# Curriculum Vitae

## Personal Details


| | |
|---|---|
| Full Name | Robert Barrington Best |
| Date of Birth | 7th October 1976, Cape Town |
| Nationality | South African, British |
| Present Position | Senior Investigator<br>Laboratory of Chemical Physics<br>National Institutes of Health<br>Bethesda, MD 20892-0520<br>U. S. A. |
| e-mail | robertbe@nih.gov |
| Tel (W) | +1-301-496-5414 Fax (W) +1-301-496-0892 |
| Web | NIH Website |
| | Google Scholar |


## Professional Experience

| | |
|---|---|
| 11/2016-present | Senior Investigator, National Institute of Diabetes and Digestive and Kidney Diseases, National Institutes of Health |
| 10/2012-11/2016 | Tenure-track investigator, National Institute of Diabetes and Digestive and Kidney Diseases, National Institutes of Health |
| 10/2008-9/2012 | College Lecturer in Chemistry, Emmanuel College, Cambridge |
| 10/2007-9/2012 | Royal Society University Research Fellow, University of Cambridge. |
| 3/2004-9/2007 | Post-doctoral research in the Laboratory of Chemical Physics, NIH, Bethesda, MD with William Eaton and Gerhard Hummer. |
| 6/2003-2/2004 | Post-doctoral research with Michele Vendruscolo, University of Cambridge. |

## Education

| | |
|---|---|
| 2000-2003 | Ph.D. in Chemistry, University of Cambridge (Advisor: Jane Clarke)<br>*High Resolution Studies of Protein Folding and Dynamics*. |
| 2000 | M.Sc. in Chemistry, University of Cape Town (Advisors: Kevin Naidoo, Graham Jackson)<br>*Combined NMR and simulation study of carbohydrate linkage dynamics*. |
| 1998 | B.Sc.(Hons) in Chemistry (First Class), University of Cape Town. |
| 1995-1997 | B.Sc. University of Cape Town, Majors in Chemistry, Biochemistry and Mathematics with distinction. |

## Professional Associations

Editorial Board Member of Biophysical Journal (from Jan 2021)

Editorial Board Member of Journal of Biological Chemistry

Developer for CHARMM molecular simulation package

Member of the American Chemical Society and Biophysical Society

## Awards

2020 Sackler Award in Biophysics

2012 Royal Society of Chemistry Marlow Award.

2006 NIDDK Scientific Director's Fellowship Award (NIH).

2000 Cambridge Commonwealth Trust Mandela Scholarship.

## Recent Meetings

2020 *November*: Invited Seminar (Virtual), Heidelberg Institute of Theoretical Studies.

*August*: Invited Speaker, (Virtual) Telluride meeting on Biomolecular Interactions in Cellular Environments.

*June*: Invited Seminar (Virtual), Martin Weigt Group.

*May*: Invited Speaker (Virtual), CUNY Biophysics Seminar Series.

*February*: Poster Presenter, Biophysical Society Meeting

*January*: Poster Presenter, Gordon Research Conference on Protein Folding and Dynamics.

2019 *November*: Invited Speaker, MOLSSI Meeting on Machine Learning, University of Maryland.

*October*: Invited Speaker, CECAM Meeting on Modelling Phase Separation in Biology, Toulouse, France.

*September*: Invited Speaker, Intrinsically Disordered Protein Regions in the Context of Polymer Physics, Oak Ridge National Lab, TN.

*August*: Invited Speaker, Single Molecule Force Spectroscopy Workshop, Duke University, NC.

*July*: Invited Speaker, TSRC Intrinsically Disordered Proteins Workshop, Telluride, CO.

*June*: Invited Speaker, Molecular Kinetics and Machine Learning Meeting, Berlin, Germany.

*May*: Invited Lecturer, IUBMB Advanced School, Spetses, Greece.

*March*: Invited Speaker, American Chemical Society Spring Meeting, Orlando, FL.

*March*: Invited Speaker, American Physical Society Meeting, JCP Editor's Choice Session, Boston, MA.

*February*: Invited Speaker, Greater Boston Area Theoretical Chemistry Lecture Series, Boston, MA.

