


Thomas-Otavio Peulen, Dr.
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Postdoctoral Researcher
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I am working on unraveling biomolecular mechanisms by integrative modeling focusing on microscopy and spectroscopy data. Previously, I was a postdoctoral researcher UCSF at Prof. Andrej Šali laboratory. I obtained a Ph.D. in Chemistry at Heinrich Heine University (Düsseldorf, Germany), a BSc and MSc degree in Water-Science at the University Duisburg-Essen.

The goal are rigorous mechanistic insights into the structure and dynamics of macromolecular complexes ideally in living systems, with emphasis on how the interaction between proteins, DNA and carbohydrates determine their biologically relevant function.

In my research I use experimental, theoretical, and computational methods from molecular biophysics, statistical mechanics, stochastic modeling, molecular modeling and scientific and statistical computing to understand how molecules work.

Curriculum vitae

2001	Community service
2002-2004	Pre-diploma (major physics, minor computer science), University Aachen
2004-2007	B.Sc. Water-Science (analytical chemistry/microbiology), University Duisburg-Essen; Electroflotation of heavy metals, supervision: Prof. Dr. Maria de Oliveira Rezende (Universidade de Sao Paulo, Brazil), Prof. Dr. Torsten C. Schmidt, Universität Duisburg
2007-2009	M.Sc. Water-Science, University Duisburg-Essen; Diffusion of nano particles in biofilms; Supervision: Prof. Dr. Kevin J. Wilkinson (Université de Montréal, Canada), Prof. Dr. Torsten C. Schmidt (Universität Duisburg-Essen)

2010-2018	Ph.D. student and postdoctoral fellow at the Institute of Molecular Physical Chemistry, Heinrich-Heine University, Düsseldorf; Supervision: Claus A.M. Seidel
2016	Ph.D. in Chemistry, graduation from Heinrich-Heine University, Düsseldorf: Mapping protein structure and dynamics by Förster Resonance Energy Transfer in vitro and in live cells; Committee: Prof. Claus A.M. Seidel and Prof. Holger Gohlke; <i>summa cum laude</i>
2019	Postdoctoral researcher at the Department of Bioengineering and Therapeutic Sciences, University of California at San Francisco; Supervision: Prof. Andrej Sali

Education and academic career

Stipends and awards

2021	Scientific advisory board of the FRET community (elected early-stage member)
2020	DFG, Walter-Benjamin: Integrative Biologie des Hefe Spindelpolkörpers (high ranked funding priority)
2019	ERC, Marie Skłodowska-Curie Actions: Integrative biology of the yeast spindle pole body (Seal of Excellence – score of 85% or more)
2015	Student Recognition Achievement Award of the Biophysical Society in Biological Fluorescence
2010-2014	Research center Jülich: Stipend of the International Helmholtz Research School of Biophysics and Soft matter
2010	Gerstel price, Duisburg-Essen: (Best M.Sc. Thesis in Analytical Chemistry)
2010	University Duisburg-Essen, Young Scientist Award
2009	Board member of the Center for Microscale Ecosystems (University Duisburg-Essen)
2007	Travel grant of the DAAD to support a B.Sc. thesis in Brazil

Major research interests

Spectroscopy, multimodal image spectroscopy, integrative modeling of biomolecules and biomolecular assemblies

Personal interests

Violin, piano, orchestra, capoeira

Languages

German (Mother tongue), Portuguese (Mother tongue), English (Proficient)

Teaching experience

2018	Heinrich Heine University, Supervision of B. Sc. Thesis, "Optical Spectroscopy of Stochastically Labeled Proteins"
2015	Supervision of BioSoft summer student
2015-2018	Training of new Ph.D. students in single-molecule spectroscopy, advanced fluorescence spectroscopy, and modeling of fluorescence observables; Heinrich Heine University, Prof. C.A.M. Seidel
2010-2018	Teaching assistant (practical courses): General chemistry (medical students); Fundamentals of physical chemistry (B.Sc., chemistry, biochemistry); Advanced physical chemistry (B.Sc., chemistry); Fluorescence spectroscopy and microscopy (M.Sc. and B.Sc., biology); Advanced fluorescence spectroscopy and microscopy (M.Sc. chemistry, biochemistry); Advanced course on molecular structures and interactions (M.Sc., biochemistry); Multiparameter fluorescence detection (M.Sc. biochemistry); Heinrich Heine University, Prof. C.A.M. Seidel
2010-2018	Teaching assistant (lectures): Fundamentals of Physical Chemistry (B.Sc. chemistry, biochemistry); Advanced physical chemistry (B.Sc. chemistry); Physical chemistry – Advanced fluorescence spectroscopy and microscopy of complex systems (M.Sc. chemistry)
2007-2009	Teaching assistant (lecture & practical course) Analytical chemistry and aquatic chemistry; University Duisburg-Essen, Prof. Dr. Torsten C. Schmidt

