# FABIAN SCHUHMANN

#### PERSONAL INFORMATION

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#### EMPLOYMENT HISTORY

research assistant 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 2023-2023 · 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 2020-2023 · Carl von Ossietzky University Oldenburg · Ph.D. student in the group of Prof. 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 2017-2019 · Ruhr-University Bochum · tutor for different mathematics service lectures for Prof. Dr.

Heinzner, Dr. Jörg Härterich, and AOR PD Dr. Kacso

assistant 2015-2019 · Hochschule Bochum · assistant with the "Institut für Mathematik und Technikdidaktik" for

Prof. Dr. Mike Scherfner

teaching assistant 2015-2019 · Hochschule Bochum · tutor for mathematics for economists for Prof. Dr. Skill

**EDUCATION** 

Dr. rer. nat 2020-2023 · CARL VON OSSIETZKY UNIVERSITY OLDENBURG · Institute of Physics

(Ph.D.) 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 2017-2019 · 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 2013-2016 · RUHR UNIVERSITY BOCHUM · Faculty of Mathematics

Thesis: Das Brunn-Minkowski Theorem und die isoperimetrische Ungleichung

Advisor: Prof. Dr. Alberto Abbondandolo

Bachelor of Science 2011-2016 · RUHR UNIVERSITY BOCHUM · Faculty of Economics

Thesis: Globaler Umweltschutz als Problem der privaten Bereitstellung eines öffentlichen Gutes

Advisor: Prof. Dr. Julio. R. Robledo

- 1. 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
- 2. 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
- 3. 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

4. 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* 

5. 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

- 6. On the energetic differences of Avian Cryptochromes 4 from selected species Maja Hanić, Anders Frederiksen, Fabian Schuhmann, Ilia A. Solov'yov *The European Physical Journal D* 2022, *Volume* 76, p. 198
- 7. The same, but different, but still the same: structural and dynamical differences of neutrophil elastase and cathersin  ${\sf G}$

Fabian Schuhmann, Xiangyin Tan, Luca Gerhards, Heloisa N. Bordallo, Ilia A. Solov'yov *The European Physical Journal D* 2022, *Volume* 76, p. 126

- 8. 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
- 9. 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
- 10. 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

- 11. 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)
- 12. 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

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 Cathersin 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, <b>2021</b>

Copenhagen, Conformational Changes in Pigeon Cryptochrome 4

Topical Meeting 2021, 2021

Copenhagen, Denmark

Denmark

User-friendly peptide modeler for biophysical applications Topical Meeting 2021, 2020

#### TEACHING EXPERIENCE

(Co)-supervisor

· (Co)-supervision of 2 Bachelor students

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  $\cdot$  Carl von Ossietzky University Oldenburg  $\cdot$  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  $\cdot$  winter term 18/19 Mathematics for Engineers II  $\cdot$  summer term 18 Mathematics for Engineers I  $\cdot$  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

01/2024  $\,\cdot\,$  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 successfull 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  $\cdot$  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 6

Prof. Daniel R. Kattnig · Cryptochrome 4 and Coarse-Graining · Living Systems Institute, University of Exeter, United Kingdom · Papers 1, 4, 10

Dr. Leonie Ryvkin · Computational Geometry · Mathematics and Computer Science, Eindhoven University of Technology, Netherlands · Paper 3

#### ACHIEVEMENTS

o2/2023 · 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

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

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

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

# Languages

German · Native

English · Fluent

# Computer Skills

LATEX · Advanced

Python · Advanced

Linux · Advanced

GIT · Basic

C++ · Basic

SLURM · Basic

TCL · Basic