mitochondrial ATP synthase**

Florian E.C. Blanc, Gerhard Hummer

*PNAS*, 2024

<https://www.pnas.org/doi/10.1073/pnas.2314199121>

### **Molecular mechanisms of inorganic-phosphate release from the core and barbed end of actin filaments**

W. Oosterheert\*, F. E. C. Blanc\*, A. Roy, A. Belyy, M. Boiero Sanders, O. Hofnagel, G. Hummer, P. Bieling, and S. Raunser. (\* equal contribution)

*Nature Structural and Molecular Biology*, 2023

<https://doi.org/10.1038/s41594-023-01101-9>

### **Antibody accessibility determines location of spike surface mutations in SARS-CoV-2 variants**

von Bülow, S., Sikora, M., Blanc, F.E.C., Covino, R., Hummer, G.

*PLOS Computational Biology*, 2023.

<https://doi.org/10.1371/journal.pcbi.1010822>

### **Computational epitope map of SARS-CoV-2 spike protein**

Sikora, M.\*, von Bülow, S.\*, Blanc, F.E.C.\*, Gecht, M.\*, Covino, R.\*, Hummer, G. (\* equal contribution)

*PLOS Computational Biology*, 2021

<https://doi.org/10.1371/journal.pcbi.1008790>

### **An Asymmetric Mechanism in a Symmetric Molecular Machine**

Florian Blanc, Marco Cecchini

*Journal of Physical Chemistry Letters*, 2021

<https://doi.org/10.1021/acs.jpclett.1c00404>

### **In situ structural analysis of SARS-CoV-2 spike reveals flexibility mediated by three hinges**

Turoňová, B., Sikora, M., Schürmann, C., Hagen, W.J.H., Welsch, S., Blanc, F.E.C., von Bülow, S., Gecht, M., Bagola, K., Hörner, C., van Zandbergen, G., Landry, J., Trevisan Doimo de Azevedo N., Mosalaganti, S., Schwarz, A., Covino, R., Mühlebach, M.D., Hummer, G., Locker, J.K., Beck, M.

*Science*, 2020

<https://doi.org/10.1126/science.abd5223>

### **An intermediate along the recovery stroke of Myosin VI revealed by X-ray crystallography and molecular dynamics**

Florian Blanc, Tatiana Isabet, Hannah Benisty, H. Lee Sweeney, Marco Cecchini, Anne Houdusse

*PNAS*, 2018

<https://doi.org/10.1073/pnas.1711512115>

### **The myosin X motor is optimized for movement on actin bundles**

Virginie Ropars\*, Zhaohui Yang\*, Tatiana Isabet\*, Florian Blanc, Kaifeng Zhou, Tianming Lin, Xiaoyan Liu, Pascale Hissier, Frédéric Samazan, Béatrice Amigues, Eric D. Yang, Hyokeun Park, Olena Pylypenko, Marco Cecchini, Charles Sindelar, H. Lee Sweeney and Anne Houdusse

*Nature Communications*, 2016

<https://doi.org/10.1038/ncomms12456>

**Myosin MyTH4-FERM structures highlight important principles of convergent evolution**

Vicente José Planelles-Herrero, Florian Blanc, Serena Sirigu, Helena Sirkia, Jeffrey Clause, Yannick Sourigues, Daniel O. Johnsrud, Béatrice Amigues, Marco Cecchini, Susan P. Gilbert, Anne Houdusse, and Margaret A. Titus

***PNAS*, 2016**

<https://doi.org/10.1073/pnas.1600736113>

## Communications

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### Invited seminars

**Revealing complex biomolecular processes with enhanced sampling Molecular Dynamics simulations**

Laboratoire de Chimie de l'ENS Lyon, invited by Natacha Gillet, July 1st, 2025

**Exploring the functional mechanisms of biomolecular machines with atomically-detailed simulations**

École Normale Supérieure de Lyon, invited by Riccardo Pellarin, November 2023

**Exploring the function of molecular machines with simulations**

Institut des Sciences Analytiques, invited by Olivier Walker, November 2021

### Oral communications

**Mechanism of Ag<sup>+</sup>-induced folding of a bacterial peptide from molecular dynamics simulations and deep dimensionality reduction**

Machine Learning in Chemistry and Physics (MLCP2025) meeting, Lyon, France, June 2025

**Mechanism and energetics of proton-powered c-ring rotation in mitochondrial ATP synthase**

Congrès du Groupe de Graphisme et Modélisation Moléculaires (GGMM), Lille, France, September 2021

### Poster presentations

**Mechanism of Ag<sup>+</sup>-induced folding of a bacterial peptide from molecular dynamics simulations**

Blanc, F. E. C.; Hologne, M.; Demontrond, M.; Chermette, H.; Walker, O.

Congrès du GGMM, Forges-les-Eaux, France, 2025

**Mechanism of Ag<sup>+</sup>-induced folding of a bacterial peptide from molecular dynamics simulations**

Blanc, F. E. C.; Hologne, M.; Demontrond, M.; Chermette, H.; Walker, O.

ML4NGP (Machine Learning for Non Globular Proteins) meeting, Vilnius, Lithuania, 2025

**A novel intermediate along the recovery stroke of Myosin VI revealed by X-ray crystallography and molecular dynamics**

Florian Blanc, Tatiana Isabet, Hannah Benisty, H. Lee Sweeney, Marco Cecchini, Anne Houdusse

Congrès du Groupe de Graphisme et Modélisation Moléculaires (GGMM), Reims, France, 2017

**A novel intermediate along the recovery stroke of Myosin VI revealed by X-ray crystallography and molecular dynamics**

Florian Blanc, Tatiana Isabet, Hannah Benisty, H. Lee Sweeney, Marco Cecchini, Anne Houdusse

EMBO Meeting, Mannheim, Germany, 2016