Ken A. Dill

Louis and Beatrice Laufer Endowed Chair of Physical and Quantitative Biology
SUNY Distinguished Professor of Physics, Chemistry, and Applied Math and Statistics
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Education

1978 – 1981	Postdoctoral Fellow, Chemistry, Stanford University. Advisor--Paul J. Flory
1971 – 1978	Ph.D. Biology Department, UC San Diego, La Jolla. Advisor--Bruno H. Zimm
1966 – 1971	S.B. and S.M., Mechanical Engineering Department, M.I.T.

Professional Experience

2012 - present	SUNY Distinguished Professor, Physics and Chemistry, Stony Brook University
2010 – present	Louis & Beatrice Laufer Endowed Chair of Physical and Quantitative Biology
2010 – present	Director, Laufer Center for Physical & Quantitative Biology, Stony Brook University
2010 – present	Professor of Chemistry & Physics, Stony Brook University
2010	Distinguished Professor, Pharmaceutical Chemistry & Biophysics, UC San Francisco
1989 – 2010	Professor, Pharmaceutical Chemistry & Biophysics, UC San Francisco
2001 – 2010	Associate Dean of Research, School of Pharmacy, UC San Francisco
1989 – 2007	Adjunct Professor, Pharmaceutics, University of Utah
1996 – present	Faculty Biochemist, Lawrence Berkeley National Lab
1985 – 1989	Associate Professor, Pharmaceutical Chemistry, UC San Francisco
1985 – 1989	Associate Adjunct Professor, University of Utah
1982 – 1985	Assistant Professor, UC San Francisco
1981 – 1982	Assistant Professor, Chemistry, University of Florida, Gainesville

Other Appointments

2017 – present	Affiliated Distinguished Professor, Applied Math and Statistics, Stony Brook University

Service to Professional Organizations

2016	Scientific and Academic Advisory Committee review of *Structural Biology*, Weizmann Institute of Science
2011	Gordon Conference on Stochastic Physics in Biology Founding Co-chair
2004	NIBIB Review Board on Intramural Activities
2003 – 2010	Bridging the Sciences Coalition, Founder and Co-Director, a coalition of 15 basic research societies, supporting deep innovation and the Life/Physical Sciences interface.
2003 – 2006	American Physical Society, Physics Policy Committee
2003 – 2006	American Physical Society, Executive Committee, Division of Biological Physics
2002 – 2005	Protein Society, Executive Committee
2001 – 2007	Biophysical Society, Public Affairs Committee, Chair

2001 – 2004	American Physical Society, Division of Biological Physics, Executive Committee
2001 – 2004	American Physical Society, Awards Committee
1998 – 2000	Biophysical Society, Joint Steering Committee for Public Policy
1998 – 1999	Biophysical Society, President
1997 – 2001	NIH BBCA study section
1996	UC San Francisco BWF Graduate Program in Quantitative Biology, Co-director
1996	NIH BBCA study section, ad hoc
1994 – 1995	UCSF Biophysics Program, Acting Director
1994	Protein Society, Nominating Committee, Chair
1993	Biophysical Society, Nominating Committee, Chair
1993	Gordon Conference on Proteins, Co-chair
1993	NIH BBCA study section, ad hoc
1992 – 1995	Biophysical Society, Council
1992	Protein Society, Nominating Committee
1992	Biophysical Society, Executive Board
1991	Biophysical Society, Nominating Committee
1990	AAAS Symposium on Protein Folding, Co-organizer

Service to Editorial/Advisory Boards

Current Annual Review of Biophysics, Editor (2013-2022),
Protein Engineering, Physical Biology, Multiscale Modeling & Simulation, Structure, Biopolymers, Biophysical Chemistry, Journal of Molecular Recognition.

Past Journal of Chemical Physics (2014-2016),
Annual Review of Biophysics, Associate Editor & Board (2009-2013),
Protein Science, Annual Reviews of Physical Chemistry, Biophysical Journal, Theochem, Chemical Physics, Current Biology.

