FABIAN SCHUHMANN

PERSONAL INFORMATION

email	fabian.schuhmann@nbi.ku.dk
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EMPLOYMENT HISTORY

research assistant

10/2023-now · **Niels Bohr Institute, University of Copenhagen** · **post-doc researcher in the group of Prof. Dr. Weria Pezeshkian**
I perform and analyse molecular dynamics simulations of proteins, membranes, and protein complexes.

research assistant

04/2023-09/2023 · Carl von Ossietzky University Oldenburg · post-doc researcher in the group of Prof. Dr. Dr. Ilia A. Solov'yov
I learned coarse-grained molecular dynamics simulations and finalized SiMBols, a trajectory analysis comparing package for Python.

research assistant

01/2020-03/2023 · Carl von Ossietzky University Oldenburg · Ph.D. student in the group of Prof. Dr. Dr. Ilia A. Solov'yov
I conducted all-atom molecular dynamics simulations of proteins in different states and derived ways to comparably analyse simulation trajectories.

teaching assistant

10/2017-04/2019 · Ruhr-University Bochum · tutor for different mathematics service lectures for Prof. Dr. Heinzner, Dr. Jörg Härterich, and AOR PD Dr. Kacso

assistant

10/2016-08/2017 · Hochschule Bochum · assistant with the "Institut für Mathematik und Technikdidaktik" for Prof. Dr. Mike Scherfner

teaching assistant

10/2015-04/2019 · Hochschule Bochum · tutor for mathematics for economists for Prof. Dr. Skill

EDUCATION

Dr. rer. nat (Ph.D.)

01/2020-02/2023 · Carl von Ossietzky University Oldenburg · Institute of Physics
Thesis: *Spotting The Difference - Tailored Tools to Analyze Protein Dynamics*;
graduated 'summa cum laude'
Advisor: Prof. Dr. Dr. Ilia A. Solov'yov

Master of Science

04/2017-02/2019 · Ruhr University Bochum · Faculty of Mathematics
Thesis: *Dynamics of billiards with emphasis on the length of the shortest periodic billiard trajectory*
Advisor: Prof. Dr. Alberto Abbondandolo

Bachelor of Science

10/2013-10/2016 · Ruhr University Bochum · Faculty of Mathematics
Thesis: *Das Brunn-Minkowski Theorem und die isoperimetrische Ungleichung (translated: The Brunn-Minkowski theorem and the isoperimetric inequality)*
Advisor: Prof. Dr. Alberto Abbondandolo

Bachelor of Science

10/2011-07/2016 · Ruhr University Bochum · Faculty of Economics
Thesis: *Globaler Umweltschutz als Problem der privaten Bereitstellung eines öffentlichen Gutes (translated: Global environmental protection as a problem of private provision of a public good)*
Advisor: Prof. Dr. Julio. R. Robledo

PUBLICATIONS (H-INDEX: 6 *google scholar, 16/07/2024*)

1. Physics-Based Protein Networks Might Recover Effectful Mutationsa Case Study on Cathepsin G
Fabian Schuhmann, Heloisa N. Bordallo, Weria Pezeshkian
Journal of Physical Chemistry B, XXX, XXX-XXX, (2024)
On the case study of neutrophil elastase and cathepsin G, we propose the utilization of the potential energy to derive inter-protein networks and pathways. A shortest path analysis shows that important sites might be recovered or predicted with the refined network approach. I conceptualized the project, performed the simulations and the formal analysis.

2. Allosteric Communication of the Dimerization and the Catalytic Domain in Photoreceptor Guanylate Cyclase
Manisha Kumari Shahu, **Fabian Schuhmann**, Siu Ying Wong, Ilia A. Solov yov, Karl-Wilhelm Koch
Biochemistry, 63, 2131-2140, (2024)
We employ experimental activity assays and molecular simulations on differentely mutated types of the photoreceptor to pinpoint an allosteric pathway spanning three domains and regulating the activity of the protein. I was in charge of the molecular dynamics simulations and the formal analysis.

3. Spurious negative eigenvalues of numerical variance-covariance matrices in many-body systems correlate with the existence of frozen degrees of freedom
Jonathan Hungerland, Ilia A. Solov'yov, **Fabian Schuhmann**
Physica Scripta, 99, 085249, (2024)
We discuss the negative eigenvalues arising in covariance matrices due to limited machine accuracy in the calculation. We correlate the negative eigenvalues to the frozen degrees of freedom to extract knowledge from the numerical error. I was the primary supervisor of the project and involved in the editing and revision of the manuscript.