2018 *December*: Invited Speaker, Protein Folding on the Ribosome, Stockholm, Sweden.

*October*: Invited Speaker, Brown University Chemistry Department, Providence, RI.

*October*: Invited Speaker, Computational Biophysics at the Molecular and Mesoscales, Qui Nhon, Vietnam.

*September*: Invited Speaker, Molecular Physiology of the Cell Membrane, Woods Hole, MA.

*July*: Invited Speaker, CHARMM Developers' meeting, Chicago.

*July*: Invited Speaker, Protein and Peptide interactions in Cellular Environments, Telluride, CO.

*May*: Invited Speaker, Statistical Mechanics of Protein Sequences, Temple University, PA.

*May*: Invited Speaker, Protein Science in Human Diseases, University of Parma, Italy.

*February*: Meeting Chair, Biophysical Society Intrinsically Disordered Proteins Subgroup, San Francisco, CA.

*January*: Session Chair, Protein folding Gordon Conference, Galveston, TX

2017 *October*: Invited Speaker, CECAM Meeting on Disordered Protein Segments, Paris, France.

*September*: Invited Speaker, Protein Folding, Evolution and Interactions Symposium, Cambridge, UK.

*July*: Invited Seminar, CHARMM Developers' meeting, Cambridge, MA.

*March*: Invited Speaker, International Center of Theoretical Physics, Trieste, Italy.

2016 *September*: Invited Speaker, Scietific Computing Internal Lecturer Series, University of Cape Town, South Africa.

*August*: Invited Speaker, American Chemical Society National Meeting, Philadelphia, PA.

*August*: Invited Speaker, CECAM/Lorentz Meeting on Reaction Coordinates, Leiden, Netherlands.

*June*: Invited Speaker, CHARMM Developers' meeting, Ann Arbor, MI.

*June*: Invited Speaker, Protein and Peptide Interactions in Cellular Environments, Telluride, CO.

*March*: Invited Speaker, American Chemical Society National Meeting, San Diego, CA.

*January*: Protein Folding Gordon Conference, Galveston, TX: Keynote Speaker

*January*: Invited Seminar, University of Calgary, Center for Molecular Simulation.

## Conferences Organised

2022 Vice chair-elect, Gordon Research Conference on Protein Folding Dynamics (co-vice chair Martin Gruebele)

2021 Chairman, Intrinsically Disordered Protein Subgroup of Biophysical Society. (co-chair Alessandro Borgia)

2018 Session Chair, Intrinsically Disordered Protein Subgroup, Biophysical Society Annual Meeting (co-chair Scott Showalter)

2015 CECAM Meeting on Intrinsically Disordered Proteins, Zürich (co-organisers Ben Schuler, Kresten Lindorff-Larsen, Birthe Kragelund)

2014 Experimental and Theoretical Approaches for Enzyme Catalysis Related to Energy Generation, London (co-organisers Jochen Blumberger, Christophe Léger, Luca de Gioia)

2013 CECAM Meeting on Intrinsically Disordered Proteins, Zürich (co-organisers Kresten Lindorff-Larsen, Birthe Kragelund)

2012 CECAM Protein Folding Meeting, Zürich (co-organisers David de Sancho, Ben Schuler)

2006 CECAM Meeting on Single Molecule Pulling Experiments, Lyon (co-organisers Emanuele Paci, Peter Olmsted)

## Current Group Members

**Thomas Dannenhofer-Lafage** (Post-doc since September 2018). Ph. D. University of Chicago, 2018. Coarse grained models for protein phase separation.

**Kathryn Lebold** (Post-doc since September 2019). Ph. D. Penn. State University, 2018. Coarse grained models for nucleic acid / protein interactions and complex coacervation.

**Layne Frechette** (Post-doc since September 2020). Ph. D. U. C. Berkeley, 2020. Sequence-based protein design and fold-switch engineering

**Grace Taumoefolau** (Co-supervised PhD Student since September 2019). Analysis of maximum likelihood theory for transition-path times using molecular simulations.