Honors

2019	Sackler Biophysics Prize (Tel Aviv University)
2019	Max Delbruck Prize for Biological Physics (American Physical Society)
2018	Dill 70th Festscrift (https://pubs.acs.org/toc/jpcbfk/122/21)
2013	American Academy of Arts and Science
2012	Distinguished Professor Chemistry and Physics, State University of New York
2012	Emily Gray Award, Biophysical Society
2010	UCSF 53rd Faculty Research Lecturer
2008	National Academy of Sciences, elected Member
2007	Biophysical Society, Distinguished Service Award
2004	Institute of Physics, elected Fellow
2002	Biophysical Society, elected Fellow
1998	Protein Society, first Hans Neurath Award
1997	AAAS, elected Fellow
1991	American Physical Society, elected Fellow
1987	UCSF Academic Senate, Distinguished Teaching Award
1987	UCSF Joseph M. Long Foundation Prize for Excellence in Teaching
1985 – 1989	Pew Scholar

1979 – 1980 Damon Runyon-Walter Winchell Postdoctoral Fellowship
1971 – 1974 National Science Foundation Pre-doctoral Fellowship

Activities at Stony Brook University

Since Oct 1, 2010

Founding and current director of the Laufer Center for Physical & Quantitative Biology—a community of 19 faculty & 3 Fellows from Stony Brook University, Cold-Spring Harbor & Brookhaven National Labs

-- Developed Physical Biology Grad Program in Physics, Chemistry, Applied Math & Statistics Departments

-- Campuswide opening event, May 2012

-- Hosted a national scientific meeting on protein folding, June 2012; northeast regional scientific meeting on protein design, June 2013; physical and quantitative biology retreats April 2015 & April 2017

-- Established the Laufer Distinguished Lecture Series

Member of the Advisory Board of the Institute of Chemical Biology & Drug Discovery
Member of the Institute for Cell & Developmental Biology in the Department of Biochemistry & Cell Biology
Member of the Provost's committee on MOOCs

Member of the search committee for a senior faculty member in Biochemistry and Cell Biology

Textbooks

PROTEIN ACTIONS, Principles & Modeling, with co-authors Ivet Bahar, Robert Jernigan, Garland Science Publishing. First edition February 2017.

MOLECULAR DRIVING FORCES, with co-author Sarina Bromberg, Garland Science Publishing. First edition 2003; Second edition 2012. A textbook of physical chemistry used in more than 150 courses worldwide; it won the Emily Gray Award from the Biophysical Society 2012.

Special Lectures

2020 Biological Physics Public Lecture (UCLA, 2020)
2019 Bing & Esther Humphrey Lecture, Chemistry (U Vermont, 2019)
2019 Daniel Kivelson Lecture, Chemistry (UCLA, 2019)
2017 Zymeworks ZED talk (Vancouver, 2017)
2017 Greater Boston Theoretical Chemistry 3-lecture series (MIT, Harvard U, BU)
2016 Fred W & Gladys E Laird Lecture, Chemistry (U British Columbia)
2016 Gary K Acker Lecturer, Gibbs Conference (Carbondale, Ill)
2016 Cyril N Hinshelwood Six Lectures, Chemistry (Oxford U)
2016 International Symposium, "The Technological Revolution in Structural Biology: Impact on Biology and Chemistry (Weizmann Institute of Science)
2016 FW Laird Lecture, Chemistry, U British Columbia
2016 60th Annual Meeting, Biophysics, Los Angeles
2016 NC3 Award Lecture, Chemistry (University Nevada-Lincoln)
2015 Sackler Symposium (Yale University)
2014 Morris Visiting Fellow, Chemistry (Hamilton College, Clinton, NY)
2012 Sackler Symposium (Yale University)
2011 Joseph Priestley Lecture (Penn State University)
2011 Eminent Scholar Lecture, Chemistry (University of Arizona)
2010 Five-campus Lecture Series (University of Massachusetts, Amherst University, Smith College, Mount Holyoke College, Hampshire College)