Original scientific publications

1. M. Hancock*, **T.O. Peulen**, B. Webb, B. Poon, J.S. Fraser, P. Adams, A. Sali; *Integration of software tools for integrative modeling of biomolecular systems*, **J. Struct. Biol.**, 2022, 107841
2. A. Barth*, O. Opanasyuk*, **T.O. Peulen***, S. Felekyan, S. Kalinin, H. Sanabria, C.A.M. Seidel; *Unraveling multi-state molecular dynamics in single-molecule FRET experiments- Part I: Theory of FRET-Lines*, **Phys. Chem. Chem. Phys.**, 2022, accepted (3 citations); (*equal contribution); Developed theory
3. O. Opanasyuk*, A. Barth*, **T.O. Peulen***, S. Felekyan, S. Kalinin, H. Sanabria, C.A.M.

- Seidel; *Unraveling multi-state molecular dynamics in single-molecule FRET experiments–Part II: Quantitative analysis of multi-state kinetic networks*, **Phys. Chem. Chem. Phys.**, 2022, in revision (1 citation); Developed theory
4. E. Lerner*, A. Barth, J. Hendrix, B. Ambrose, V. Birkedal, S.C. Blanchard, R. Börner, H.S. Chung, T. Cordes, T.D. Craggs, A.A. Deniz, J. Diao, J. Fei, R.L. Gonzalez, I.V. Gopich, T. Ha, C.A. Hanke, G. Haran, N.S. Hatzakis, S. Hohng, S.C. Hong, T. Hugel, A. Ingargiola, C. Joo, A.N. Kapanidis, H.D. Kim, T. Laurence, N.K. Lee, T.H. Lee, E.A. Lemke, E. Margeat, J. Michaelis, X. Michalet, S. Myong, D. Nettels, **T.O. Peulen**, E. Ploetz, Y. Razvag, N.C. Robb, B. Schuler, H. Soleimaninejad, C. Tang, R. Vafabakhsh, D.C. Lamb, C.A.M. Seidel, S. Weiss; *FRET-based dynamic structural biology: Challenges, perspectives and an appeal for open-science practices*; **eLife**; e60416, 2021 (36 citations)
 5. M. Dimura*, **T.O. Peulen**, H. Sanabria, D. Rodnin, K. Hemmen, C.A. Hanke, C.A.M. Seidel, H. Gohlke; *Automated and optimally FRET-assisted structural modeling*; **Nat. Commun.**, 2020, 11 (16 citations); Data analysis
 6. H. Sanabria*, D. Rodnin*, K. Hemmen*, **T.O. Peulen**, S. Felekyan, M.R. Fleissner, M. Dimura, F. Koberling, R. Kühnemuth, W. Hubbell, H. Gohlke, and C.A.M. Seidel; *Resolving dynamics and function of transient states in single enzyme molecules*. **Nat. Commun.**, 2020, 11 (36 citations); Analysis software development, data analysis
 7. **T.O. Peulen***, O. Opanasyuk, and C.A.M. Seidel; *Combining Graphical and Analytical Methods with Molecular Simulations to Analyze Time-Resolved FRET Measurements of Labeled Macromolecules Accurately*. **J. Phys. Chem. B**, 2017. **121**(35): 8211-8241; (47 citations); Theory & software development, simulations, data acquisition & analysis
 8. M. Dimura*, **T.O. Peulen***, C.A. Hanke, A. Prakash, H. Gohlke, and C.A.M. Seidel; *Quantitative FRET studies and integrative modeling unravel the structure and dynamics of biomolecular systems*. **Curr. Opin. Struc. Biol.**, 2016. **40**: p. 163-185.; (123 citations) Software developed, data analysis
 9. A. Greife*, S. Felekyan, Q.J. Ma, C.G.W. Gertzen, L. Spomer, M. Dimura, **T.O. Peulen**, C. Wöhler, D. Häussinger, H. Gohlke, V. Keitel, and C.A.M. Seidel; *Structural assemblies of the di- and oligomeric G-protein coupled receptor TGR5 in live cells: an MFIS-FRET and integrative modelling study*. **Sci. Rep.**, 2016. **6**. (20 citations); Theory, simulations, software development, data analysis
 10. E. Kravets*, D. Degrandi*, Q.J. Ma*, **T.O. Peulen**, V. Klumpers, S. Felekyan, R. Kühnemuth, S. Weidtkamp-Peters, C.A.M. Seidel, and K. Pfeffer; *Guanylate binding proteins directly attack Toxoplasma gondii via supramolecular complexes*. **eLife**, 2016. **5**.(93 citations); Theory, software, and data analysis
 11. T. Vöpel*, C.S. Hengstenberg*, **T.O. Peulen***, Y. Ajaj, C.A.M. Seidel, C. Herrmann, and J.P. Klare; *Triphosphate Induced Dimerization of Human Guanylate Binding Protein 1 Involves Association of the C-Terminal Helices: A Joint Double Electron-Electron*

