Joseph F. Rudzinski, Ph.D.

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Professional experience

Max Planck Institute for Polymer Research, Mainz, Germany

Group Leader — **Jan 2020–**
- Structurally- and kinetically-consistent coarse-grained simulation models
- Automated analysis of molecular simulation trajectories
- Interactions and conformational dynamics of disordered proteins

Independent Postdoctoral Researcher — **Mar 2018-Dec 2019**
- Methods for coarse-grained structure and dynamics

Alexander von Humboldt Postdoctoral Fellow — **Mar 2016-Feb 2018**
- Topic: *Dynamical Properties of Coarse-Grained Models for Peptides*

Postdoctoral Researcher (Dr. Tristan Bereau, Prof. Kurt Kremer) — **Jan 2015-Feb 2016**
- Methods for consistent coarse-grained kinetics

The Pennsylvania State University, State College, PA, USA

Graduate Research Assistant (Prof. Will Noid) — **Jun 2009–Oct 2014**
- Methods for bottom-up coarse-grained models
- Applications to peptides and ionomers
- Software development and management

University of California, Santa Barbara, Santa Barbara, CA, USA

Undergraduate Research Assistant
- Aptamer binding in micro-fluidic systems (Prof. Paul J. Atzberger) — **Jan 2008–Jun 2009**
- Electrochemical deposition of Pt in H_2 fuel cells; Optics of electrochemically-etched Silicon Bragg mirrors (Prof. Steven K. Buratto) — **Feb 2007–Aug 2008**

Education

The Pennsylvania State University, State College, PA, USA

Ph.D., Theoretical Chemistry (Advisor: Prof. Will Noid) — **Sep 2009–Oct 2014**

Hierarchical coarse-graining via a generalized Yvon-Born-Green framework: many-body correlations, mappings, and structural accuracy

University of California, Santa Barbara, Santa Barbara, CA, USA

B.Sc. Chemistry; B.Sc. Mathematics — **Sep 2004–Jun 2009**

Funding and Awards

Max Planck Institute for Polymer Research, Mainz, Germany

Postdoctoral Fellowship, Alexander von Humboldt Foundation — **Mar 2016–Feb 2018**
- **full salary**

The Pennsylvania State University, State College, PA, USA

Academic Computing Fellowship — **Sep 2012–Jun 2014**
- **full tuition and stipend**

Graduate Travel Awards
- American Conference on Theoretical Chemistry — **2014**
- Telluride School of Theoretical Chemistry — **2013**
- American Chemical Society National Meeting — **2012**

Graduate Achievement Award — **2012**
- stipend supplement

Dan H. Waugh Memorial Teaching Award — **2010**
- stipend supplement

1st Year Graduate Fellowship — **2009**
- stipend supplement

Braddock Graduate Fellowship — **2009**
- summer stipend

University of California, Santa Barbara, Santa Barbara, CA, USA

Summer Undergraduate Research Fellowship	**2008**
Undergraduate Research and Creative Activities Award	**2008**
Research Internships in Science and Engineering	**Sep 2007-Jun 2009**

Publications

20. Y. Zhao; R. Cortes-Huerto; K. Kremer; **J. F. Rudzinski**, Investigating the conformational ensembles of intrinsically disordered proteins with a simple physics-based model, *J. Phys. Chem. B*, **2020**, 124, 4097-4113

19. Y. Bozkurt Varolgüneş, T. Bereau, **J. F. Rudzinski**, Interpretable embeddings for molecular kinetics using Gaussian mixture variational autoencoders, *Mach. Learn.: Sci. Technol.*, **2020**, 1, 015012

18. S. J. Wörner, T. Bereau, K. Kremer, **J. F. Rudzinski**, Direct route to reproducing pair distribution functions with coarse-grained models via transformed atomistic cross correlations *J. Chem. Phys.*, **2019**, 244110

17. **J. F. Rudzinski**, Recent progress towards chemically-specific coarse-grained simulation models with consistent dynamical properties, *Computation*, **2019**, 7(3), 42

16. **J. F. Rudzinski**, M. Radu, T. Bereau, Automated detection of many-particle solvation states for accurate characterizations of diffusion kinetics, *J. Chem. Phys.*, **2019** MMMK, 024102

    – Special issue: *Markov Models of Molecular Kinetics*

15. T. Bereau, **J. F. Rudzinski**, Accurate structure-based coarse-graining leads to consistent barrier-crossing dynamics, *Phys. Rev. Lett.*, **2018** 121, 256002

