

# Oliver Beckstein

CV current as of December 8, 2017

Dept. of Physics & Center for Biological Physics  
College of Liberal Arts and Sciences  
Arizona State University  
P.O. Box 871504  
Tempe AZ 85287-1504

Office phone: +1 (480) 727-9765  
Office fax: +1 (480) 965-7954  
E-mail: [oliver.beckstein@asu.edu](mailto:oliver.beckstein@asu.edu)  
Web: <http://becksteinlab.physics.asu.edu>

## Education

- 2005            **DPhil in Biochemistry**, Laboratory of Molecular Biophysics, **University of Oxford**, UK. Advisor: Prof. M.S.P. Sansom. Dissertation: *Principles of Gating Mechanisms of Ion Channels*
- 1999            **Diplom Physik**, Department of Physics, **Friedrich-Alexander Universität Erlangen-Nürnberg** (Germany). Advisor: Prof. O. Pankratov. Thesis: *Structural and electronic properties of platinum silicides from ab-initio calculations*

## Positions and Employment

- 01/2012–present    **Assistant Professor**, Department of Physics, Arizona State University
- 09/2008–12/2011    **Research Associate** with Prof. M.S.P. Sansom, Department of Biochemistry, University of Oxford, UK
- 01/2006–12/2007    **Postdoctoral Fellow** with Prof. T.B. Woolf, Department of Physiology, Johns Hopkins University, School of Medicine
- 09/2004–08/2008    **Junior Research Fellow**, Merton College, University of Oxford, UK

## Scientific Interests

*Computational biophysics*: Quantitatively predicting the function and activity of proteins from the knowledge of their structures alone and so to better understand biological phenomena at the molecular level, in particular transmembrane transport processes catalyzed by membrane proteins such as secondary active transporters and ion channels. This work contributes to the fields of structural biology, physiology, nanobiotechnology, and drug discovery. *Computational method and software development*: Development of novel algorithms to sample and analyze molecular systems and distribution as open source software.

## Professional Development

- 2013    *Promotion and Tenure Workshop* (Provost's Office, Arizona State University)  
OKED ASU National Science Foundation Day (workshop on funding opportunities at the NSF) at Arizona State University  
OKED ASU NIH Day (workshop on grant writing for NIH) at Arizona State University
- 2012    *AAPT Workshop for New Physics and Astronomy Faculty*; a 3.5 day intense workshop introducing new pedagogical methods that focus on student-learning
- 2011    *Managing people—an introductory course*; e-learning course on how to lead and manage employees and students effectively

- 2005 *Learning and Teaching in Higher Education* at the Oxford Learning Institute (University of Oxford); a year-long course for more experienced teachers who wish to improve their understanding of student learning, improve their own teaching practice, and develop ideas for educational enhancement.
- 2004 *Teaching undergraduate students*, a two-day seminar run by the university's Learning Institute to introduce graduate students to teaching techniques for undergraduate classes and tutorials
- 2003 *UKGRADschool*, a week-long workshop that developed leadership and teamwork skills.

## Awards

- 2012 top prediction in the *SAMPL3 challenge* to blindly predict hydration free energies (with Bogdan Iorga, ICSN CNRS, France). [Publication 23]
- 2009 elected *Supernumerary Fellow* of Merton College, Oxford, 2009–2011
- 2008 *Physical Biology 2008 Citations Award* for the most cited article in the journal (O. Beckstein & M.S.P. Sansom, *Physical Biology* 1 (2004), 42–52) [Publication 39]
- 2005 *Visions of Science Photographic Award\** for my computer-generated image “Ion channel in the nervous system” [Publication 36] (\*a national competition for the best scientific images, sponsored by Novartis and the Daily Telegraph newspaper)
- 2004 *Junior Research Fellowship* (£70,000) at Merton College, Oxford, 2004–2008
- 2003 *Merton Graduate Prize Scholarship* (£500), Merton College, Oxford
- 2000 *Wellcome Trust Prize Studentship* in Structural Biology, The Wellcome Trust (£150,000), 2000–2004  
*Georg Simon Ohm Preis 2000* for an outstanding Diploma thesis at the Friedrich-Alexander Universität Erlangen-Nürnberg [Publication 58]
- 1992 *Stipendium nach dem Bayerischen Begabtenförderungsgesetz* (€ 25,000), State of Bavaria, 1993–1999

## RESEARCH

### Publications

Google Scholar

[scholar.google.com/citations?user=4BfuubAAAAAJ](http://scholar.google.com/citations?user=4BfuubAAAAAJ):

h-index: 22, citations: 2938

ISI Web of Science (AU=Beckstein O\*):

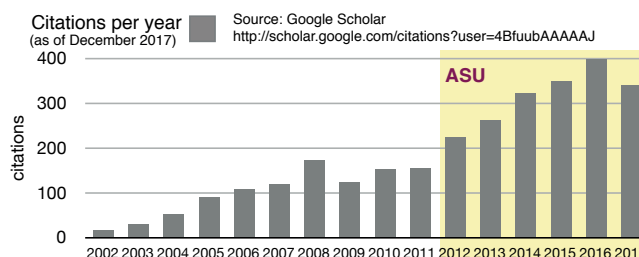
h-index: 20, citations: 2241

ORCID 0000-0003-1340-0831;

ResearcherID C-9095-2009

**Author order convention in the field: Students first, principal investigator(s) last**, joint first-authorship may be indicated.

**Bold:** supervised students (at ASU); asterisk (“\*”): joint first-authorship; dagger (“†”): communicating author. Citation counts according to Google Scholar (December 2017).



## Reviews, News&Views

Peer-reviewed reviews and similar publications (at ASU):

1. J. K. Hilton, P. Rath, C. V. M. Helsell, O. Beckstein, and W. D. Van Horn. *Understanding thermosensitive TRP channels as versatile polymodal cellular sensors*. *Biochemistry*, 54 (2015), 2401–2413. doi:[10.1021/acs.biochem.5b00071](https://doi.org/10.1021/acs.biochem.5b00071) (20 citations)
2. **S.L. Seyler**, O. Beckstein<sup>†</sup>. *Sampling large conformational transitions: AdK as a testing ground*. *Molecular Simulations* 40 (2014), 855–877. doi:[10.1080/08927022.2014.919497](https://doi.org/10.1080/08927022.2014.919497) (Invited review) (15 citations)
3. E. J. Denning, O. Beckstein<sup>†</sup>. *Influence of lipids on protein-mediated transmembrane transport*. *Chemistry and Physics of Lipids*. 169 (2013), 57–71. doi:[10.1016/j.chemphyslip.2013.02.007](https://doi.org/10.1016/j.chemphyslip.2013.02.007) (Invited review) (22 citations)

Prior to ASU:

4. S. Weyand, T. Shimamura, O. Beckstein, M.S.P. Sansom, S. Iwata, P.J.F. Henderson, and A.D. Cameron. *The Alternating Access Mechanism of Transport as Observed in the Sodium-Hydantoin Transporter Mhp1*. *J. Synchrotron Radiation* 37 (2011), 20–23. doi:[10.1107/S0909049510032449](https://doi.org/10.1107/S0909049510032449) (34 citations)
5. O. Beckstein<sup>†</sup>. *New and Notable: Teaching old coefficients new tricks: New insight into the osmotic and diffusive permeation coefficients*. *Biophys J* 96 (2009), 763–764. doi:[10.1016/j.bpj.2008.10.048](https://doi.org/10.1016/j.bpj.2008.10.048) (1 citation)
6. O. Beckstein, P.C. Biggin, P. Bond, J.N. Bright, C. Domene, A. Grottesi, J. Holyoake, and M.S.P. Sansom, *Ion channel gating: insights via molecular simulations*, *FEBS Letters* 555 (2003), 85–90. doi:[10.1016/S0014-5793\(03\)01151-7](https://doi.org/10.1016/S0014-5793(03)01151-7) (128 citations)
7. M. S. P. Sansom, P. Bond, O. Beckstein, P. C. Biggin, J. Faraldo-Goméz, R. J. Law, G. Patargias, D. P. Tieleman, *Water in ion channels and pores—simulation studies*, in *Novartis Foundation Symposia* 245 (2002), 66–83. doi:[10.1002/0470868759.ch6](https://doi.org/10.1002/0470868759.ch6) (21 citations)

## Articles

Peer reviewed research articles (at ASU):

8. Antonio N Calabrese, Scott M Jackson, Lynsey Jones, Oliver Beckstein, Florian Heinkel, Joerg Gsponer, David Sharples, Marta Sans, Maria Kokkinidou, Arwen Pearson, Sheena E Radford, Alison E Ashcroft, Peter JF Henderson. *Topological dissection of the membrane transport protein Mhp1 derived from cysteine accessibility and mass spectrometry*. *Analytical Chemistry*. 89 (2017), 8844–8852. doi:[10.1021/acs.analchem.7b01310](https://doi.org/10.1021/acs.analchem.7b01310) (0 citations)
9. J. Domański, O. Beckstein<sup>†</sup>, and B. I. Iorga<sup>†</sup>. *Ligandbook — an online repository for small and drug-like molecule force field parameters*. *Bioinformatics*, 33 (2017), 1747–1749. doi:[10.1093/bioinformatics/btx037](https://doi.org/10.1093/bioinformatics/btx037) (1 citation)
10. N. Coudray, **S. Seyler**, R. Lasala, Z. Zhang, K. M. Clark, M. E. Dumont, A. Rohou, O. Beckstein, and D. L. Stokes. *Structure of the SLC4 transporter Bor1p in an inward-facing conformation*. *Protein Sci*, 26 (2017), 130–145. doi:[10.1002/pro.3061](https://doi.org/10.1002/pro.3061) (2 citations)

11. Y. Huang, W. Chen, **D. L. Dotson**, O. Beckstein, and J. Shen. Mechanism of pH-dependent activation of the sodium-proton antiporter NhaA. *Nature Communications* 7 (2016), 12940 EP. doi:[10.1038/NCOMMS12940](https://doi.org/10.1038/NCOMMS12940) (6 citations)
12. **I. M. Kenney**, O. Beckstein<sup>†</sup>, and B. I. Iorga. Prediction of cyclohexane-water distribution coefficients for the SAMPL5 data set using molecular dynamics simulations with the OPLS-AA force field. *J Comput Aided Mol Des*, 30 (2016), 1045–1058. doi:[10.1007/s10822-016-9949-5](https://doi.org/10.1007/s10822-016-9949-5). (5 citations)
13. M. Coincon, P. Uzdavinyas, E. Nji, **D. L. Dotson**, I. Winkelmann, S. Abdul-Hussein, A. D. Cameron, O. Beckstein, and D. Drew. Crystal structures reveal the molecular basis of ion-translocation in sodium/proton antiporters. *Nature Struct. Mol. Biol.* 23 (2016), 248–255. doi:[10.1038/nsmb.3164](https://doi.org/10.1038/nsmb.3164) (22 citations)
14. **S. L. Seyler**, A. Kumar, M. F. Thorpe, and O. Beckstein<sup>†</sup>. Path similarity analysis: a method for quantifying macromolecular pathways. *PLoS Comput. Biol.*, 11 (2015), e1004568. doi:[10.1371/journal.pcbi.1004568](https://doi.org/10.1371/journal.pcbi.1004568) (6 citations)
15. M. B. Ulmschneider, J. K. Leman, H. Fennell, and O. Beckstein. *Peptide folding in translocon-like pores*. *J Membrane Biology* 248 (2015), 407–417. doi:[10.1007/s00232-015-9808-7](https://doi.org/10.1007/s00232-015-9808-7) (4 citations)
16. C. Lee\*, S. Yashiro\*, **D.L. Dotson\***, P. Uzdavinyas, S. Iwata, M. S. P. Sansom, C. von Ballmoos, O. Beckstein<sup>†</sup>, D. Drew<sup>†</sup>, and A. D. Cameron<sup>†</sup>. *Crystal structure of the sodium-proton antiporter NhaA dimer and new mechanistic insights*. *J Gen Physiol* 144 (2014), 529–544. doi:[10.1085/jgp.201411219](https://doi.org/10.1085/jgp.201411219). (Cover image) (25 citations)
17. K. J. Simmons, S. M. Jackson, F. Brückner, S. G. Patching, O. Beckstein, E. Ivanova, T. Geng, S. Weyand, D. Drew, J. Lannigan, D. J. Sharples, M. S. P. Sansom, S. Iwata, C. W. Fishwick, A. P. Johnson, A. D. Cameron, and P. J. Henderson. *The molecular mechanism of ligand recognition by a membrane transport protein*. *EMBO J* 33 (2014), 1831–1844. doi:[10.15252/embj.201387557](https://doi.org/10.15252/embj.201387557) (26 citations)
18. O. Beckstein, A. Fourier, B.I. Iorga. *Prediction of hydration free energies for the SAMPL4 diverse set of compounds using molecular dynamics simulations with the OPLS-AA force field*. *J Computer-Aided Molecular Design*. 28 (2014), 265–276. doi:[10.1007/s10822-014-9727-1](https://doi.org/10.1007/s10822-014-9727-1) (17 citations)
19. L.S. Stelzl, P.W. Fowler, M.S.P. Sansom, O. Beckstein<sup>†</sup>. *Flexible gates generate occluded intermediates in the transport cycle of LacY*. *J Mol Biol* 426 (2014), 735–751. doi:[10.1016/j.jmb.2013.10.024](https://doi.org/10.1016/j.jmb.2013.10.024) (28 citations)
20. P.W. Fowler, E. Abad, O. Beckstein, M.S.P. Sansom. *Energetics of multi-ion conduction pathways in potassium ion channels*. *J. Chem. Theo. Comput.* 9 (2013), 5176–5189 doi:[10.1021/ct4005933](https://doi.org/10.1021/ct4005933) (17 citations)
21. C. Lee, H.J. Kang, C. von Ballmoos, S. Newstead, P. Uzdavinyas, **D.L. Dotson**, S. Iwata, O. Beckstein, A.D. Cameron, and D. Drew. *A two-domain elevator mechanism for sodium/proton antiport*. *Nature* 501 (2013), 573–577, doi:[10.1038/nature12484](https://doi.org/10.1038/nature12484) (86 citations)
22. P.W. Fowler, O. Beckstein, E. Abad, and M.S.P. Sansom. *Detailed Examination of a Single Conduction Event in a Potassium Channel*. *J Phys Chem Lett* 4 (2013), 3104–3109. doi:[10.1021/jz4014079](https://doi.org/10.1021/jz4014079) (6 citations)
23. O. Beckstein and B. I. Iorga. *Prediction of hydration free energies for aliphatic and aromatic chloro derivatives using molecular dynamics simulations with the OPLS-AA force field*. *J Computer-Aided Molecular Design* 26 (2012), 635–645. doi:[10.1007/s10822-011-9527-9](https://doi.org/10.1007/s10822-011-9527-9) (14 citations)