- Resonance and FRET Study. **Biochemistry**, 2014. **53**(28): 4590-4600. (38 citations);*
Data acquisition & analysis, simulations, software development
12. S. Kalinin*, **T.O. Peulen**, S. Sindbert, P.J. Rothwell, S. Berger, T. Restle, R.S. Goody, H. Gohlke, and C.A.M. Seidel; *A toolkit and benchmark study for FRET-restrained high-precision structural modeling. Nature Methods, 2012. **9**(12): p. 1218-U129. (370 citations);* Data analysis
13. **T.O. Peulen***, K.J. Wilkinson; Diffusion of nanoparticles in a biofilm. **Environ. Sci. Technol.**, 2011, *45*(8), 3367-3373. (328 citations); Sample preparation, data acquisition & analysis

Preprints & manuscripts in preparation

1. **T.O. Peulen***, C.S. Hengstenberg*, R. Biehl, M. Dimura, C. Lorenz, A. Valeri, S. Ince, T. Vöpel, B. Faragó, H. Gohlke, J.P. Klare, A. Stadler, C.A.M. Seidel, C. Herrmann: *An integrative approach maps motions and conformers essential for oligomerization of the large GTPase hGBP1* (2 citations); Sample preparation, data acquisition & analysis, software development
2. A. Greife*, **T.O. Peulen***, M. Somssich, R. Kühnemuth, N. Steffens, Y. Stahl, R. Simon, S. Weidtkamp-Peters, C.A.M. Seidel; *Functional FRET imaging: Revealing structural features and affinities of protein complexes in living cells with sub-nanometer resolution*; Data analysis software development
3. **T.O. Peulen***, A. Sali; *Bayesian Fluorescence Framework for integrative modeling of biomolecules*; Theory & software development, data acquisition & analysis
4. J. Dittrich*, **T.O. Peulen***, J. Kubiak, M. Popara, M. Dimura, B. Schepers, N. Verma, B. Schmitz, F. Kovacic, K.E. Jaeger, C.A.M. Seidel, H. Gohlke; *Multiple prior ensembles can yield multiple posterior ensembles in maximum entropy refinements*; Theory & software development, data analysis
5. **T.O. Peulen***, K. Hemmen, D. Mondal, R. Ramachandran, B. Webb, N. van der Voort, A. Greife, S. Felekyan, P. Wang, R.C. Stevens, A. Sali, C.A.M. Seidel, H. Sanabria, K.G. Heinze; *tttrlib integrates time-resolved fluorescence, image spectroscopy, and molecular modeling*; Software development & data analysis

References	<p>Prof. Dr. Claus A.M. Seidel <i>Institute of Physical Chemistry II, Heinrich-Heine-University of Düsseldorf Universitätstr. 1, 40225 Düsseldorf, Germany Phone: +49 (0)211-81-15881; Fax: +49 (0)211-81-12803 E-mail: cseidel@hhu.de</i></p>
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	<p>Prof. Hugo Sanabria <i>Department of Physics and Astronomy, Clemson University, Clemson, S.C., U.S.A. 214 Kinard Lab, Clemson, S.C. 29634-0978, U.S.A. Phone: +1 (0)864-656-1749 E-mail: hsanabr@clemson.edu</i></p>
	<p>Prof. Kevin J. Wilkinson <i>Chimie biologique, analytique et environnementale, Département de Chimie, Université de Montréal, C.P. 6128, Succursale Centre-Ville Montréal, QC, Canada, H3C 3J7 Phone: +1 (514) 343-6741 E-mail: kj.wilkinson@umontreal.ca</i></p>