2008 Gary Griffin Lecture (University of New Orleans)
2006 Engbretsons Lecture (North Dakota State University)
2004 Inaugural Harrison Shull Lecture, Chemistry (Indiana University)
2002 Nieuwland-Reilly Lectures, Chemistry (Notre Dame University)
2001 Meloche Lecture, Chemistry (University of Wisconsin)
1998 Norman Hascoe Lecture, Physics (University Connecticut)
1998 Harland G. Wood Lecture, Biochemistry (Case-Western Reserve University)
1998 Clayton Foundation Regents Lectures (University of Texas)
1997 Keynote Lecture, Texas Folders Meeting
1997 Moses Gomberg Lecture (University of Michigan)
1996 National Lecture, Biophysical Society
1996 Joseph F. Foster Lecture (Purdue University)
1996 C.B. Anfinsen Lecture, Johns Hopkins Folding meeting
1995 Warren L. McCabe Lecture (North Carolina State University)
1993 Jesse W. Beams Lectures (University of Virginia)
1993 Wesleyan Lectures (Wesleyan University)
1992 Merck Lecture (Purdue University)
1991 Dartmouth Lectures (Dartmouth College)
1989 Bayer/Mobay Lecture (University of Pittsburgh)

PhD Students

1986 – 1990 Linda De Young, Ph.D., Head, Product Development, NuMedii
1984 – 1991 Kevin Scott, Ph.D., AstraZeneca
1985 – 1991 Darwin O. V. Alonso, Ph.D., retired, University of Washington, Seattle
1986 – 1994 David P. Yee, Ph.D., Translational Sci Project Leader, Novartis Inst for BioMedical Research
1987 – 1994 Klaus M. Fiebig, Ph.D., Senior Director Strategic Programs, Ontario Bioscience Innovation Organization
1991 – 1996 Paul D. Thomas, Ph.D., Associate Professor, Norris Cancer Center, U Southern Cal
1991 – 1997 Kevin A. T. Silverstein, Ph.D., RISS Operations Manager and Scientific Lead, Supercomputing Institute, U Minnesota
1991 – 1997 Karen E. S. Tang, Ph.D., Biochem, Molec Bio & Biophysics Department, U Minnesota
1994 – 1997 David W. Miller, Ph.D., Open Eye Software
1994 – 1999 Kent Kirshenbaum, Ph.D. Professor of Chemistry at NYU
1994 – 2000 Rachel Brem, Ph.D., Associate Professor, Buck Institute for Aging, Marin, CA
1996 – 2000 Jack Schonbrun, Ph.D., Director Software Engineering - Analytics, Pandora
1998 – 2001 Noel Southall, Ph.D., NIH, National Center for Advancing Translational Sciences
1999 – 2006 John Chodera, Assistant Member, Memorial Sloan-Kettering Cancer Center, NYC
2001 – 2006 Vince Voelz, Associate Professor of Chemistry, Temple University
2001 – 2006 Byoung-Chul Lee, 23 & Me
2004 – 2006 Justin Bradford, Information Systems, Consultant, Genentech
2008 – 2013 Gabriel Rocklin, Senior Fellow, Department of Biochemistry, Univ of Washington
2008 – 2013 Charlie Kehoe, Software Engineer, Google
2009 – 2012 Jack Peterson, Co-founder and lead develop at Augur
2009 – 2013 Geoff Rollins, Decision Analytics, Dropbox
2010 – 2012 Relly Brandman, Product Manager, Google
2012 – 2016 Eliza Guseva, data scientist, Gartner, Inc., Stamford

2012 – 2016 Michael Hazoglou, postdoc, UC San Diego
2012 – 2017 Mariola Szenk (join with Gabor Balazsi), Translational Partnerships Lead, nrerence, Boston)
2015 – 2016 Valentin Walther (MS student), now a Ph.D. student Aarhus University
2016 – present Luca Agozzino, postdoc at Stony Brook University
2016 – present Cong Liu, Stony Brook University
2016 – present Corey Weistuch, Stony Brook University
2017 – present Roy Nassar, Stony Brook University
2019 – present Jonathan Pachter, Stony Brook University
2020 – present Charles Kocher, Stony Brook University
2020 – present Chris Fortran, Stony Brook University

