

# David R. Slochower

## Curriculum Vitae

April 2019

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🌐 [slochower](https://github.com/slochower)

### Education and positions

- 2015- **Postdoctoral scholar**, University of California, San Diego  
Advisor: Michael K. Gilson, M.D., Ph.D.  
Topic: Biophysical modeling and computational chemistry
- 2014 **Instructor**, University of Pennsylvania  
Course: “Molecular physiology and cellular engineering”
- 2007-2014 **Ph.D. in Biochemistry and Molecular Biophysics**, University of Pennsylvania  
Advisor: Paul A. Janmey, Ph.D.  
Thesis: Multiscale simulations of phosphatidylinositol bisphosphate: understanding its biological role through physical chemistry
- 2003-2007 **A.B. cum laude in Physics with distinction**, Kenyon College  
Research: high energy nuclear imaging

### Research interests

- Nonequilibrium statistical mechanics of molecular motors
- New methods for computing binding free energies
- Improving force fields using open source science
- Physical chemistry of biological membranes

### Previous research

- 2017- **Force field development with the open force field consortium**  
[Open Force Field Group](#)
- 2016- **Thermodynamics of host-guest molecular recognition**  
Advisor: Michael K. Gilson, M.D., Ph.D. (University of California, San Diego)
- 2015- **Theory of molecular motors**  
Advisor: Michael K. Gilson, M.D., Ph.D. (University of California, San Diego)
- 2014-2015 **Simulations and docking of macrocycles**  
Advisors: Ravi Radhakrishnan, Ph.D. (University of Pennsylvania) and Mark A. Lemmon, Ph.D. (Yale University)
- 2009-2014 **Quantum, all-atom, and coarse-grained molecular dynamics of membranes**  
Advisor: Paul A. Janmey, Ph.D. (University of Pennsylvania)
- 2008 **Simulations of viral entry into cells**  
Advisors: William DeGrado, Ph.D. (University of California, San Francisco) and Michael L. Klein, Ph.D. (Temple University)
- 2007 **Experimental single molecule biophysics**  
Advisor: Yale E. Goldman, M.D., Ph.D. (University of Pennsylvania)
- 2007 **Computational design of synthetic peptides**  
Advisor: Jeffery Saven, Ph.D. (University of Pennsylvania)
- 2006-2008 **Coded aperture imaging**

Advisors: John Idoine, Ph.D. (Kenyon College), John Frangioni, M.D., Ph.D. (Harvard University), and Richard Lanza, Ph.D. (Massachusetts Institute of Technology)

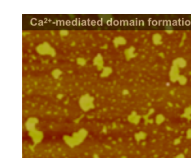
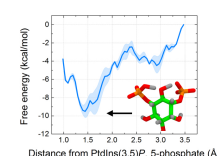
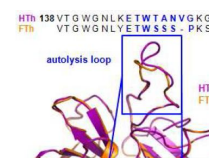
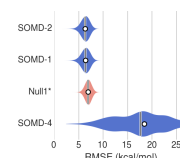
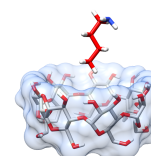
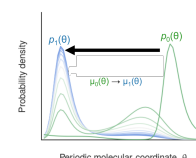
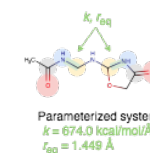
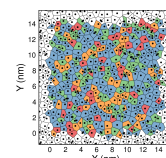
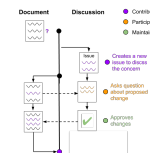
2005

### Analysis of protein hydration shells in simulations

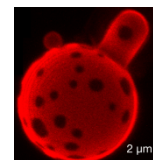
Advisor: Matthias Buck, Ph.D. (Case Western Reserve University)