Peer-reviewed research articles (prior to ASU):

24. M. Lindau, B.A. Hall, A. Chetwynd, O. Beckstein, M.S.P. Sansom. *Coarse-Grain Simulations Reveal Movement of the Synaptobrevin C-Terminus in Response to Piconewton Forces*. *Biophys J* 103 (2012), 959–969. doi:[10.1016/j.bpj.2012.08.007](https://doi.org/10.1016/j.bpj.2012.08.007) (30 citations)
25. R. Webster, S. Maxwell, H. Spearman, K. Tai, O. Beckstein, M.S.P. Sansom, D. Beeson. *A novel congenital myasthenic syndrome due to decreased acetylcholine receptor ion channel conductance*. *Brain* 135 (2012), 1070–1080. doi:[10.1093/brain/aws016](https://doi.org/10.1093/brain/aws016) (5 citations)
26. P. Pongprayoon, O. Beckstein, and M.S.P. Sansom. *Biomimetic design of a brush-like nanopore: Simulation studies*. *J Phys Chem B* 116 (2012), 462–468. doi:[10.1021/jp206754w](https://doi.org/10.1021/jp206754w) (15 citations)
27. N. Michaud-Agrawal, E. J. Denning, T. B. Woolf, O. Beckstein<sup>†</sup>. *MDAnalysis: A Toolkit for the Analysis of Molecular Dynamics Simulations*. *J. Comp. Chem.* 32 (2011), 2319–2327. doi:[10.1002/jcc.21787](https://doi.org/10.1002/jcc.21787) (370 citations)
28. J. R. Perilla, O. Beckstein, E. J. Denning, and T. B. Woolf. *Computing ensembles of transitions from stable states: Dynamic importance sampling*. *J. Comp. Chem.* 32 (2011), 196–209. doi:[10.1002/jcc.21564](https://doi.org/10.1002/jcc.21564) (34 citations)
29. J. Domański and P. J. Stansfeld and M. S. P. Sansom and O. Beckstein<sup>†</sup>. *Lipidbook: A Public Repository for Force-Field Parameters Used in Membrane Simulations*. *J Memb. Biol.* 236 (2010), 255–258. doi:[10.1007/s00232-010-9296-8](https://doi.org/10.1007/s00232-010-9296-8) (108 citations)
30. T. Shimamura\*, S. Weyand\*, O. Beckstein\*, N. G. Rutherford, J. M. Hadden, D. Sharples, M. S. P. Sansom, S. Iwata, P. J. F. Henderson, and A. D. Cameron. *Molecular Basis of Membrane Transport by the Sodium-Hydantoin Transporter, Mhp1*. *Science* 328 (2010), 470–473. doi:[10.1126/science.1186303](https://doi.org/10.1126/science.1186303) (218 citations)
31. P. Pongprayoon, O. Beckstein, C. L. Wee, and M. S. P. Sansom. *Simulations of anion transport through OprP reveal the molecular basis for high affinity and selectivity for phosphate*. *Proc. Natl. Acad. Sci. USA* 106 (2009), 21614–21618. doi:[10.1073/pnas.0907315106](https://doi.org/10.1073/pnas.0907315106) (41 citations)
32. O. Beckstein<sup>†\*</sup>, E. J. Denning\*, J. R. Perilla, and T. B. Woolf. *Zippering and Unzippering of Adenylate Kinase: Atomistic Insights into the Ensemble of Open ↔ Closed Transitions*. *J. Mol. Biol* 394 (2009), 160–176. doi:[10.1016/j.jmb.2009.09.009](https://doi.org/10.1016/j.jmb.2009.09.009) (88 citations)
33. S. Furini, O. Beckstein, and C. Domene. *Permeation of water through the KcsA K<sup>+</sup> channel*. *Proteins* 74 (2009), 437–448. doi:[10.1002/prot.22163](https://doi.org/10.1002/prot.22163) (22 citations)
34. C. Millar, R. Madathil, O. Beckstein, M. S. P. Sansom, S. Roy, and A. Asenov. *Brownian simulation of charge transport in α-haemolysin*. *J. Comput. Electron.* 7 (2008), 28–33. doi:[10.1007/s10825-008-0230-6](https://doi.org/10.1007/s10825-008-0230-6) (2 citations)
35. C. Millar, S. Roy, O. Beckstein, M. S. P. Sansom, and A. Asenov, *Continuum vs particle simulations of model nano-pores*, *J. Comput. Electron.* 6 (2007), 367–371. doi:[10.1007/s10825-006-0131-5](https://doi.org/10.1007/s10825-006-0131-5) (3 citations)
36. O. Beckstein<sup>†</sup> and M. S. P. Sansom, *A Hydrophobic Gate in an Ion Channel: The Closed State of the Nicotinic Acetylcholine Receptor*, *Phys. Biol.* 3 (2006), 147–159. doi:[10.1088/1478-3975/3/2/007](https://doi.org/10.1088/1478-3975/3/2/007) (142 citations)