4. A Computer Laboratory for the Calculation of the Heat Capacity of a Peptide Unfolding Transition
Lau Blom Grøndahl, **Fabian Schuhmann**, Dennis Bruhn, Vikas Dubey, Ilia A. Solov'yov, Himanshu Khandelia
TheBiophysicist 2024; DOI: 10.35459/tbp.2024.000251
In this work, we discuss the possibility of using the VIKING online platform to employ molecular dynamics simulations for a bachelor level class dealing with the phase transition in a peptide chain with increasing temperature. I wrote the technical sections involving VIKING and did the first level technical support during the classes.

5. Different receptor models show differences in ligand binding strength and location: a computational drug screening for the tick-borne encephalitis virus
Felicitas Finke, Jonathan Hungerland, Ilia A. Solov'yov, **Fabian Schuhmann**
Molecular Diversity, 2024, DOI: 10.1007/s11030-024-10850-8
The work is the result of the bachelor project of Felictias Finke, whom I supervised throughout the process. I was the lead in coverting her thesis to a publishable manuscript.

6. Structural Rearrangements of Pigeon Cryptochrome 4 Undergoing a Complete Redox Cycle
Fabian Schuhmann, Jessica L. Ramsay, Daniel R. Kattnig, Ilia A. Solov'yov
Journal of Physical Chemistry B 2024, Volume 128, p. 3844-3855 (chosen for cover)

7. Introducing the Automated Ligand Searcher
Luise Jacobsen, Jonathan Hungerland, Vladimir Bačić, Luca Gerhards, **Fabian Schuhmann**, Ilia A. Solov'yov
Journal of Chemical Information and Modeling 2023, Volume 63, p. 7518-7528
ALISE is part of the master's project of Luise Jacobsen. After her master's was completed, I was involved in rerunning simulations, writing the original draft and organizing the project and its people through the publication process. My role made me a corresponding author.

8. Across atoms to crossing continents: Application of similarity measures to biological location data
Fabian Schuhmann, Leonie Ryvkin, James D. McLaren, Luca Gerhards, Ilia A. Solov'yov
Plos ONE 2023, Volume 18, p. e0284736

9. Effects of Dynamical Degrees of Freedom on Magnetic Compass Sensitivity: A Comparison of Plant and Avian Cryptochromes
Gesa Grüning, Siu Ying Wong, Luca Gerhards, **Fabian Schuhmann**, Daniel R. Kattnig, P. J. Hore, Ilia A. Solov'yov
Journal of the American Chemical Society 2022, Volume 144, p. 22902-22914
I built the theory on how to unify and create the orthonormal system, which is the base for most calculations in in the manuscript and I was involved in the review and editing of the manuscript.

10. On the energetic differences of avian cryptochromes 4 from selected species
Maja Hanić, Anders Frederiksen, **Fabian Schuhmann**, Ilia A. Solov'yov
The European Phyiscal Journal D 2022, Volume 76, p. 198
I assisted in the analysis of the simulation data and performing statistical tests. I was also involved in the review and editing of the manuscript.

11. The same, but different, but still the same: structural and dynamical differences of neutrophil elastase and cathepsin G
Fabian Schuhmann, Xiangyin Tan, Luca Gerhards, Heloisa N. Bordallo, Ilia A. Solov'yov
The European Phyiscal Journal D 2022, Volume 76, p. 126

12. Computational Reconstruction and Analysis of Structural Models of Avian Cryptochrome 4
Maja Hanić, **Fabian Schuhmann**, Anders Frederiksen, Corinna Langebrake, Georg Manthey, Miriam Liedvogel, Jingjing Xu, Henrik Mouritsen, Ilia A. Solov'yov
Journal of Physical Chemistry B 2022, Volume 126, p. 4623-4635
I assisted in the molecular dynamics simulation, the statistical analysis and the clustering analysis. I was also involved in the review and editing of the manuscript.

13. The Transition of Photoreceptor Guanylate Cyclase Type 1 to the Active State
Manisha Kumari Shahu, **Fabian Schuhmann**, Alexander Scholten, Ilia A. Solov'yov, Karl-Wilhelm Koch
International Journal of Molecular Sciences 2022, Volume 23, p. 4030
I was responsible for the computational part of the study and directly involved in the writing of the original manuscript.