## Former Group Members

**Pengfei Tian** (Post-doc 2014–2018) Misfolding of multidomain proteins, co-evolutionary models for sequence design, Co-translational protein folding. *Current: Research Scientist, Novozymes*

**Matthias Bellaiche** (NIH/Oxcam Ph. D. student 2014–2018) Mechanism of secondary nucleation of amyloid fibers, Markov State Models for amyloid formation. *Current: Guidehouse Consulting*

**Jan Domanski** (NIH/Wellcome Ph. D. student 2013–2017). Molecular simulation of membrane protein folding and association *Current: Co-founder, Labstep.*

**Wenfei Li** (Visiting Scholar, 2017–18). Prof., Dept. of Physics, Nanjing University, China. Coarse-grained models for amyloid formation, and kinetics. Interpretation of protein folding $\psi$-values versus $\phi$-values.

**Wenwei Zheng** (Post-doc 2014–2017). Internal friction in protein folding, interpretation of scattering experiments on disordered proteins. *Current: Assistant Professor, Arizona State University.*

**Travis Hoppe** (Post-doc 2014-2016). Contact potentials for intrinsically disordered proteins, role of intrinisically disordered proteins in protein interaction networks. *Current: Grant Analyst, NIH Office of the Director.*

**David De Sancho** (Post-doc 2010–2014). Kinetics of helix formation, downhill folding, protein internal friction, ligand transport in proteins, Markov State Models. *Current: Ramón y Cahal Fellow at the University of the Basque Country and the Donostia International Physics Center.*

**Christopher M. Baker** (Post-doc 2012–2013). Development of systematic coarse-grained models, binding of intrinsically disordered proteins to DNA. *Current: Head of Physical Chemistry at Syngenta UK.*

**Michael Knott** (Post-doc 2010–2013). Multistate models for intrinsically disordered proteins, models for chaperonin function. *Current: Signal/spectral analysis at CRFS, Cambridge.*

**Anshul Sirur** (Ph. D. student 2010–2013). Models for action of chaperonins on substrate proteins, Markov State Models. *Current: Senior Developer, UK Government Digital Service.*

**Thomas Graham** (M.Phil. Student 2009). Effect of mechanical force on protein unfolding mechanism. *Current: Post-doctoral fellow University of California, Berkeley.*

**James Carter** (project student 2012). Markov State Models for protein folding. *Current: Ph. D. Student, Imperial College, London.*

## Jointly Supervised/Visiting Students

**Sandro Bottaro** (Visiting Ph. D. 2011). Systematic derivation of implicit solvent models. *Current: Post-doc, University of Lugano.*

**Ian Tunbridge** (Shared Ph.D.). Development of GPU code for coarse-grained simulations. *Current: Professional Software Development.*

**Yaw-Sing Tan** (Shared Ph. D. Student 2011-2012). Discovery of cryptic binding pockets in Polo-like kinase. *Current: Research Associate, A*STAR Bioinformatics Institute, Singapore.*

**Petra Kührová** (Visiting Ph. D. Student 2011). Folding of peptides and RNA. *Current: Assistant Professor, Palack University, Olomoac, Czech Republic.*

**Digvijay Singh** (Summer Student, 2012). Ising-like models for force-induced protein unfolding. *Current: Post-doc, University of California, San Diego.*

## Journal Articles (Google Scholar h-index: 60)


[1] Andrea Sottini, Alessandro Borgia, Madeleine B. Borgia, Katrine Bugge, Daniel Nettels, Aritra Chowdhury, Petur O. Heidarsson, Franziska Zosel, Robert B. Best, Birthe B. Kragelund, and Benjamin Schuler. Polyelectrolyte interactions reconcile high affinity and fast kinetics in disordered protein complexes. *Nat. Commun., in press*, 2020.

[2] Pengfei Tian and Robert B. Best. Exploring the fitness landscape of a bridge between protein folds. *PLoS Comput. Biol., in press*, 2020.

[3] Gregory Dignon, Robert B. Best, and Jeetain Mittal. Biomolecular phase separation: from molecular driving forces to macroscopic properties. *Annu. Rev. Phys. Chem.*, 71:53–75, 2020.