## Peer-reviewed publications

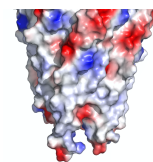
1. Himmelstein DS, **Slochower DR**, Malladi VS, Greene CS, Gitter, A. "Open Collaborative Writing with Manubot" *Accepted with minor revisions at PLOS Computational Biology* 2019 · [GitHub \(code\)](#) · [GitHub \(manuscript\)](#) · [Nature TechBlog](#)
2. Bradley RP\*, **Slochower DR\***, Janmey PA, Radhakrishnan R. "Molecular modeling of divalent cation-specific nano-clusters of phosphoinositides in physiologically-composed bilayers" *Under Review at JACS* 2018 · [GitHub](#)
3. Mobley DL, Bannan CC, Bayly CI, Rizzi A, Chodera JD, Lim VT, Lim NM, Beauchamp KA, **Slochower DR**, Shirts MR, Gilson MK, Eastman PK. "Escaping Atom Types in Force Fields Using Direct Chemical Perception" *Journal of Chemical Theory and Computation*, 14 6706-6092, 2018 · [GitHub](#)
4. **Slochower DR**, Gilson MK. "Motor-like Properties of Nonmotor Enzymes" *Biophysical Journal* 114:9, 2018 · [bioRxiv](#) · [DOI](#) · [GitHub](#) · [New and Notable](#) · [UCSD In the News](#)
5. Yin J, Henriksen NM, **Slochower DR**, Gilson MK. "The SAMPL5 host-guest challenge: computing binding free energies and enthalpies from explicit solvent simulations by the attach-pull-release (APR) method" *Journal of Computer-Aided Molecular Design* 1:31 133-145, 2017 · [DOI](#)
6. Yin J, Henriksen NM, **Slochower DR**, Shirts MR, Chiu MW, Mobley DL, Gilson MK. "Overview of the SAMPL5 host-guest challenge: Are we doing better?" *Journal of Computer-Aided Molecular Design* 1:31 1-19, 2017 · [DOI](#) · [GitHub](#)
7. Smith JR, Galie PA, **Slochower DR**, Weisshaar CL, Janmey PA, Winkelstein BA. "Salmon-derived thrombin inhibits development of chronic pain through an endothelial barrier protective mechanism dependent on APC" *Biomaterials* 80 96-105, 2016 · [DOI](#)
8. **Slochower DR**, Wang Y-H, Radhakrishnan R, Janmey PA. "Physical chemistry and membrane properties of two phosphatidylinositol biphosphate isomers" *Physical Chemistry Chemical Physics* 17:19 12608-12615, 2015 · [DOI](#)
9. Wang Y-H, **Slochower DR**, Janmey PA. "Counterion-mediated cluster formation by polyphosphoinositides" *Chemistry and Physics of Lipids* 182 38-51, 2014 · [DOI](#)



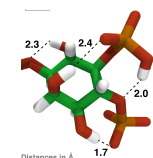
10. **Slochower DR**, Wang Y-H, Tourdot RW, Radhakrishnan R, Janmey PA. "Counterion-mediated pattern formation in membranes containing anionic lipids" *Advances in Colloid and Interface Science* 208 177-188, 2014 · [DOI](#)



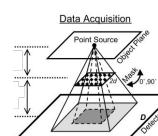
11. Janmey PA, **Slochower DR**, Wang Y-H, Wen Q, Ceber A. "Polyelectrolyte properties of filamentous biopolymers and their consequences in biological fluids" *Soft Matter* 10:10 1439-1449, 2014 · [DOI](#)



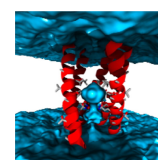
12. **Slochower DR**, Huwe PJ, Radhakrishnan R, Janmey PA. "Quantum and All-Atom Molecular Dynamics Simulations of Protonation and Divalent Ion Binding to Phosphatidylinositol 4,5-Bisphosphate (PIP<sub>2</sub>)" *The Journal of Physical Chemistry B* 117:28 8322-8329, 2013 · [DOI](#)



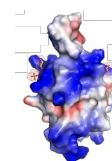
13. Fujii, H, Idoine JD, Gioux S, Accorsi R, **Slochower DR**, Lanza R, Frangioni JV. "Optimization of Coded Aperture Radioscintigraphy for Sentinel Lymph Node Mapping" *Molecular Imaging and Biology* 14:2 173-182, 2012 · [DOI](#)



14. Donald JE, Zhang Y, Fiorin G, Carnevale V, **Slochower DR**, Gai F, Klein ML, De-Grado WF. "Transmembrane orientation and possible role of the fusogenic peptide from parainfluenza virus 5 (PIV5) in promoting fusion" *Proceedings of the National Academy of Sciences* 108:10 3958-3963, 2011 · [DOI](#)



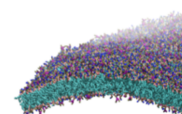
15. Moravcevic K, Mendrola JM, Schmitz KR, Wang Y-H, **Slochower DR**, Janmey PA, Lemmon MA. "Kinase Associated-1 Domains Drive MARK/PAR1 Kinases to Membrane Targets by Binding Acidic Phospholipids" *Cell* 143:6 966-977, 2010 · [DOI](#)



\* These authors contributed equally.

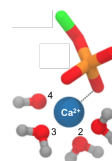
## Book chapters

1. **Slochower DR**, Wang Y-H, Radhakrishnan R, Janmey PA. "Lipid membrane shape evolution and the actin cytoskeleton" in *Handbook of Lipid Membranes, Molecular and Materials Aspects*, Eds. Safinya C, Rädler, J. (2018)



## Ph.D. thesis

**Slochower DR**. "Multiscale simulations of phosphatidylinositol bisphosphate: understanding its biological role through physical chemistry" *University of Pennsylvania*, 2014



## Software packages and contributions

pAPRika	<a href="#">GitHub</a>	Free energy calculations with AMBER and OpenMM
speakeasy	<a href="#">GitHub</a>	Automates the conversion of SMIRNOFF parameters to AMBER force field files
smirnovert	<a href="#">GitHub</a>	Convert host-guest systems into SMIRNOFF force fields
manubot	<a href="#">GitHub</a>	Automated scholarly publishing
BioPhysCode	<a href="#">GitHub</a>	Tools for building and analyzing membrane simulations