14. Navigation of migratory songbirds: a quantum magnetic compass sensor
Siu Ying Wong, Anders Frederiksen, Maja Hanić, **Fabian Schuhmann**, Gesa Grüning, P. J. Hore, Ilia A. Solov'yov
Neuroforum 2021, Volume 27, Issue 3, p. 141-150
I performed and wrote the necessary tasks for the molecular dynamics section in this review.

15. Exploring Post-activation Conformational Changes in Pigeon Cryptochrome 4
Fabian Schuhmann, Daniel R. Kattnig, Ilia A. Solov'yov
The Journal of Physical Chemistry B 2021, Volume 125, Issue 34, p. 9652-9659 (chosen for cover)

16. Introducing Pep McConst—A user-friendly peptide modeler for biophysical applications
Fabian Schuhmann, Vasili Korol, Ilia A. Solov'yov
Journal of Computational Chemistry 2021, Volume 42, Issue 8, p. 572-580

presentations / posters

Copenhagen, Denmark — Introducing the Automated Ligand Searcher (ALISE)
ISBUC Innovation Day **2024**

Toledo, Spain — Experimental data informs computational protein cluster prediction in Mitochondria
ECMTB 2024 **2024**

Drübeck, Germany — Experimental data informs computational protein cluster prediction in Mitochondria
International Membrane Biophysics Meeting "From Model to Cellular Membranes" **2024**

Lyon, France — Experimental data informs computational protein cluster prediction in Mitochondria
CECAM Workshop **2024**

Berlin, Germany — Introducing SiMBols - Similarity Measures for Biological Systems
DPG Frühjahrstagung **2024**

Copenhagen, Denmark — Introducing the Automated Ligand Searcher (ALISE)
Joint Symposium 2024 - Junior ISBUC and Young Medical Chemists **2024**

Copenhagen, Denmark — Structural Rearrangements of pigeon cryptochrome 4 undergoing a complete redox cycle
DANEMO Symposium **2024**

Odense, Denmark — Structural Rearrangements of pigeon cryptochrome 4 undergoing a complete redox cycle
PhyLife Seminar, invited by Prof. Himanshu Khandelia **2024**

Copenhagen, Denmark — Introducing SiMBols - Similarity Measures for Biological Systems
Advanded Methods in MD **2023**

Copenhagen, Denmark — Introducing SiMBols - Similarity Measures for Biological Systems
Linderstrøm-Lang Centre Symposium **2023**

Copenhagen, Denmark — Introducing SiMBols - Similarity Measures for Biological Systems
ISBUC Anual Meeting **2023**

Cambridge, United Kingdom — Introducing SiMBols - Similarity Measures for Biological Systems
Isaac Newton Institute, Workshop: USMW02 **2023**

Kraków, Poland — Introducing SiMBols - Similarity Measures for Biological Systems
BioNano 8, **2023**

Egmond aan Zee, Netherlands — ALISE: An Improved And Automated Virtual Drug Screening Procedure
BioSB, **2023**

Amsterdam, Netherlands — The Same, But Different – Discovering Differences Between Neutrophil Elastase and Cathepsin G
SIAM CSE 2023, **2023**

Borstel, Germany — Introducing SiMBols - Similarity Measures for Biological Systems
14th North German Biophysics Meeting, **2023**

Oldenburg, Germany — Coarse grained pigeon cryptochrome and its conformational changes
ERC Quantum Birds, **2023**

Copenhagen, Denmark — The Same, But Different – Discovering Differences Between Neutrophil Elastase and Cathepsin G
ISBUC Symposium, **2022**

Heidelberg, Germany — The Same, But Different – Discovering Differences Between Neutrophil Elastase and Cathepsin G
ECMTB 2022, **2022**

Copenhagen, Denmark — The Same, But Different – Discovering Differences Between Neutrophil Elastase and Cathepsin G
Topical Meeting 2022, **2022**

Paris, France — Conformational Changes in Pigeon Cryptochrome 4
FENS 2022, **2022**

Exeter, United Kingdom — Conformational Changes in Pigeon Cryptochrome 4
Living Systems Institute Ph.D. Seminar, **2022**

Oxford, United Kingdom — Conformational Changes in Pigeon Cryptochrome 4
ERC Quantum Birds, **2022**