[4] Grant Kemp, Ola B. Nilsson, Pengfei Tian, Robert B. Best, and Gunnar von Heijne. Cotranslational folding cooperativity of contiguous domains of $\alpha$-spectrin, in press. *Proc. Natl. Acad. Sci. U. S. A.*, pages 1–8, 2020.

[5] Jan Domański, Mark S. P. Sansom, Phillip J. Stansfeld, and Robert B. Best. Atomistic mechanism of transmembrane helix association. *PLoS Comput. Biol.*, 16:e1007919, 2020.

[6] Xuemin Chen, Yanxiang Cui, Robert B. Best, Huaibin Wang, Z. Hong Zhou, Wei Yang, and Martin Gellert. Cutting antiparallel DNA strands in a single active site. *Nat. Struct. Mol. Biol.*, 27:119–126, 2020.

[7] Robert B. Best. Emerging consensus on the collapse of unfolded and intrinsically disordered proteins in water. *Curr. Opin. Struct. Biol.*, 60:27–38, 2020.

[8] Eiji Yamamoto, Jan Domanski, Fiona B. Naughton, Robert B. Best, Antreas C. Kalli, Philip J. Stansfeld, and Mark S. P. Sansom. Multiple lipid binding sites determine the affinity of ph domains for phosphoinositide-containing membranes. *Sci. Adv.*, 6:eaay5736, 2020.

[9] Aleix Lafita, Pengfei Tian, Robert B. Best, and Alex Bateman. Tandem domain swapping: determinants of multidomain protein misfolding. *Curr. Opin. Struct. Biol.*, 58:97–104, 2019.

[10] Erik D. Holmstrom, Zhaowei Liu, Daniel Nettels, Robert B. Best, and Benjamin Schuler. Disordered RNA chaperones can enhance nucleic acid folding via local charge screening. *Nat. Commun.*, 10:2453, 2019.

[11] Gül H. Zerze, Wenwei Zheng, Robert B. Best, and Jeetain Mittal. Evolution of all-atom protein force fields to improve local and global properties. *J. Phys. Chem. Lett.*, pages 2227–2234, 2019.

[12] Petra Kührová and Vojtech Mlýnsky and Marie Zgarbová and Miroslav Krepl and Giovanni Bussi and Robert B. Best and Michal Otyepka and Jiri Sponer and Pavel Banás. Improving the Performance of the Amber RNA Force Field by Tuning the Hydrogen-Bonding Interactions. *J. Chem. Theory Comput.*, 15:3288–3305, 2019.

[13] Aleix Lafita, Pengfei Tian, Robert B. Best, and Alex Bateman. TADOSS: computational estimation of tandem domain swap stability. *Bioinformatics*, 35(14):2507–2508, 2019.

[14] Renuka Kudva, Pengfei Tian, Fátima Pardo-Aliva, Marta Carroni, Robert B. Best, Harris D. Bernstein, and Gunnar von Heijne. The shape of the bacterial ribosome exit tunnel affects cotranslational protein folding. *Elife*, 7:e36326, 2018.

[15] Erik D. Holmstrom, Andrea Holla, Wenwei Zheng, Daniel Nettels, Robert B. Best, and Benjamin Schuler. Accurate transfer efficiencies, distance distributions, and ensembles of unfolded and intrinsically disordered proteins from single-molecule FRET. *Methods Enzym.*, 611:287–325, 2018.

[16] Matthias M. J. Bellaiche and Robert B. Best. Molecular determinants of A$\beta_{42}$ adsorption to amyloid fibril surfaces. *J. Phys. Chem. Lett.*, 9:6437–6443, 2018.

[17] Emily J. Guinn, Pengfei Tian, Mia Shin, Robert B. Best, and Susan Marqusee. A small single-domain protein folds through the same pathway on and off the ribosome. *Proc. Natl. Acad. Sci. U. S. A.*, 115(48):12206–12211, 2018.

[18] Pengfei Tian, Annette Steward, Renuka Kudva, Ting Su, Patrick J. Shilling, Adrian A. Nickson, and Robert B. Best. The folding pathway of an ig domain is conserved on and off the ribosome. *Proc. Natl. Acad. Sci. U. S. A.*, 115:E11284–E11293, 2018.