37. S. Amiri, K. Tai, O. Beckstein, P. C. Biggin and M. S. P. Sansom, *The  $\alpha 7$  nicotinic acetylcholine receptor: molecular modelling, electrostatics, and energetics*, *Molec. Memb. Biol.* 22 (2005), 151–162. doi:[10.1080/09687860500063340](https://doi.org/10.1080/09687860500063340) (29 citations)
38. O. Beckstein, K. Tai, and M. S. P. Sansom, *Not ions alone: Barriers to ion permeation in nanopores and channels* *J. Am. Chem. Soc.* 126 (2004), 14694–14695. doi:[10.1021/ja045271e](https://doi.org/10.1021/ja045271e) (146 citations)
39. O. Beckstein<sup>†</sup> and M. S. P. Sansom, *The influence of geometry, surface character and flexibility on the permeation of ions and water through biological pores*, *Phys. Biol.* 1 (2004), 42–52. doi:[10.1088/1478-3967/1/1/005](https://doi.org/10.1088/1478-3967/1/1/005) (201 citations)
40. O. Beckstein and Mark S. P. Sansom, *Liquid-vapor oscillations in hydrophobic nanopores*, *Proc. Natl. Acad. Sci. USA* 100 (2003), 7063–7068. doi:[10.1073/pnas.1136844100](https://doi.org/10.1073/pnas.1136844100) (340 citations)
41. O. Beckstein, P. C. Biggin and M. S. P. Sansom, *A hydrophobic gating mechanism for nanopores*, *J. Phys. Chem B* 105 (2001), 12902–12905. doi:[10.1021/jp012233y](https://doi.org/10.1021/jp012233y) (242 citations)
42. J. E. Klepeis, O. Beckstein, O. Pankratov, G. L. W. Hart, *Chemical bonding, elasticity, and valence force field models: a case study for  $\alpha$ -Pt<sub>2</sub>Si and PtSi*, *Phys. Rev. B* 64 (2001), 155110. doi:[10.1103/PhysRevB.64.155110](https://doi.org/10.1103/PhysRevB.64.155110) (22 citations)
43. O. Beckstein, J. E. Klepeis, G. L. W. Hart, and O. Pankratov, *First-principles elastic constants and electronic structure of  $\alpha$ -Pt<sub>2</sub>Si and PtSi*, *Phys. Rev. B* 63 (2001), 134112. doi:[10.1103/PhysRevB.63.134112](https://doi.org/10.1103/PhysRevB.63.134112) (323 citations)

## Conference papers

Competitively selected and peer-reviewed (at ASU)

44. **M. Khoshlessan**, I. Paraskevagos, S. Jha, and O. Beckstein<sup>†</sup>. Parallel analysis in MDAnalysis using the Dask parallel computing library. In Katy Huff, David Lippa, Dillon Niederhut, and M. Pacer, editors, *Proceedings of the 16th Python in Science Conference*, pages 64–72, Austin, TX, 2017. SciPy. (0 citations)
45. **D. L. Dotson**, **S. L. Seyler**, M. Linke, R. J. Gowers, and O. Beckstein<sup>†</sup>. datreant: persistent, Pythonic trees for heterogeneous data. In S. Benthall and S. Rostrup, editors, *Proceedings of the 15th Python in Science Conference*, pages 51–56, Austin, TX, 2016. <http://datreant.org>. (0 citations)
46. R. J. Gowers, M. Linke, J. Barnoud, T. J. E. Reddy, M. N. Melo, **S. L. Seyler**, **D. L. Dotson**, J. Domański, S. Buchoux, **I. M. Kenney**, and O. Beckstein<sup>†</sup>. MDAnalysis: A Python package for the rapid analysis of molecular dynamics simulations. In S. Benthall and S. Rostrup, editors, *Proceedings of the 15th Python in Science Conference*, pages 102–109, Austin, TX, 2016. SciPy. <http://mdanalysis.org>. (11 citations)

## Book chapters and encyclopedia entries

Invited contributions but not peer-reviewed (prior to ASU):

47. S. M. Jackson, E. Ivanova, K. Simmons, S. G. Patching, S. Weyand, T. Shimamura, F. Brückner, S. Iwata, D. J. Sharples, S. A. Baldwin, M. P. Sansom, O. Beckstein, A. D. Cameron, and P. J. Henderson. *Na<sup>+</sup>-hydantoin membrane transport protein, Mhp1*. In G. Roberts, editor, *Encyclopedia of Biophysics*. Springer, 2013. (0 citations)

48. A. D. Cameron, O. Beckstein, and P. J. Henderson. *The 5-helix inverted repeat superfamily of membrane transport proteins*. In G. Roberts, editor, *Encyclopedia of Biophysics*. Springer, 2013. (0 citations)
49. S. Weyand, P. Ma, M. Saidijam, J. Baldwin, O. Beckstein, S. Jackson, S. Suzuki, S. G. Patching, T. Shimamura, M. S. P. Sansom, S. Iwata, A. D. Cameron, S. A. Baldwin, and P. J. F. Henderson. *The nucleobase-cation-symport-1 family of membrane transport proteins (met 268)*. In Albrecht Messerschmidt, editor, *Handbook of Metalloproteins*. Wiley, 2010. doi:[10.1002/0470028637.met268](https://doi.org/10.1002/0470028637.met268) (4 citations)
50. Y. Arinaminpathy, O. Beckstein, P. C. Biggin, P. J. Bond, C. Domene, A. Pang and M. S. P. Sansom, *Large Scale Biomolecular Simulations: Current Status and Future Prospects*, in Proc. UK e-Science All Hands Meeting 2003, ed. Simon J. Cox. Swindon: EPSRC (2003), 901-907. ISBN [1-904425-11-9](https://www.amazon.com/dp/1904425119) (2 citations)

## Preprints and Technical Reports

Not peer-reviewed but citable (at ASU).

51. **M. Khoshlessan** and O. Beckstein<sup>†</sup>. *Parallel analysis in the MDAnalysis Library: Benchmark of Trajectory File Formats*. Technical report, Arizona State University, Tempe AZ. figshare 2017. doi:[10.6084/m9.figshare.4695742](https://doi.org/10.6084/m9.figshare.4695742) (0 citations)
52. G. Fox, J. Quiu, D. Crandall, G. von Laszewski, S. Jha, J. Paden, F. Wang, O. Beckstein, and T. E. Cheatham III. *Datanet: CIF21 DIBBs: Middleware and high performance analytics libraries for scalable data science NSF14-43054 progress report*. Technical report, Indiana University, Rutgers University, Virginia Tech, University of Kansas, Stony Brook, Arizona State University, University of Utah. ResearchGate. 2016. doi:[10.13140/RG.2.2.31163.21289](https://doi.org/10.13140/RG.2.2.31163.21289) (0 citations)
53. **R. Delgado** and O. Beckstein<sup>†</sup>. *Technical Report: SPIDAL summer REU 2016: Distance array and RMSD speed-up in MDAnalysis*. Technical report, Arizona State University, Tempe, AZ. figshare 2016. doi:[10.6084/m9.figshare.3823293](https://doi.org/10.6084/m9.figshare.3823293)
54. **I. M. Kenney**, O. Beckstein<sup>†</sup>. *Technical Report: SPIDAL Summer REU 2015: Biomolecular benchmark systems*. Technical report, Arizona State University, Tempe, AZ. figshare. 2015. doi:[10.6084/m9.figshare.1588804](https://doi.org/10.6084/m9.figshare.1588804) (0 citations)

Prior to ASU:

55. S. E. Rogers, K. Tai, O. Beckstein, and M. S. P. Sansom. *Opening a hydrophobic gate: the nicotinic acetylcholine receptor as an example*. [arXiv:0902.1417v1](https://arxiv.org/abs/0902.1417v1) [q-bio.BM] (1 citation)
56. O. Beckstein. *Elastic Constants How-To*. figshare. 2001. doi:[10.6084/m9.figshare.1164130](https://doi.org/10.6084/m9.figshare.1164130) (2 citations)

## Theses

All theses were produced prior to ASU.