Postdoctoral Associates and Junior Fellows

1981 – 1984 Robert S. Cantor, Ph.D., Professor, Dartmouth College
1983 – 1986 Jeffrey A. Marqusee, Ph.D., Chief Scientist, Noblis, Inc, Falls Church, VA
1985 – 1989 Kit Lau, Ph.D., Principal, TBS Analytics
1986 – 1987 Ling-Chu Li, Ph.D.
1987 – 1998 Hue Sun Chan, Ph.D., Canada Research Chair Professor,
Department of Biochemistry, University of Toronto
1989 – 1991 Gregg B Fields, Ph.D., Professor of Chemistry, Florida Atlantic University
1989 – 1996 Sarina Bromberg, Ph.D., Biophysics writer, editor, illustrator
1990 – 2000 Kaizhi Yue, Ph.D., Owner, Conformational Search Solutions, San Francisco
1993 – 1995 Shaojian Sun, Ph.D.
1994 – 1999 Shi-Jie Chen, Ph.D., Professor of Physics & Astronomy, University of Missouri
1995 – 1997 Thomas Beutler, Ph.D., Swiss Banking System
1996 – 1997 Annelise Barron, Ph.D., Associate Professor of Bioengineering, Stanford University
1997 – 2000 Kenneth Foreman, Ph.D., Coferon, Inc.
1999 – 2001 Keith Ball, Ph.D., Senior HPC Engineer, RedLine, Falls Church, VA
1999 – 2001 Adam Lucas, Ph.D., Lecturer, Department of Statistics, Univ of California, Berkeley
2000 – 2001 Nick Braun, Ph.D.
2000 – 2002 Thomas Truskett Ph.D., Professor & Chair, Chemical Engineering, Univ of Texas, Austin
2000 – 2003 Matteo Palassini, Ph.D., Professor of Physics, University of Barcelona, Spain
2000 – 2003 Thomas Weikl, Ph.D., Group Leader, Max Planck Institute, Potsdam, Germany
2000 – 2004 Chaok Seok, Professor, Chemistry, Seoul National University, Korea
2002 – 2006 Kingshuk Ghosh, Ph.D., Associate Professor of Physics, University of Denver
2003 – 2005 Ilya Chorny, Ph.D., Senior Manager of Product Marketing, Illumina, San Diego, CA
2003 – 2006 Banu Ozkan, Ph.D., Associate Professor of Physics, Arizona State University
2004 – 2005 Ke Fan, Ph.D.
2004 – 2005 Huafeng Xu, Ph.D. DE Shaw Research Co.
2004 – 2007 Guo-Hong (Albert) Wu, Ph.D.
2004 – 2007 Julia Hockenmaier, Ph.D., Assoc Prof of Computer Sci, U Illinois, Urbana-Champaign
2004 – 2008 David Mobley, Ph.D., Associate Professor, Chemistry & Pharm Sci, UC Irvine
2005 – 2006 Bosco Ho, Ph.D., Scientific and web programmer
2005 – 2007 M. Scott Shell, Ph.D., Associate Professor of Chemical Engineering, UC Santa Barbara
2007 – 2010 Jeremy Schmit, Ph.D., Assistant Professor of Physics, Kansas State University
2007 – 2013 Christopher Fennell, Ph.D., Associate Professor of Chemistry, Oklahoma State Univ
2007 – 2014 Justin MacCallum, Ph.D., Assoc Prof of Chemistry, Canada Research Chair, Univ of Calgary
2008 – 2013 Steve Presse, Ph.D., Assistant Professor of Physics, Arizona State University
2011 – 2013 Daniel W. Farrell, Ph.D., Data Scientist, Facebook