[19] Wenwei Zheng, Hagen Hofmann, Benjamin Schuler, and Robert B. Best. Origin of internal friction in disordered proteins depends on solvent quality. *J. Phys. Chem. B*, 122:11478–11487, 2018.

[20] Joerg Schoenfelder, David De Sancho, Robert Best Ronen Berkovich, Victor Munoz, and Raul Perez-Jiminez. Reversible two-state folding of the ultrafast protein gpw under mechanical force. *Comms. Chem.*, 54:57–87, 2003.

[21] Gregory Dignon, Wenwei Zheng, Robert B. Best, Young C. Kim, and Jeetain Mittal. Relation between single-molecule properties and phase behaviour of intrinsically disordered proteins. *Proc. Natl. Acad. Sci. U. S. A.*, 115:9929–9934, 2018.

[22] Robert B. Best, Wenwei Zheng, Alessandro Borgia, Karin Buholzer, Madeleine B. Borgia, Hagen Hofmann, Andrea Soranno, Daniel Nettels, Klaus Gast, Alexander Grishaev, and Benjamin Schuler. Comment on "Innovative scattering analysis shows that hydrophobic disordered proteins are expanded in water". *Science*, 361:eaar7101, 2018.

[23] David de Sancho, Jörg Schönfelder, Robert B. Best, Raul Perez-Jiminez, and Victor Muñoz. Instrumental effects in the dynamics of an ultrafast folding protein under mechanical force. *J. Phys. Chem. B*, 2018.

[24] Wenwei Zheng and Robert B. Best. An extended Guinier analysis for intrinsically disordered proteins. *J. Mol. Biol.*, 430:2540–2553, 2018.

[25] Pengfei Tian, John M. Louis, James L. Baber, Annie Aniana, and Robert B. Best. Coevolutionary fitness landscapes for sequence design. *Angew. Chem. Intl. Ed.*, 130:5776–5780, 2018.

[26] Robert B. Best. Race to the native state. *Proc. Natl. Acad. Sci. U. S. A.*, 115:2267–2269, 2018.

[27] Jan Domański, Mark S. P. Sansom, Phillip J. Stansfeld, and Robert B. Best. Balancing force field protein-lipid interactions to capture transmembrane helix-helix association. *J. Chem. Theor. Comput.*, 14:1706–1715, 2018.

[28] Wenwei Zheng, Gul H. Zerze, Alessandro Borgia, Jeetain Mittal, Benjamin Schuler, and Robert B. Best. Inferring properties of disordered chains from FRET transfer efficiencies. *J. Chem. Phys.*, 148:123329, 2018.

[29] Gregory Dignon, Wenwei Zheng, Young C. Kim, Robert B. Best, and Jeetain Mittal. Sequence determinants of protein phase behaviour from a coarse-grained model. *PLoS Comput. Biol.*, 14:e1005941, 2018.

[30] Alessandro Borgia, Madeleine B. Borgia, Katrine Bugge, Vera M. Kissling, Petur O. Heidarsson, Catarina B. Fernandes, Andrea Sottini, Karin J. Buholzer, Daniel Nettels, Birthe B. Kragelund, Robert B. Best, and Benjamin Schuler. Extreme disorder in an ultra-high-affinity protein complex. *Nature*, 555:61–66, 2018.

[31] Fanjie Meng, Mathias M. J. Bellaiche, Jae-Yeol Kim, Gul H. Zerze, Robert B. Best, and Hoi-Sung Chung. Highly disordered amyloid-beta monomer probed by single-molecule FRET and MD simulation. *Biophys. J.*, 114(4):870–884, 2018.

[32] Zachary Monahan, Veronica H. Ryan, Abigail M. Janke, Kathleen A. Burke, Gul H. Zerze, Robert O'Meally, Gregory L. Dignon, Alexander E. Conicella, Wenwei Zheng, Robert B. Best, Robert N. Cole, Jeetain Mittal, Frank Shewmaker, and Nicholas L. Fawzi. Low complexity domain phosphorylation disrupts FUS phase separation, aggregation and toxicity. *EMBO J.*, page e201696394, 2017.