14. **J. F. Rudzinski**, T. Bereau, Structural-kinetic-thermodynamic relationships identified from physics-based molecular simulation models, *J. Chem. Phys.*, **2018** 148, 204111

13. **J. F. Rudzinski**, T. Bereau, The role of conformational entropy in the determination of structural-kinetic relationships for helix-coil transitions, *Computation*, **2018**, 6(1)

    – Special issue: *Computation in Molecular Modeling*

12. Nicholas J.H. Dunn, Kathryn M. Lebold, Michael R. DeLyser, **J. F. Rudzinski**, W. Noid, BOCS: Bottom-up Open-source Coarse-graining Software, *J. Phys. Chem. B*, **2017**, 122(13)

    – Special issue: *Benjamin Widom Festschrift*

11. **J. F. Rudzinski**, K. Lu, S. T. Miller, J. K. Maranas, W. Noid, Extended ensemble approach to transferable potentials for low-resolution coarse-grained models of ionomers, *J. Chem. Theory Comput.*, **2017**, 13(5)

10. **J. F. Rudzinski**, T. Bereau, Concurrent parametrization against static and kinetic information leads to more robust coarse-grained force fields, *Eur. Phys. J. Special Topics*, **2016**, 225(8-9)

    – Special issue: *Modern simulation approaches in soft matter science: from fundamental understanding to industrial applications*

9. **J. F. Rudzinski**, K. Kremer, T. Bereau, Communication: Consistent interpretation of molecular simulation kinetics using Markov state models biased with external information, *J. Chem. Phys.*, **2016**, 144(5)

8. **J. F. Rudzinski**, W. Noid, A generalized-Yvon-Born-Green method for coarse-grained modeling: Advances, challenges, and insight, *Eur. Phys. J. Special Topics*, **2015**, 224(12)

    – Special issue: *Discussion and debate: Recurrent problems in scale bridging techniques in molecular simulation – What are the current options?*

7. **J. F. Rudzinski**, W. Noid, Bottom-up coarse-graining of peptide ensembles and helix-coil transitions, *J. Chem. Theory Comput.*, **2015**, 11(3)

6. **J. F. Rudzinski**, W. Noid, Investigation of coarse-grained mappings via an iterative generalized Yvon-Born-Green method, *J. Phys. Chem. B*, **2014**, 118(28)

    – Special issue: *James L. Skinner Festschrift*

5. K. Lu, **J. F. Rudzinski**, W. Noid, S. T. Miller, J. K. Maranas, Scaling behavior and local structure of ion aggregates in single-ion conductors, *Soft Matter*, **2014**, 10

4. J. Wang, **J. F. Rudzinski**, Q. Gong, H. T. Soh, P. J. Atzberger, Influence of target concentration and background binding on in vitro selection of affinity reagents, *PLoS ONE*, **2012**, 7

3. **J. F. Rudzinski**, W. Noid, The role of many-body correlations in determining potentials for coarse-grained models of equilibrium structure, *J. Phys. Chem. B*, **2012**, 116(29)

   – Special issue: *Macromolecular systems understood through multiscale and enhanced sampling techniques*

2. **J. F. Rudzinski**, W. Noid, Coarse-graining entropy, forces, and structures, *J. Chem. Phys.*, **2011**, 135

   – Most downloaded paper from JCP in 12/2011

1. C. R. Ellis, **J. F. Rudzinski**, W. Noid, Generalized Yvon-Born-Green model of toluene, *Macromol. Theory Simul.*, **2011**, 20

   – Ellis and Rudzinski contributed equally
   – Special issue: *Novel simulation approaches for polymeric and soft matter systems*