2011 – 2014 Arijit Maitra, Ph.D., Assistant Professor, BML Munjal University, India
2011 – 2014 Libo Li, Ph.D., Associate Professor, South China University of Technology, Guangzhou
2011 – 2014 Arijit Roy, Ph.D., Scientist, TCS Innovation Labs, India
2014 – 2016 Joseph Morrone, Researcher, IBM, Thomas J. Watson Research Center, NY
2016 – 2017 Lane Votapka, Ph.D., Assistant Professor of Chemistry, Point Loma Nazarene University
2010 – present Alberto Perez, Ph.D., Assistant Professor, Univ Florida, Gainesville
2012 – present Adam De Graff, Ph.D., Sr Research Scientist, Methuselah Health UK LTD, Cambridge
2013 – present Emiliano Brini, Ph.D., Laufer Junior Fellow, Stony Brook University
2013 – present Mantu Santra, Ph.D., Indian Institute of Technology, Goa, India
2013 – present Jason Wagoner, Ph.D., Laufer Junior Fellow, Stony Brook University
2013 – 2017 Li Guo, Ph.D. (joint with Ron Zuckermann), Jiangsu University, China
2016 – present James Robertson, Ph.D., Scientist, Janssen Pharmaceutical, Philadelphia
2018 – present Bhanita Sharma, Stony Brook University
2019 – present Gregory Dignon, Stony Brook University
2019 – present Sridip Parui, Stony Brook University
2020 –present Luca Agozzino, Stony Brook University

Publications

333. C. Liu, E. Brini, A. Perez, K. A. Dill, Computing Ligands Bound to Proteins Using MELD-Accelerated MD. *Journal of Chemical Theory and Computation*, 10.1021/acs.jctc.0c00543 (2020).

332. L. Agozzino, G. Balázsi, J Wang, and K. A. Dill, How Do Cells Adapt? Stories Told in Landscapes. *Annual Review of Chemical and Biomolecular Engineering*, 11: 155-82 (2020).

331. D. Padhorny, K.A. Porter, M. Ignatov, A. Alekseenko, D. Beglov, S. Kotelnikov, R. Ashizawa, I. Desta, N. Alam Z. Sun, E. Brini, K.A. Dill, O. Schueler-Furman, S. Vajda, and D. Kozakov, ClusPro in rounds 38 to 45 of CAPRI: Toward combining template-based methods with free docking. *Proteins: Structure Function and Bioinformatic*, doi:10.1002/prot.25887 (2020).

330. L.R. Mujica-Parodi, A. Amgalan, S.F. Sultan, B. Antal, X. Sun, S. Skiena, A. Lithen, N. Adra, E.-M. Ratai, C. Weistuch, S.T. Govindarajan, H.H. Strey, K.A. Dill, S.M. Stufflebeam, R.L. Veech, and K. Clarke, Diet modulates brain network stability, a biomarker for brain aging, in young adults. *Proc Natl Acad Sci USA*, 117 (11): doi:10.1073/pnas.1913042117 (2020).

329. K. Ghosh, P.D. Dixit, L. Agozzino, K.A. Dill, The Maximum Caliber Variational Principle for Nonequilibria. *Annual Review of Physical Chemistry*, 71: doi: 10.1146/annurev-physchem-071119-040206 (2020).

328. M. Ignatov, C. Liu, A. Alekseenko, Z. Sun, D. Padhorny, S. Kotelnikov, A. Kazennov, I. Grebenkin, Y. Kholodov,I. Kolosvari, A. Perez, K.A. Dill, and D. Kozakov, Monte Carlo on the manifold and MD refinement for binding pose prediction of protein–ligand complexes: 2017 D3R Grand Challenge. *J Comput Aided Mol Des*, 33(1): 119-127 (2019).

327. A. Khramushin,O. Marcu,N. Alam,O. Shimony,D. Padhorny,E. Brini,K.A. Dill,S. Vajda,D. Kozakov,O. Schueler-Furman, Modeling beta-sheet peptide-protein interactions: Rosetta FlexPepDock in CAPRI rounds 38-45. *Proteins: Structure Function and Bioinformatic*, (2019).

326. M. Santra, K. A. Dill, A. M.R. de Graff, Proteostasis collapse is a driver of cell aging and death. *Proc Natl Acad Sci USA*, 116 (44): 22173-8 (2019).

325. J. Wagoner, K.A. Dill, Opposing pressures of speed and efficiency guide the evolution of molecular machines. *Molecular Biology and Evolution*, (2019).