[33] Pengfei Tian and Robert B. Best. How many protein sequences fold to a given structure? a co-evolutionary analysis. *Biophys. J.*, 113:1719–1730, 2017.

[34] Robert B. Best. Computational and theoretical advances in studies of intrinsically disordered proteins. *Curr. Opin. Struct. Biol.*, 42:147–154, 2017.

[35] Adam Kubas, Christophe Orain, David De Sancho, Laure Saujet, Matteo Sensi, Charles Gauquelin, Isabelle Meynial-Salles, Philippe Soucaille, Hervé Bottin, Carole Baffert, Vincent Fourmond, Robert B. Best, Jochen Blumberger, and Christophe Léger. Mechanism of $O_2$ diffusion and reduction in FeFe hydrogenases. *Nat. Chem.*, 9:88–95, 2017.

[36] Jan Domański, George Hedger, Robert B. Best, Phillip J. Stansfeld, and Mark S. P. Sansom. Convergence and sampling in determining free energy landscapes for membrane protein association. *J. Phys. Chem. B*, 121:3364–3375, 2016.

[37] David de Sancho and Robert B. Best. Reconciling intermediates in mechanical unfolding experiments with two-state protein folding in bulk. *J. Phys. Chem. Lett.*, 7:3798–3803, 2016.

[38] Alessandro Borgia, Wenwei Zheng, Karin Buholzer, Madeleine B. Borgia, Anja Schüler, Hagen Hofmann, Andrea Soranno, Daniel Nettels, Klaus Gast, Alexander Grishaev, Robert B. Best, and Benjamin Schuler. Consistent view of polypeptide chain expansion in chemical denaturants from multiple experimental methods. *J. Am. Chem. Soc.*, 138:11714–11726, 2016.

[39] Wenwei Zheng, Alessandro Borgia, Karin Buholzer, Alexander Grishaev, Benjamin Schuler, and Robert B. Best. Probing the action of chemical denaturant on an intrinsically disordered protein by simulation and experiment. *J. Am. Chem. Soc.*, 138:11702–11713, 2016.

[40] Petra Kührová, Robert B. Best, Sandro Bottaro, Giovanni Bussi, Jiri Sponer, Michal Otyepka, and Pavel Banás. Computer folding of RNA tetraloops: identification of key force field deficiencies. *J. Chem. Theory Comput.*, 12:4534–4548, 2016.

[41] Pengfei Tian and Robert B. Best. Structural determinants of misfolding in multidomain proteins. *PLOS Comput. Biol.*, 12:e1004933, 2016.

[42] Wenwei Zheng, David De Sancho, and Robert B. Best. Modulation of folding internal friction by local and global barrier heights. *J. Phys. Chem. Lett.*, 7:1028–1034, 2016.

[43] Robert B. Best and Gerhard Hummer. Microscopic interpretation of folding $\phi$-values using the transition path ensemble. *Proc. Natl. Acad. Sci. U. S. A.*, 113:3263–3268, 2016.

[44] Anshul Sirur, David De Sancho, and Robert B. Best. Markov state models of protein misfolding. *J. Chem. Phys.*, 144:075101, 2016.

[45] Gül H. Zerze, Jeetain Mittal, and Robert B. Best. Diffusive dynamics of contact formation in disordered polypeptides. *Phys. Rev. Lett.*, page 068102, 2016.

[46] Wenwei Zheng and Robert B. Best. Reduction of all-atom folding dynamics to one-dimensional diffusion. *J. Phys. Chem. B*, 119:15247–15255, 2015.

[47] Gül H. Zerze and Robert B. Best and Jeetain Mittal. Sequence and temperature-dependent properties of unfolded and disordered proteins from atomistic simulations. *J. Phys. Chem. B*, 119:14622–14630, 2015.

[48] Wenwei Zheng, Alessandro Borgia, Madeleine B. Borgia, Benjamin Schuler, and Robert B. Best. Empirical optimization of interactions between proteins and chemical denaturants in molecular simulations. *J. Chem. Theor. Comput.*, 11:5543–5553, 2015.

