## Joseph F. Rudzinski, Ph.D.

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### Professional experience

**Max Planck Institute for Polymer Research**, Mainz, Germany
Postdoctoral Researcher (Dr. Tristan Bereau, Dr. Kurt Kremer) **Jan 2015–**
– Methods for consistent coarse-grained kinetics
Alexander von Humboldt Postdoctoral Fellow **Mar 2016-Feb 2018**
– Topic: *Dynamical Properties of Coarse-Grained Models for Peptides*

**The Pennsylvania State University**, State College, PA, USA
Graduate Research Assistant (Dr. 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 (Dr. Paul J. Atzberger) **Jan 2008–Jun 2009**
– Electrochemical deposition of Pt in $H_2$ fuel cells; Optics of electrochemically-etched Silicon Bragg mirrors (Dr. Steven K. Buratto) **Feb 2007–Aug 2008**

### Education

**The Pennsylvania State University**, State College, PA, USA
Ph.D., Theoretical Chemistry (Advisor: Dr. 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**
– summer stipend
Undergraduate Research and Creative Activities Award **2008**
– cash prize
Research Internships in Science and Engineering **Sep 2007-Jun 2009**
– per hour salary

## Presentation Highlights

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| *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, CA | **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

Svenja Wörner, Ph.D. student **Jan 2016–**
– *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*

## Software

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|---|---|
| BOCS: Bottom-up Open-source Coarse-graining Software | github |
| Dynamical reweighting of Markov state models using external reference data | github |