324. L. Agozzino, K. A. Dill, Minimal constraints for maximum caliber analysis of dissipative steady-state systems. *Phys. Rev. E*, (2019).

323. J.C. Robertson, R. Nassar, C. Liu, E. Brini, K.A. Dill, A. Perez, NMR-assisted protein structure prediction with MELDxMD. *Proteins*, doi: 10.1002/prot.25788: (2019).

322. E. Brini, D. Kozakov, K.A. Dill, Predicting Protein Dimer Structures Using MELD × MD. *J. Chem. Theory Comput*., (2019).

321. J. Wagoner, K.A. Dill, Mechanisms for achieving high speed and efficiency in biomolecular machines. *Proc Natl Acad Sci USA*, 116: 5902-07 (2019).

320. P.D. Dixit, K.A. Dill, Building Markov state models using optimal transport theory. *The Journal of Chemical Physics*, 150: 54105 (2019).

319. T. Urbic, K.A. Dill, Water Is a Cagey Liquid. *J. of the American Chemical Society*, DOI: 10.1021/jacs.8b08856: (2018).

318. L. Agozzino, K. A. Dill, Protein evolution speed depends on its stability and abundance and on chaperone concentrations*. Proc Natl Acad Sci USA*, 115 (37): 9092 (2018).

317. M. Santra, K. A. Dill, A. M.R. de Graff, How Do Chaperones Protect a Cell's Proteins from Oxidative Damage?. *Cell Systems*, 743-751 (2018).

316. K. A. Dill, Colleagues of Ken A. Dill. *The Journal of Physical Chemistry B*, 5267 (2018).

315. K. A. Dill, Autobiography of Ken A. Dill. *The Journal of Physical Chemistry B*, 5263 (2018).

314. B. Hribar-Lee, C. Seok, E. Coutsias, and M. Lukšič, Tribute to Ken A. Dill. *The Journal of Physical Chemistry B*, 5261 (2018).

313. A. Perez, F. Sittel, G. Stock, and K.A. Dill, MELD-Path Efficiently Computes Conformational Transitions, Including Multiple and Diverse Paths. *J. Chem. Theory Comput*., 14: 2109 (2018).

312. P.D. Dixit, J. Wagoner, C. Weistuch, S. Pressé, K. Ghosh, K.A. Dill,, Perspective: Maximum Caliber is a General Variational Principle for Dynamical Systems. *J. Chem. Phys*., 148 (1): 10901 (2018).

311. E Brini, CJ Fennell, M Fernandez-Serra, B Hribar-Lee, M Luksic, KA Dill, How water's properties are encoded in its molecular structure and energies. *Chemical Reviews*. (2017).

310. T Urbic, KA Dill, Analytical theory of the hydrophobic effect of solutes in water. *Physical Review* E 96 (3), 032101. (2017).

309. M Szenk, KA Dill, AMR de Graff, Why Do Fast-Growing Bacteria Enter Overflow Metabolism? Testing the Membrane Real Estate Hypothesis. *Cell Systems*. (2017).

308. A Perez, JA Morrone, KA Dill, Accelerating physical simulations of proteins by leveraging external knowledge. *Wiley Interdisciplinary Reviews: Computational Molecular Science*. (2017).

307. M Santra, DW Farrell, KA Dill, Bacterial proteostasis balances energy and chaperone utilization efficiently.

Proceedings of the National Academy of Sciences, 201620646. (2017).

306. KA Dill, MF Holovko, B Hribar-Lee, N Malikova, The scientific life of Vojko Vlachy. *Journal of Molecular Liquids* 228, 1-3. (2017)

305. I Bahar, RL Jernigan, KA Dill, *Protein Actions: Principles and Modeling*. Garland Science. (2017).

304. JA Wagoner, K Dill, Molecular Motors have Evolved to Optimize Thermodynamic Performance. *Biophysical Journal* 112 (3), 279a. (2017).

303. JA Morrone, A Perez, J MacCallum, KA Dill, Computed binding of peptides to proteins with MELD-accelerated molecular dynamics. *Journal of chemical theory and computation* 13 (2), 870-876. (2017).