[49] Alessandro Borgia, Katherine R. Kemplen, Madeleine B. Borgia, Andrea Soranno, Sarah Shammas, Bengt Wunderlich, Daniel Nettels, Robert B. Best, Jane Clarke, and Benjamin Schuler. Transient misfolding dominates multidomain protein folding. *Nature Comm.*, 6:8861, 2015.

[50] Julien Roche, John M. Louis, Ad Bax, and Robert B. Best. Pressure-induced structural transition of mature HIV-1 protease from a combined NMR/MD simulation approach. *Proteins*, 83:2117–2123, 2015.

[51] Robert B. Best, Hagen Hofmann, Daniel Nettels, and Ben Schuler. Quantitative interpretation of FRET experiments via molecular simulation: force field and validation. *Biophys. J.*, 108:2721–2731, 2015.

[52] David de Sancho, Adam Kubas, Po hung Wang, Jochen Blumberger, and Robert B. Best. Identification of mutational hot spots for substrate diffusion: application to myoglobin. *J. Chem. Theor. Comput.*, 11:1919–1927, 2015.

[53] Wenwei Zheng, David de Sancho, Travis Hoppe, and Robert B. Best. Dependence of internal friction on folding mechanism. *J. Am. Chem. Soc.*, 137:3283–3290, 2015.

[54] Robert B. Best, Cayla Miller, and Jeetain Mittal. Role of solvation in pressure-induced helix stabilization. *J. Chem. Phys.*, 141:22D522, 2014.

[55] Robert B. Best, Wenwei Zheng, and Jeetain Mittal. Balanced protein-water interactions improve properties of disordered proteins and non-specific protein association. *J. Chem. Theor. Comput.*, 10:5113–5124, 2014.

[56] Gül H. Zerze and Robert B. Best and Jeetain Mittal. Modest influence of FRET chromophores on the properties of unfolded proteins. *Biophys. J.*, 107:1654–1660, 2014.

[57] Robert B. Best. Bootstrapping new protein folds. *Biophys. J.*, 107:1040–1041, 2014.

[58] David de Sancho and Robert B. Best. Molecular origins of internal friction effects on protein-folding rates. *Nature Commun.*, 5:4307, 2014.

[59] Michael Knott and Robert B. Best. Discriminating binding mechanisms of an intrinsically disordered protein via a multistate coarse-grained model. *J. Chem. Phys.*, 140:175102, 2014.

[60] Rene Wuttke, Hagen Hofmann, Daniel Nettels, Madeleine B. Borgia, Jeetain Mittal, Robert B. Best, and Benjamin Schuler. Temperature-dependent solvation modulates the dimensions of disordered proteins. *Proc. Natl. Acad. Sci. U. S. A.*, 111:5213–5218, 2014.

[61] Adam Kubas, David de Sancho, Robert B. Best, and Jochen Blumberger. Aerobic damage of [FeFe] hydrogenases: activation barriers for $O_2$ chemical attachment. *Angew. Chem.*, 126:4165–4168, 2014.

[62] Anshul Sirur, Michael Knott, and Robert B. Best. Effects of interactions with the chaperonin cavity on protein folding and misfolding. *Phys. Chem. Chem. Phys.*, 16:6358–6366, 2014.

[63] Robert B. Best. Folding and binding: when the force is against you. *Biophys. J.*, 105:2611–2612, 2013.

[64] Sandro Bottaro, Kresten Lindorff-Larsen, and Robert B. Best. Variational optimization of an all-atom implicit solvent force field to match explicit solvent simulation data. *J. Chem. Theor. Comput.*, 9:5641–5652, 2013.

[65] James W. Carter, Christopher M. Baker, Robert B. Best, and David de Sancho. Engineering folding dynamics from two-state to downhill: application to $\lambda$-repressor. *J. Phys. Chem. B*, 117:13435–13443, 2013.

[66] Robert B. Best, Gerhard Hummer, and William A. Eaton. Native contacts determine protein folding mechanisms in atomistic simulations. *Proc. Natl. Acad. Sci. U. S. A.*, 110:17874–17879, 2013.