57. O. Beckstein, Doctoral Thesis: Principles of Gating Mechanisms of Ion Channels (2004), University of Oxford. BLDSC reference no.: D233707. doi:[10.6084/m9.figshare.1166494](https://doi.org/10.6084/m9.figshare.1166494)
58. O. Beckstein, Diploma thesis: Strukturelle und elektronische Eigenschaften der Platinsilizide aus ab initio-Rechnungen (1999). Friedrich-Alexander Universität Erlangen-Nürnberg. doi:[10.6084/m9.figshare.1166496](https://doi.org/10.6084/m9.figshare.1166496)

## Software Portfolio

Most of my software is open source and available from [github.com/Becksteinlab](https://github.com/Becksteinlab) or [github.com/orbeckst](https://github.com/orbeckst). A number of noteworthy packages are listed below, with my own contributions described for collaborative projects:

**MDAnalysis** is a versatile, object-oriented Python toolkit for analyzing Molecular Dynamics trajectories and developing new tools that go beyond what is typically found in established packages. New releases are downloaded more than 2000 times and there are about 150 subscribers on the mailing list. International core developer team with about six members, over 40 contributors. ¶Estimated cost to produce the software (47k lines of code, 11 person-years): US\$ 630,000 (source: [OpenHUB.net/p/mdanalysis](https://OpenHUB.net/p/mdanalysis)) ¶URL: [mdanalysis.org](https://mdanalysis.org) ¶My contribution: Project leader, lead developer, founder (with N. Michaud-Agrawal and E. J. Denning). ¶Publications [27](#), [14](#), [46](#), [44](#) [51](#), [53](#), [54](#)

**DIMS in CHARMM** *Dynamic importance sampling* (DIMS) code in the CHARMM software package (released in c35b2). ¶My contribution: conceptual and algorithm development, validation, documentation. ¶Publications [14](#), [19](#), [28](#), [30](#), [32](#)

**GromacsWrapper** is a Python package for running the Gromacs tools from within Python scripts. It provides error handling and command logging and makes it feasible to modularize and re-use small building blocks and set up a plugin analysis architecture. ¶Estimated cost to produce the software (10k lines of code, 2 person-years): US\$ 120,000 (source: [OpenHUB.net/p/GromacsWrapper](https://OpenHUB.net/p/GromacsWrapper)) ¶URL: [github.com/Becksteinlab/GromacsWrapper](https://github.com/Becksteinlab/GromacsWrapper) ¶My contribution: Project leader, lead developer, founder

**Ligandbook website** [ligandbook.org](https://ligandbook.org) is a chemically-aware public repository for force field parameters for small and drug-like molecules. ¶My contribution: Concept and design (with B. Iorga and J. Domański). ¶Publication [9](#)

**Lipidbook website** [lipidbook.bioch.ox.ac.uk](https://lipidbook.bioch.ox.ac.uk) is a public repository for force field parameters with a special emphasis on lipids, detergents, and similar molecules that are of interest when simulating biological membranes. It acts as a warehouse for parameter files that are supplied by the community. ¶My contribution: Project manager and developer (with J. Domański). ¶Publication [29](#)

**Hop** is a Python package based on *MDAnalysis* to analyze solvation dynamics in terms of “hopping graphs”. ¶URL [github.com/Becksteinlab/hop](https://github.com/Becksteinlab/hop) ¶My contribution: Project leader, lead developer

**MDPOW** is a Python package based on *GromacsWrapper* that facilitates the calculation of hydration free energies and solvent-water partition coefficients for small molecules as a means for validating force field parametrizations. ¶URL [github.com/Becksteinlab/MDPOW](https://github.com/Becksteinlab/MDPOW) ¶My contribution: Project leader, lead developer ¶Publications [23](#), [18](#), [12](#)

**alchemlyb** is a Python package for the calculation of free energies that provides a common user interface to a range of calculation methods. ¶URL [github.com/alchemistry/alchemlyb](https://github.com/alchemistry/alchemlyb) ¶My contribution: Project leader

**BornProfiler** is a Python package (based on APBS) that estimates energetics of ion permeation via a Poisson-Boltzmann approach. ¶URL [github.com/Becksteinlab/BornProfiler](https://github.com/Becksteinlab/BornProfiler) ¶My contribution: Project leader, lead developer ¶Publications [19](#)

**gridcount** is an analysis tool for Gromacs that creates 3D (number) densities from molecular dynamics trajectories. ¶URL: [github.com/orbeckst/gridcount](https://github.com/orbeckst/gridcount) ¶My contribution: sole developer ¶Publications: [40](#), [39](#), [36](#)

**g\_count and g\_flux** are Gromacs tools that characterizes movement of solvent particles inside a cylindrical region such as the pore of an ion channel or a carbon nanotube. *g\_count* analyzes thermodynamic properties (such as occupancies) whereas *g\_flux* returns kinetic properties such as the flux. ¶URL: [github.com/orbeckst/g\\_count](https://github.com/orbeckst/g_count) ¶My contribution: sole developer ¶Publications [41](#), [40](#), [38](#), [39](#), [36](#)



## Invited Presentations

### Invited Conference Presentations

Invited while at ASU:

- 2017 **APS 4 Corners Section Meeting**, Colorado State University, Ft Collins, CO  
254th **ACS National Meeting**: Symposium on “Membrane Proteins” (Washington, DC)  
**Telluride Workshop** on Ion Channels, Telluride, CO  
**Telluride Workshop** on Protein Electrostatics, Telluride, CO
- 2016 251st **ACS National Meeting**: Symposium on “Computer Simulations of Thermodynamics & Long-Time Kinetics of Molecular Events” (San Diego, CA)  
**NSF Molecular Science Cyberinfrastructure (MolSSI) Workshop**, Rice University, Houston, TX  
Honoring Dr Stuart Lindsay for His Achievements in Science Workshop, ASU, Tempe, AZ
- 2015 **Telluride Workshop** on Ion Channels, Telluride, CO  
Extended Software Development **CECAM Workshop**, Jülich, Germany
- 2012 Workshop on Physics, Chemistry, and Biology of Membrane Proteins, **Arizona State University**

Invited before coming to ASU:

- 2011 Lecture at the **International School of Biophysics** on Channels and Transporters (Erice, Sicily, Italy).
- 2010 **Gordon Research Conference** on Membrane Transport Proteins.
- 2003 **2nd Conference on Applied Statistical Physics**, Puerto Vallarta, Mexico.