302. JA Morrone, A Perez, Q Deng, SN Ha, MK Holloway, TK Sawyer, Bradley S Sherborne, Frank K Brown, Ken A Dill, Molecular simulations identify binding poses and approximate affinities of stapled α-helical peptides to MDM2 and MDMX. *Journal of chemical theory and computation* 13 (2), 863-869. (2017).

301. A. Perez, J.A. Morrone, E. Brini, J. L. MacCallum, K.A. Dill, Blind protein structure prediction using accelerated free-energy simulations. *Science Advance*, 2: e1601274 (2016).

300. E. Brini, S.S. Paranahewage, C.J. Fennell, K.A. Dill, Adapting the semi-explicit assembly solvation model for estimating water-cyclohexane partitioning with the SAMPL5 molecules. *Journal of Computer-Aided Molecular Design*, doi:10.1007/s10822-016-9961-9 (2016).

299. K. Ghosh, A.M.R. de Graff,L Sawle and K.A. Dill, Role of Proteome Physical Chemistry in Cell Behavior. *Journal of Physical Chemistry B*, web: (2016).

298. J.A. Wagoner and K.A. Dill, Molecular Motors: Power Strokes Outperform Brownian Ratchets. *Journal of Physical Chemistry B,* DOI: 10.1021/acs.jpcb.6b02776 (2016).

297. A. Maitra and K.A. Dill, Modeling the Overproduction of Ribosomes when Antibacterial Drugs Act on Cells. *Biophysical Journal*, 110: 743-748 (2016).

296. A. Perez, J.A. Morrone, C. Simmerling and K.A. Dill, Advances in free-energy-based simulations of protein folding and ligand binding. *Current Opinion in Structural Biology*, 36: 25-31 (2016).

295. A.M.R de Graff, M.J. Hazoglou, and K.A. Dill, Highly Charged Proteins: The Achilles' Heel of Aging Proteomes. *Structure*, 24: 1 (2016).

294. A. Perez, J. L. MacCallum, E.A. Coutsias, and K.A. Dill, Constraint methods that accelerate free-energy simulations of biomolecules. *Journal of Chemical Physics*, 143: 243143 (2015).

293. P.D. Dixit, A. Jain, G. Stock, and K.A. Dill, Inferring Transition Rates of Networks from Populations in Continuous-Time Markov Processes. *Journal of Chemical Theory and Computation*, DOI: 10.1021/acs.jctc.5b00537 (2015).

292. A. Perez, J. L. MacCallum, E. Brini, C. Simmerling, and K.A. Dill, Grid-Based Backbone Correction to the ff12SB Protein Force Field for Implicit-Solvent Simulations. *Journal of Chemical Theory and Computation*, DOI: 10.1021/acs.jctc.5b00662: (2015).

291. M.J. Hazoglou, V. Walther, P.D. Dixit and K.A. Dill, Communication: Maximum caliber is a general variational principle for nonequilibrium statistical mechanics. *Journal of Chemical Physics*, 143: 51104 (2015).

290. S. Presse, K. Ghosh, J. Lee and K.A. Dill, Reply to C. Tsallis' "Conceptual Inadequacy of the Shore and Johnson Axioms for Wide Classes of Complex Systems". *Entropy*, 17: 5043-5046 (2015).

289. A.Perez, J.L. MacCallum, K. A. Dill, Accelerating molecular simulations of proteins using Bayesian inference on weak information. *PNAS*, 112: 11846-11851 (2015).

288. J.L. MacCallum, A.Perez, K. A. Dill, Determining protein structures by combining semireliable data with atomistic physical models by Bayesian inference. *PNAS*, 112: 6985-6990 (2015) PMID: PMC4460504.

287. A. Maitra, K. A. Dill, Bacterial growth laws reflect the evolutionary importance of energy efficiency. *PNAS*, 112: 406-411 (2015).

286. M. Kastelica, Y.V. Kalyuzhnyib, B. Hribar-Leea, K.A. Dillc and V. Vlachy, Protein aggregation in salt solutions. *PNAS*, 112(10): 6766–6770 (2015).