Presentation Highlights

Invited talk, Big Data Summer School, Platya d'Aro, Spain **Sep 2019**
Invited talk, American Chemical Society Fall Meeting, San Diego, USA **Aug 2019**
Invited talk, Dept. of Physics, University of Luxembourg, Luxembourg **Jun 2019**
Contributed talk, Mainz Molecular Simulation Days, Mainz, Germany **Jun 2019**
Contributed talk, Biophysical Society Spring Meeting, Baltimore, USA **Mar 2019**
Invited talk, Dept. of Physics, University of Delaware, Delaware, USA **Feb 2019**
Invited talk, Dept. of Chemistry, University of Wisonsin-Madison, Madison, USA **Jan 2019**
Invited talk, Dept. of Chemical and Biological Eng., Koç University, Istanbul, Turkey **Oct 2018**
Lecture, Introduction to Markov state models, Koç University, Istanbul, Turkey **Oct 2018**
Contributed talk, CECAM workshop on coarse-graining, Mainz, Germany **Sep 2018**
Invited talk, Heidelberg Institute for Theoretical Studies, Heidelberg, Germany **July 2018**
Invited talk, Dept. of Physics, Darmstadt University, Darmstadt, Germany **May 2018**
Invited talk, Max Planck Institute for Biophysics, Frankfurt am Main, Germany **Jan 2018**
Invited talk, Dept. of Biochemistry, University of Zurich, Zurich, Switzerland **Jun 2017**
Contributed talk, ACS National Meeting, San Francisco, USA **Apr 2017**
Contributed talk, workshop on simulations of macromolecules, Hünfeld, Germany **Mar 2017**
Invited talk, CECAM school on multiscale simulations, Mainz, Germany **Oct 2016**
Invited talk, TRR146 seminar series, Johannes Gutenberg Universität, Mainz, Germany **Mar 2015**
Software tutorial, CECAM school on biomolecular modeling, Lausanne, Switzerland **Oct 2011**

Committees, Leadership, Outreach

Organizer, CECAM workshop, Mainz, Germany **Sep 2018**
– "New frontiers in particle-based multiscale and coarse-grained modeling"
Organizer, TRR146 mini-workshop, Mainz, Germany **Dec 2015**
– "Transferability issues in multiscale modeling of hierarchical phenomena"
Postdoctoral Representative, TRR146 organization committee, Mainz, Germany **2015**
– organization of lecture series and representative for MPIP members
Organizer, Theoretical chemistry seminar series, State College, PA, USA **Sep 2011–Jun 2012**
Instructor, Upward Bound Math and Science Program, State College, PA, USA **Jul 2010**
– chemistry instruction for underrepresented high school students
Exhibit Leader, Exploration Day, State College, PA, USA **May 2010**
– chemistry demonstrations for a county-wide science gathering for kids

Teaching and Mentoring

Max Planck Institute for Polymer Research, Mainz, Germany

Polymer physics and soft-matter theory course, University of Mainz — **Fall 2019**
– co-taught with Dr. Burkhard Dünweg and Dr. Robin Cortes-Huerto

Hanne Zillmer, Masters student — **Mar 2020–**
– *Interactions and phase behavior of polyubiquitin chains*

Daniel Chavez, Ph.D. student — **Jan 2020–**
– *Multiscale investigation of peptide aggregation dynamics*

Atreyee Banerjee, Postdoctoral researcher — **Sep 2019–**
– *Free-energy landscapes and kinetics of polymer polymorphism*

Yasemin Bozkurt, Postdoctoral researcher/Ph.D. student — **Nov 2018–**
– *Characterizing diffusion kinetics with deep learning methods*

Yani Zhao, Postdoctoral researcher — **Jun 2018–**
– *Conformational dynamics of intrinsically-disordered proteins*

Svenja Wörner, Ph.D. student — **Jan 2016–Dec 2019**
– *Kinetic properties of liquid crystals from multiscale simulations*

The Pennsylvania State University, State College, PA, USA

Addison Leedy, undergraduate student — **Sep 2011–Jun 2012**
– *Mixed resolution simulations of the DNA-Histone complex*

Brian Sirovetz, Research Experience for Undergraduates (REU) student — **Summer 2011**
– *Bottom-up coarse-grained models for alkane-toluene mixtures*

Nadia Ahlborg, Research Experience for Undergraduates (REU) student — **Summer 2010**
– *Molecular dynamics study of water adsorption onto NaCl crystals*

PSU Dept. of Chemistry, *General Chemistry Teaching Assistant* — **Sep 2009-Dec 2010**

University of California, Santa Barbara, Santa Barbara, CA, USA

UCSB Campus Learning Assistance Services, *General Chemistry Tutor* — **Sep 2008-Jun 2009**

Journal referee

https://publons.com/a/1298433/

Computer Physics Communications, *Journal of Chemical Physics*, *Journal of Chemical Theory and Computation*, *Journal of Physical Chemistry*, *Journal of Physical Chemistry Letters*, *Nanomaterials*

Software

BOCS: Bottom-up Open-source Coarse-graining Software — github

Dynamical reweighting of Markov state models using external reference data — github

Languages

English native; German B2