Santa Margherita Ligure, Italy — VIKING and its featured multiscale tools
DySon-ISACC 2021, **2021**

Copenhagen, Denmark — Conformational Changes in Pigeon Cryptochrome 4
Topical Meeting 2021, **2021**

Copenhagen, Denmark — User-friendly peptide modeler for biophysical applications
Topical Meeting 2021, **2020**

TEACHING EXPERIENCE

(Co)-supervisor · (Co)-supervision of **2** Bachelor students and 1 Ph.D. student (ongoing)

Teacher 2023 · Carl von Ossietzky University Oldenburg · In charge of a semester-accompanying introduction to Python and teaching assistant for the module "Einführung in die theoretische Physik"

Teacher 2021 · Carl von Ossietzky University Oldenburg · In charge of a two-weeks mathematics course to bridge the gap between school mathematics and university mathematics

Tutor 2020 · Carl von Ossietzky University Oldenburg · Mathematical Modelling for future teachers · summer term 2020

Tutor 2017-2019 · Ruhr University Bochum
Mathematics for Biologists · winter term 18/19
Mathematics for Engineers II · summer term 18
Mathematics for Engineers I · winter term 17/18

Assistant 2016-2018 · Hochschule Bochum · 'Institut für Mathematik und Technikdidaktik'.

Tutor 2015-2019 · Hochschule Bochum · Mathematics for Economists

INVITED PRESENTATIONS, GRANTS, HONORS, AND AWARDS

07/2024 · ECMTB 2024, Toledo · received ESMTB Travel Award

01/2024 · Invited presenter at the PhyLife Group Seminar in Odense

08/2023 · Mathematical mechanical biology: old school and new school, methods and applications, Cambridge · Award covering the workshop registration fee

02/2023 · SIAM CSE 2023, Amsterdam · received SIAM Travel Award and ESMTB Travel Award

10/2022 · Invited presenter at the ISBUC Symposium in Copenhagen

05/2022 · Research stay at the Living Systems Institute, University of Exeter · guest of Dr. Daniel Kattnig · Funded by the German Academic Exchange Service (DAAD), Program: 57595508

01/2022 · assisted in writing a successful high performance computing application to HLRN (NPL 910,000, eqv. 241,800€)

PROFESSIONAL SERVICE

2021-2023 · Doctoral representative on the board of the Research Training School "GRK 1885 - Molecular Basis of Sensory Biology"
Carl von Ossietzky University Oldenburg

2015-2018 · Member of the Faculty Council Mathematics
Ruhr University Bochum

2014-2018 · Member of the student representations Mathematics, responsible for finances (2015-2017)
Ruhr University Bochum

COLLABORATIONS

Prof. Heloisa N. Bordallo · Experimental data and Validation · Niels Bohr Institute, University of Copenhagen, Denmark · Paper 11, 1

Prof. Daniel R. Kattnig · Cryptochrome 4 and Coarse-Graining · Living Systems Institute, University of Exeter, United Kingdom · Papers 6, 9, 15

Dr. Leonie Ryvkin · Computational Geometry · Mathematics and Computer Science, Eindhoven University of Technology, Netherlands · Paper 8

ACHIEVEMENTS

02/2023 · OLTECH Certificate · Successfully passed the Ph.D. programme "Neurosensory Science and Systems"

02/2023 · SIAM Hackathon 2023, Amsterdam · Member of a team which made it to finals

REVIEW ACTIVITY

2024 · ACS Omega · 1 paper

2023 · Computational and Structural Biotechnology Journal · 1 paper

2022 · The Journal of Physical Chemistry B · 1 paper

OTHER QUALIFICATIONS

Workshops and additional training

Workshop on finances and booking for the public sector (Germany)

Trainer licence C for general sports

Workshop on teaching mathematics by ZAB at Ruhr University Bochum

Workshop on "Introduction to University Pedagogy" by the PhD School of SCIENCE, University of Copenhagen

Voluntary work

2010-2011 · Voluntary Social Year
CVJM Westbund e.V. Wuppertal (YMCA)

2009-2016 · Youth Badminton Trainer
TV Frisch-Auf Altenbochum e.V.

Languages

GERMAN · Native

ENGLISH · Fluent (C2)

DANISH · Basic (A2)

Computer Skills

LATEX · Advanced

PYTHON · Advanced

LINUX · Advanced

GIT · Basic

C++ · Basic

SLURM · Basic

TCL · Basic

October 3, 2024