285. L. Li, K.A. Dill, C.J. Fennell, Testing the semi-explicit assembly model of aqueous solvation in the SAMPL4 challenge. *J Comput Aided Mol Des*., 28: 259-264 (2014).

284. L. Li, C. J. Fennell, and K. A. Dill, Small molecule solvation changes due to the presence of salt are governed by the cost of solvent cavity formation and dispersion. *Journal of Chemical Physics*, 141: 22D518 (2014).

283. M. Luksic, C. J. Fennell, K. A. Dill, Using Interpolation for Fast and Accurate Calculation of Ion−Ion Interactions. *Journal of Physical Chemistry B* Article ASAP, (2014).

282. G. J. Rocklin, D. L. Mobley, K. A. Dill, P. H. Hunenberger, Calculating the binding free energies of charged species based on explicit-solvent simulations employing lattice-sum methods: An accurate correction scheme for electrostatic finite-size effects. *Journal of Chemical Physics*, 139: 184103 (2013).

281. S. Pressé, K. Ghosh, J. Lee, K. A. Dill, Principles of maximum entropy and maximum caliber in statistical physics. *Rev. Mod. Phys*., 85 (3): 1115-41 (2013).

280. S. Pressé, K.Ghosh, J.Lee, K. A. Dill, Nonadditive Entropies Yield Probability Distributions with Biases not Warranted by the Data. *Phys. Rev. Lett*., 111: 180604 (2013).

279. S. Pressé, J.Lee, K. A. Dill, Extracting Conformational Memory from Single-Molecule Kinetic Data*. J. Phys. Chem. B*, 117 (2): 495-502 (2013).

278. A. Roy, A.Perez, K. A. Dill, J. MacCallum, Computing the Relative Stabilities and the Per-Residue Components in Protein Conformational Changes. *Structure*, 22: 168-175 (2013).

277. Rocklin GJ, Mobley DL, Dill KA, Calculating the sensitivity and robustness of binding free energy calculations to force field parameters, *J Chem Theory Comput*. 2013 Jul 9; 9(7):3072-3083

276. Rocklin GJ, Boyce SE, Fischer M, Fish I, Mobley DL, Shoichet BK, Dill KA, Blind Prediction of Charged Ligand Binding Affinities in a Model Binding Site. *J Mol Biol*. 2013 Jul 26. doi:pii: S0022-2836(13)00477-4. 10.1016/j.jmb.2013.07.030.

275. Dill KA, *Annu Rev Biophys*. 2013; 42. doi: 10.1146/annurev-bb-42-050113-100001. Biophysics. Introduction.

274. Rocklin GJ, Mobley DL, Dill KA, Separated topologies--a method for relative binding free energy

calculations using orientational restraints, *J Chem Phys*. 2013 Feb 28;138(8):085104. doi: 10.1063/1.4792251.

273. Kortkhonjia E, Brandman R, Zhou JZ, Voelz VA, Chorny I, Kabakoff B, Patapoff TW, Dill KA, Swartz TE, Probing antibody internal dynamics with fluorescence anisotropy and molecular dynamics simulations, *MAbs*. 2013 Mar-Apr;5(2):306-22. doi: 10.4161/mabs.23651. *Epub* 2013 Feb 8.

272. E. Kortkhonjia, R. Brandman, J. Z. Zhou, V. A. Voelz, I. Chorny, B. Kabakoff, T. W. Patapoff, K. A. Dill, T. E. Swartz, Probing antibody internal dynamics with fluorescence anisotropy and molecular dynamics simulations, *MAbs 5*, (2): 306-322 (2013).

271. K. A. Dill and J. L. MacCallum, The protein folding problem, 50 years on, *Science* 338, 1042-1046 (2012). (PDF) (Full Text Online) (podcast)

270. A. Perez, Z. Yang, I. Bahar, K. A. Dill, and J. L. MacCallum, FlexE: Using elastic network models to compare models of protein structure, *Journal of Chemical Theory and Computation 8*: 3985–3991 (2012). (PDF)

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