### Invited Colloquia and Seminars

Invited while at ASU:

- 2017 Department of Pharmacological Sciences, **UC Irvine**, Irvine CA  
Department of Chemistry, **UC Riverside**, Riverside CA
- 2016 **Sandia National Labs**, Albuquerque NM  
Beckman Institute, **University of Illinois at Urbana-Champaign**, Urbana, IL  
Department of Cell Biology, Microbiology and Molecular Biology, **University of Southern Florida**, Tampa, FL
- 2015 **Max Planck Institute for Biophysics**, Frankfurt, Germany  
Department of Biology, **University of Erlangen-Nuremberg**, Germany
- 2014 Weill Medical College, **Cornell University**, NY  
Department of Materials Sciences and Engineering, **Johns Hopkins University**, MD  
Department of Pharmacology, **University of Maryland, Baltimore**, MD  
Department of Chemistry and Biochemistry, **Arizona State University**  
Department of Physiology, **Johns Hopkins University**, MD  
Institute for Lung and Blood Diseases, **NIH**, Bethesda, MD
- 2013 Physical Sciences Oncology Center Think Tank, Department of Physics, **Arizona State University**
- 2012 Department of Physics and Astronomy, **University of Delaware**  
Department of Physics and Astronomy, Colloquium, **Brigham Young University**  
Department of Chemistry and Biochemistry, **Arizona State University**  
Graduate Lunch Talk, Department of Physics, **Arizona State University**

Invited before coming to ASU:

- 2010 Department of Physiology and Pharmacology, **Oregon Health & Science University**.  
Department of Physiology, **Johns Hopkins University, School of Medicine**.  
Department of Pharmacology, **University of Maryland**, Baltimore.  
Institut de Biologie Physico-Chimique, **CNRS**, Paris.  
**Institut Pasteur**, Paris.  
Institut de Chimie des Substances Naturelles, **CNRS**, Gif-sur-Yvette, France.  
Laboratory of Molecular Biophysics, **University of Oxford**.
- 2008 Bionanotechnology Seminars, Department of Physics, **University of Oxford**.  
MRC Laboratory of Molecular Biology, **University of Cambridge**.  
Presentation to the **Warden and Junior Research Fellows of Merton College**, Oxford.
- 2005 Merton-Christ Church-St. Johns Junior Research Fellows' Seminar, **Merton College**.  
IRC Seminar at the Department of Physics, **University of Oxford**.  
**Scripps Research Institute**, La Jolla, CA.
- 2003 Weill Medical College, **Cornell University**, New York NY, USA.
- 2002 Beckman Institute, **University of Urbana-Champaign** IL, USA.
- 2001 MRC Laboratory of Molecular Biology, **University of Cambridge**.

## Contributed presentations

\*Talks at some meetings (in particular the Annual Meeting of the Biophysical Society) are competitively selected and are marked with an asterisk.

Contributed presentations while at ASU.

†Presentations by my students are also listed and marked with a dagger.

- 2017 Talk\* at the **61st Annual Meeting of the Biophysical Society**, New Orleans, LA, USA  
Talk† (presented by Sean Seyler), ASU **Biophest 2017**, Tempe, AZ  
Poster† (presented by Taylor Colburn), ASU, **Biophest 2017**, Tempe, AZ  
Poster† (presented by Mahzad Khoshlessan), ASU, **Biophest 2017**, Tempe, AZ  
Poster† (presented by Kathleen Clark-Reidy), ASU, **Biophest 2017**, Tempe, AZ
- 2016 Talk\* at the **15th Python in Science Conference, SciPy 2016**, Austin, TX  
Talk\*† (presented by David Dotson) at the **15th Python in Science Conference, SciPy 2016**, Austin, TX  
Talk\*† (presented by Sean Seyler) at the **60th Annual Meeting of the Biophysical Society**, Los Angeles, CA, USA  
Poster† (presented by David Dotson) at the **60th Annual Meeting of the Biophysical Society**, Los Angeles, CA, USA  
Talk\*† (presented by Taylor Colburn), **APS 4C and TX Section Meeting**, Las Cruces, NM  
Talk† (presented by David Dotson), U of Arizona **Biophest 2016**, Tucson, AZ  
Poster† (presented by Taylor Colburn), U of Arizona **Biophest 2016**, Tucson, AZ  
Poster† (presented by Ian Kenney), U of Arizona **Biophest 2016**, Tucson, AZ  
Poster† (presented by Kathleen Clark-Reidy), U of Arizona **Biophest 2016**, Tucson, AZ
- 2015 Talk\* at the **59th Annual Meeting of the Biophysical Society**, Baltimore MD, USA  
Talk\*† (presented by David Dotson) at the **59th Annual Meeting of the Biophysical Society**, Baltimore MD, USA  
Talk at the American Physical Society **APS March Meeting**, San Antonio, TX

- Poster<sup>†</sup> (presented by Sean Seyler) at the American Physical Society **APS March Meeting**, San Antonio, TX
- Poster<sup>†</sup> (presented by David Dotson) at **14th Python in Science Conference, SciPy 2015**, Austin, TX
- Talk<sup>†</sup> (presented by Sean Seyler), ASU **Biophest 2015**, Tempe, AZ
- Poster<sup>†</sup> (presented by David Dotson), ASU **Biophest 2015**, Tempe, AZ
- Poster<sup>†</sup> (presented by Ian Welland), ASU **Biophest 2015**, Tempe, AZ
- Poster<sup>†</sup> (presented by Ian Kenney), ASU **Biophest 2015**, Tempe, AZ
- Talk<sup>†</sup> (presented by Sean Seyler), ASU **APS 4 Corners Meeting 2015**, Tempe, AZ
- Poster<sup>†</sup> (presented by Ian Kenney), **APS 4 Corners Meeting 2015**, Tempe, AZ
- 2014 Poster at the **58th Annual Meeting of the Biophysical Society**, San Francisco, CA, USA
- Talk<sup>†</sup> (presented by David Dotson), U of Arizona **Biophest 2014**, Tucson, AZ
- Talk<sup>†</sup> (presented by Sean Seyler), U of Arizona **Biophest 2014**, Tucson, AZ
- 2013 Talk\* at the **57th Annual Meeting of the Biophysical Society**, Philadelphia, PA, USA
- Poster at the **Gordon Research Conference** on Membrane Transport Proteins
- Talk\*<sup>†</sup> (presented by Sean Seyler), **American Physical Society 4CS Meeting**, Denver, CO
- Poster<sup>†</sup> (presented by David Dotson), **American Physical Society 4CS Meeting**, Denver, CO
- Talk<sup>†</sup> (presented by David Dotson), ASU **Biophest 2013**, Tempe, AZ
- Talk<sup>†</sup> (presented by Sean Seyler), ASU **Biophest 2013**, Tempe, AZ

Contributed conference presentations before coming to ASU:

- 2011 Talk\* at the **55th Annual Meeting of the Biophysical Society**, Baltimore, MD, USA
- Talk at the **EDICT General Assembly**, Madrid, Spain.
- 2010 Talk\* at the **54th Annual Meeting of the Biophysical Society**, San Francisco, CA.
- Talk at the **EDICT General Assembly**, Tallinn, Estonia.
- 2009 Departmental seminar at **SBCB, Oxford**.
- Poster at **Molecular Kinetics '09**, Berlin, Germany.
- Two posters at the **53rd Annual Meeting of the Biophysical Society**, Boston, MA.
- 2008 Departmental seminar at **SBCB, Oxford**.
- Poster at **OXION Day**, Oxford.
- Poster at the **ENI-Net Workshop on Neuronal Ion Channels**, UCL London.
- Poster at the **Oxford University Research Staff Society (OURSS) Poster Session**, Oxford.
- Poster at the Wellcome Trust Conference **Nicotinic Receptors 2008**, Cambridge, UK.
- 2007 Poster at the **51st Annual Meeting of the Biophysical Society**, Baltimore, MD, USA.
- 2006 Departmental seminar, **Department of Physiology, Johns Hopkins University**.
- Poster at the **50th Annual Meeting of the Biophysical Society**, Salt Lake City, UT, USA.
- 2005 Poster at **OXION Day**, Oxford.
- Poster at the **MGMS Annual International Meeting**, Oxford.
- Departmental Seminar, **Laboratory of Molecular Biophysics, University of Oxford**.
- Poster at the **49th Annual Meeting of the Biophysical Society**, Long Beach CA, USA.
- 2004 Talk\* at the **48th Annual Meeting of the Biophysical Society**, Baltimore MD, USA.
- Poster at the **Final Year Students' Meeting at The Wellcome Trust**, London, UK.
- 2003 Talk\* at the **4th European Biophysics Congress**, Alicante, Spain.
- Poster at **Bionanotechnology**, Granada, Spain.
- Talk\* at the **CLRC Workshop on Advances in the Fundamental Properties of Confined Fluids**, Abingdon, UK.

- 2002 Presentation at the **CCP5 Summer School 2002**, London.  
 Poster at **Bionanotechnology**, Oxford, UK.
- 1999 Talk at the **Frühjahrstagung der Deutschen Physikalischen Gesellschaft**, Münster, Germany.

## TEACHING AND MENTORING

### Arizona State University (ASU)

I am a member of the graduate faculty in the PhD programs in **Physics** and in the **School of Molecular Sciences**, as well as Honors Faculty with Barrett, The Honors College at Arizona State University.

#### Courses taught at ASU

PHY542 / NAN542	<i>Topics in Biophysics I</i> Lecture (3h/week). 13 students	(Fall 2017)
PHY494	<i>Topic: Computational Methods in Physics</i> Interactive Lecture (3h/week). 16 students	(Spring 2017)
PHY542 / NAN542	<i>Topics in Biophysics I</i> Lecture (3h/week). 9 students	(Fall 2016)
PHY494	<i>Topic: Computational Methods in Physics</i> Interactive Lecture (3h/week). 20 students	(Spring 2016)
PHY542 / NAN542	<i>Topics in Biophysics I</i> Lecture (3h/week). 17 students	(Fall 2015)
PHY315	<i>Quantum Physics II</i> Lecture (3h/week). 48 students	(Spring 2015)
PHY542 / NAN542	<i>Topics in Biophysics I</i> Lecture (3h/week). 16 students	(Fall 2014)
PHY315	<i>Quantum Physics II</i> Lecture (3h/week). 55 students	(Spring 2014)
PHY542/494 / NAN542	<i>Topics in Biophysics I</i> Lecture (3h/week). 16 students	(Fall 2013)
PHY598/494 / CHM598	<i>Simulation approaches to Bio- and Nanophysics</i> Lecture/Computer lab (3h/week). 12 students	(Spring 2013)
PHY598/494	<i>Simulation approaches to Bio- and Nanophysics</i> Lecture/Computer lab (3h/week). 6 students	(Spring 2012)

#### Individual lectures taught at ASU

CHM501	introductory seminar for new graduate students in Chemistry and Biochemistry	(Fall 2014)
HON394	Barrett Honors seminar <i>A Century of Physics in a Smartphone</i> , two lectures	(Spring 2013)
PHY542/NAN542	one lecture on simulations of transport proteins	(Fall 2012)

#### Completed PhD Theses

David L. Dotson. *Solving the Mechanism of Na<sup>+</sup>/H<sup>+</sup> Antiporters Using Molecular Dynamics Simulations*,

Department of Physics, ASU (11/2016)

Sean L. Seyler. *Computational Approaches to Simulation and Analysis of Large Conformational Transitions in Proteins*, Department of Physics, ASU (11/2017)

### Completed Master's Theses

Lennard van der Feltz. *Calculation of Ion Channel Electrostatics*, Department of Physics, ASU (9/2014)

Ben Folsom. *Density Functional Theory Simulation of Rhodium Nanoframes and Carbon Nanotube-Graphene Pillars*, Professional Science Master's in Nanoscience, Department of Physics, ASU (4/2014). Now: PhD program in Physics at the University of Lund and the European Spallation Source, Sweden

### Completed Honors Theses

Ian Welland. *Quantifying Solvent Kinetics in Molecular Dynamics Simulations of Biomolecules*, Barrett, The Honors College, ASU (4/2015).

### Postdoctoral fellows

David Dotson (2017)

### Graduate students

David Dotson (graduated 2016; Publications [11](#), [13](#), [16](#), [21](#), [45](#), [46](#)), Sean Seyler (graduated 2017; Publications [10](#), [14](#), [2](#), [45](#), [46](#)), Mahzad Khoshlessan (since Fall 2016; Publications [44](#), [51](#)), Anton Kononenko (Spring 2017), Julio Candanedo (since Spring 2017, jointly supervised with Prof. John Spence), Ian Kenney (since Fall 2017)  
past rotation students: Shujie Fan (Fall 2017), Rick Sexton (Fall 2017), Armin Zjajo (Fall 2016), Alexander Cochran (Spring 2016), Bedabrata Choudhury (Fall 2014), Long Liang (Spring 2013)

### Undergraduate students

Ryan Heilman (Fall 2016), Kathleen Clark-Reidy (since Summer 2016), Taylor Colburn (since Fall 2015), Ian Kenney (research student, Spring 2014 – Summer 2017; publications [12](#), [46](#), [54](#))  
past undergraduate students: Ian Welland (honors thesis Summer 2015, research student Fall 2012 – Summer 2014, honors credit Spring 2013), Will Nobles (research student, Spring 2015),

### Honors enrichment projects

Alejandro Martinez (PHY 494, Spring 2015), *Simulation and Analysis of a Double Pendulum*

### Highschool students (Outreach) (also see [Outreach](#))

Kathleen Clark-Reidy (Fall 2015 – Spring 2016)

### Examination Committees

Chair, Dissertation Committee: David Dotson (2016), Sean Seyler (2017), Mahzad Khoshlessan (Mechanical and Aerospace Engineering, since Fall 2016), Anton Kononenko (since Spring 2017), Julio Candanedo (since Spring 2017, co-chair with Prof. John Spence), Ian Kenney (since Fall 2017)

Member, Dissertation Committee: Hadi Dinpajoo (Chemistry and Biochemistry, 2016), Garret Nelson (2015), Ashini Bolia (Chemistry and Biochemistry, 2015), Bryant Doss (2015), Avishek Kumar (2014), Alan Friesen (2012), Parminder Kaur (2012)

Lucas Madeira (since 2016), Cody Petrie (since 2016), Varda Faghir Hagh (since 2016), Tushar Modi (since 2016), Bryce Davis (since 2014), Rong Chen (since 2014), Morteza Moghimi Waskasi (Chemistry and Biochemistry, since 2014), Long Liang (since 2014), Seyed Salman Seyedi (since 2014)

Chair, Professional Science Master's (PSM) Thesis Committee: Ben Folsom (Fall 2013 – Spring 2014)

## University of Oxford, UK

### Teaching

- 2005 Lecturer (Bionanotechnology option for final year undergraduates) in the Department of Biochemistry)
- 2005 Lecturer (Bionanoscience lecture series of the Life Sciences Interface doctoral training centre programme) in Department of Biochemistry and Department of Physics
- 2004–2005 Tutor and Lecturer (Thermodynamics and Statistical Mechanics) at Merton College
- 2003, 2004, 2008 Teaching Assistant (Mathematics for Biochemists) in the Department of Biochemistry

**Graduate students** Lukas Stelzl (rotation project, 2010, Publication [19](#)), Prapasiri Pongprayoon (co-advisor with Mark Sansom, 2008–2010, Publications [26](#), [31](#)).