## Software skills

- Proficient programming in Python and Jupyter Notebooks with knowledge of Bash, C++, FORTRAN, and Perl.
- Active user of GitHub and continuous integration platforms; experienced writing unit, integration, and regression tests.
- Expert with molecular dynamics simulations using AMBER and OpenMM; familiar with Gromacs, CHARMM, and LAMMPS.
- Used Schrödinger and MOE software suites
- Accomplished using OpenEye Toolkits; familiar with KNIME and RDKit

## Invited talks, posters, abstracts, and workshops (selected)

- 2019 Talk **Binding free energy calculations using the attach-pull-release method**  
2019 AMBER developers' meeting
- 2019 Talk **Benchmarking emerging force fields with binding thermodynamics calculations**  
2019 University of California Chemical Symposium
- 2017 Talk **Directional motion in chiral molecules out of equilibrium**  
253rd American Chemical Society Meeting
- 2017 Poster **Directional and driven motion in enzymes out of equilibrium**  
61st Annual Biophysical Society Meeting
- 2014 Talk **Multiscale modeling of polyphosphoinositides**  
University of California, San Diego
- 2014 Talk **Physical chemistry of phosphatidylinositol isomers**  
University of California, Irvine
- 2013 Talk **Membranes: Polyphosphoinositides**  
Friday Research Discussions, University of Pennsylvania
- 2013 Poster **Quantum and All-atom Molecular Dynamics Simulations of Proton Binding to Phosphatidylinositol 4,5-bisphosphate (PIP<sub>2</sub>)**  
57th Biophysical Society Meeting
- 2012 Talk **Molecular Dynamics Simulations of Ion Binding and Protonation of Phosphatidylinositol Bisphosphate (PIP<sub>2</sub>)**  
244th American Chemical Society Meeting
- 2012 Talk **Simulations of membrane electrostatics with PtdInsP<sub>2</sub>**  
George W. Raiziss 30th Annual Retreat
- 2012 Poster **Molecular Dynamics Simulations of Phosphatidylinositol Bisphosphate (PIP<sub>2</sub>)**  
American Physical Society, March Meeting
- 2011 Talk **Molecular Dynamics Simulations of Membranes**  
47th New England Complex Fluids Workshop
- 2011 Poster **Molecular Dynamics Simulations of Monolayers and Membranes with Phosphatidylinositol Bisphosphate**  
55th Biophysical Society Meeting
- 2010 Talk **Simulating highly charged monolayers**  
Mechanistic Studies in Membrane Biophysics: Experiments and Theory, Tel-luride Science and Research Workshop
- 2010 Poster **Simulations of Monolayers with Phosphatidylinositol Bisphosphate**  
Gotham-Metro Condensed Matter Meeting

## Awards and grants

2012-2013 NIH T32 Structural Biology Training Grant  
2011 Juan Grana Graduate Teaching Assistantship  
2010-2012 NIH T32 Interdisciplinary Cardiovascular Training Grant  
2007 Distinction in Physics (best research), Kenyon College  
2007 Sigma Xi, The Scientific Honor Society  
2004-2007 Dean's List, Kenyon College  
2005 Best Summer Project (biophysics), Case Western Reserve University  
2001 Science Olympiad, National Champion Team

## Teaching and mentoring experience

Fall 2014 Molecular Physiology & Cellular Engineering – University of Pennsylvania  
I was responsible for creating the syllabus, giving lectures, designing project assignments, and grading for one-half of this course.

Spring 2011 Macromolecular Biophysics II – University of Pennsylvania  
I was in charge of arranging lectures, holding office hours and regular review sessions, grading homework and exams for first and second year graduate students.

2009- Mentored high school, undergraduate, and graduate students in research.

Spring 2005 Programming I – Kenyon College  
I designed regression tests for weekly project assignments, graded, and then posted my own solutions to the class.

## Service

- Reviewer for *Soft Matter*
- Reviewer for *European Biophysics Journal*
- Reviewer for *Scientific Reports*
- Reviewer for *Nature Structural & Molecular Biology*
- Member, Biophysical Society
- Member, American Chemical Society

## References

Michael K. Gilson, M.D., Ph.D.  
Professor and Chair in Computer-Aided Drug Design  
Co-Director UC San Diego Center for Drug Discovery Innovation  
Skaggs School of Pharmacy and Pharmaceutical Sciences  
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Paul A. Janmey, Ph.D.  
Professor of Physiology  
Associate Director, Institute for Medicine and Engineering  
University of Pennsylvania  
1010 Vagelos Research Laboratories  
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Ravi Radhakrishnan, Ph.D.  
Professor of Bioengineering & Chemical and Biomolecular Engineering  
Department of Bioengineering  
University of Pennsylvania  
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Professor of Pharmaceutical Sciences and Chemistry  
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