**Undergraduate students** Jan Domański (summer project funded by the Wellcome Trust; Publication [29](#))

## University of Erlangen-Nürnberg, Germany

### Teaching

- 1998–1999 Teaching Assistant (Quantum Mechanics; Statistical Mechanics and Thermodynamics) in the Department of Physics

## SERVICE

### Editorial board membership

European Biophysics Journal (Advisory Editorial Board)

### Professional reviewer activities

Grant reviewer for the French National Research Agency (ANR), the Environmental and Physical Sciences Research Council (EPSRC, UK), BBSRC, Israel Science Foundation

Journal reviewer (about 2 reviews per month): *Nature*, *Proc. Natl. Acad. Sci. USA*, *Physical Review Letters*, *Nature Struct. Molec. Biol.*, *Nature Communications*, *J Am Chem Soc*, *Biophysical Journal*, *PLoS Comp Biol*,

*PLoS ONE, Biochemistry, Physical Review B, Physical Review E, J Phys Chem, J Comp Chem, BBA Biomembranes, BBA General Subjects, J Phys:Cond Matt, J Expt Nano Sci, Proteins, Physical Biology, J Membrane Biol, J Computer-Aided Molec Design, Chemical Neuroscience, European Biophys J*

## **Conference and Seminar Organization**

- 2017 Organizer, Biological Physics Seminar series (Center for Biological Physics and Center for Applied Structural Discovery, ASU)  
Organizer, BioPhest 2017 (joint annual University of Arizona and Arizona State University event) at Arizona State University
- 2016 Organizer, Biological Physics Seminar series (Center for Biological Physics and Center for Applied Structural Discovery, ASU)
- 2015 Session co-Chair, “Molecular Dynamics Methods” at the 59th Meeting of the Biophysical Society  
Organizer, Center for Biological Physics Seminar series (ASU)  
Organizer, BioPhest 2015 (joint annual University of Arizona and Arizona State University event) at Arizona State University
- 2013 Organizer, BioPhest 2013 at Arizona State University  
Session co-Chair, “Membrane Transporters and Exchangers” at the 57th Meeting of the Biophysical Society
- 2012 Co-Organizer, Center for Biological Physics Workshop “Physics, Chemistry, and Biology of Membrane Proteins”
- 2011 Session co-Chair, “Membrane Transporters and Exchangers” at the 55th Meeting of the Biophysical Society
- 2009 Session co-Chair, “Protein Dynamics” at the 53rd Meeting of the Biophysical Society

## **Professional Societies**

Member, American Physical Society  
Member, Biophysical Society  
Member, American Chemical Society  
Member, British Biophysical Society  
Member, Deutsche Physikalische Gesellschaft

## **University Service (at Arizona State University)**

- 2017 Member, Working Group on Research Computing at ASU
- 2016 Member, Working Group on Research Computing at ASU
- 2015 Member, Steering Committee for Research Computing at ASU (OKED)

## **Department Service (at Arizona State University)**

### **Standing Committees**

- 2017 Chair, Technology Committee (Physics)  
Member, Committee on Committees (Physics)  
Member, Graduate Program Committee (Physics)
- 2016 Chair, Technology Committee (Physics)  
Member, Graduate Program Committee (Physics)
- 2016 Chair, Technology Committee (Physics)  
Member, Graduate Program Committee (Physics)
- 2015 Member, Graduate Program Committee (Physics)  
Member, Technology Committee (Physics)  
Member, Biophysics representation on Web Taskforce
- 2014 Chair, Committee on Committees (Physics)  
Member, Graduate Examinations Committee (Physics)  
Member, Graduate Program Committee (Physics)  
Member, Technology Committee (Physics)
- 2013 Chair, Committee on Committees (Physics)  
Member, Graduate Examinations Committee (Physics)
- 2012 Member, Graduate Examinations Committee (Physics)  
Member, Committee on Committees (Physics)

#### **Faculty Searches**

- 2016 Member, Modelling and Structure Methods Search (School of Molecular Sciences and Biodesign)
- 2012 Member, Experimental Biodesign Search (Physics and Biodesign)

## **Outreach**

### **Arizona State University**

- 2017 Google: *Google Summer of Code 2017* with MDAnalysis (our open source project); one student will be working on our project for 3 months during the summer with full funding at \$5,000  
*REU: CIF21 DIBBs: Middleware and High Performance Analytics Libraries for Scalable Data Science* (Research Experience for Undergraduates) ten-week research program in computational biophysics for 1 undergraduate student
- 2016 Google: *Google Summer of Code 2016* with MDAnalysis (our open source project); two students (Cal Poly and Oxford, UK) worked on our project for 3 months during the summer and were fully funded at \$5,000 each  
*NSF REU: CIF21 DIBBs: Middleware and High Performance Analytics Libraries for Scalable Data Science* (Research Experience for Undergraduates) ten-week research program in computational biophysics for 1 undergraduate student (Robert Delgado, Cornell University)  
*NSF BioXFEL STC* young researchers: one high school student and one undergraduate student work in the lab for at least one semester  
*Sundial\** Summer Program: Lunch with Biophysics students
- 2015 *NSF REU: CIF21 DIBBs: Middleware and High Performance Analytics Libraries for Scalable Data Science* (Research Experience for Undergraduates) ten-week research program in computational biophysics for 1 undergraduate student (Ian Kenney, Arizona State University)  
*NSF BioXFEL STC BioVizSim Village*: three high school students and one undergraduate spent two weeks in the lab working on interactive simulation and visualization



NSF *BioXFEL STC* young researchers: one high school student and one undergraduate student work in the lab for at least one semester

*Sundial*\* Summer Program: Tour of the lab for incoming Physics freshmen

2014 *Sundial*\* Summer Program: Tour of the lab for incoming Physics freshmen

\*The *Sundial* Project is a student-led initiative in the Department of Physics at ASU that aims to create a tight community amongst students and so increase retention rates.

### **University of Oxford**

2010 Open Day lecture to prospective students, Department of Biochemistry, University of Oxford.

2009 Open Day lecture to prospective students, Department of Biochemistry, University of Oxford.