[67] Eric R. Henry, Robert B. Best, and William A. Eaton. Comparing a simple theoretical model for protein folding with all-atom molecular dynamics simulations. *Proc. Natl. Acad. Sci. U. S. A.*, 110:17880–17885, 2013.

[68] Maksym Tsytlonok, Patricio O. Craig, Elin Sivertsson, David Serquera, Sarah Perrett, Robert B. Best, Peter G. Wolynes, and Laura S. Itzhaki. Complex energy landscape of a giant repeat protein. *Structure*, 21:1954–1965, 2013.

[69] Stephanie M. Cope, Sandip Shinde, Robert B. Best, Giovanna Ghirlanda, and Sara M. Vaiana. Cyclic N-terminal loop of amylin forms non-amyloid fibers. *Biophys. J.*, 105:1661–1669, 2013.

[70] Robert B. Best. How well does a funneled energy landscape capture the folding mechanism of spectrin domains. *J. Phys. Chem. B*, 117:13235–13244, 2013.

[71] Yue Shi, Zhen Xia, Robert Best, Chuanjie Wu, Jay W. Ponder, and Pengyu Ren. Polarizable atomic multipole-based AMOEBA force field for proteins. *J. Chem. Theor. Comput.*, 9:4046–4063, 2013.

[72] Christopher M. Baker and Robert B. Best. Insights into the binding of intrinsically disordered proteins from molecular dynamics simulation. *WIREs Comput. Mol. Sci.*, pages 182–198, 2013.

[73] Christopher M. Baker and Robert B. Best. Matching of additive and polarizable force fields for multiscale condensed phase simulations. *J. Chem. Theory. Comput.*, 9:2826–2837, 2013.

[74] Robert B. Best. A "slow" protein folds quickly in the end. *Proc. Natl. Acad. Sci. U. S. A.*, 110:5744–5745, 2013.

[75] Petra Kührová, Pavel Banás, Robert B. Best, Jiri Sponer, and Michal Otyepka. Computer folding of RNA tetraloops? Are we there yet? *J. Chem. Theor. Comput.*, 9:2115–2125, 2013.

[76] Anshul Sirur and Robert B. Best. Effects of interactions with the GroEL cavity on protein folding rates. *Biophys. J.*, 104:1098–1106, 2013.

[77] David de Sancho, Jeetain Mittal, and Robert B. Best. Folding kinetics and unfolded state dynamics of the GB1 hairpin from molecular simulation. *J. Chem. Theor. Comput.*, 9:1743–1753, 2013.

[78] Jihyun Shim, Xiao Zhu, Robert B. Best, and Alexander D. Mackerell. (Ala)4-X-(Ala)4 as a model system for the optimization of the $\chi_1$ and $\chi_2$ amino acid side-chain dihedral empirical force field parameters. *J. Comput. Chem.*, 34:593–603, 2013.

[79] Robert B. Best, Jeetain Mittal, Michael Feig, and Alexander D. Mackerell. Inclusion of many-body effects in the additive CHARMM all-atom protein CMAP potential results in enhanced cooperativity of $\alpha$-helix and $\beta$-hairpin formation. *Biophys. J.*, 103:1045–1051, 2012.

[80] Robert B. Best, Xiao Zhu, Jihyun Shim, Pedro Lopes, Jeetain Mittal, Michael Feig, and Alexander D. Mackerell. Optimization of the additive CHARMM all-atom protein force field targeting improved sampling of the backbone $\phi, \psi$ and side-chain $\chi_1$ and $\chi_2$ dihedral angles. *J. Comp. Theor. Comput.*, 8:3257–3273, 2012.

[81] Yaw-Sing Tan, Paweł Śledź, Steffen Lang, Christopher J. Stubbs, David R. Spring, Chris Abell, and Robert B. Best. Using ligand-mapping simulations to design a ligand selectively targeting a cryptic surface pocket of polo-like kinase 1. *Angew. Chem. Int. Ed.*, 51:10078–10081, 2012.

[82] Apratim Bhattacharya, Robert B. Best, and Jeetain Mittal. Smoothing of the GB1 hairpin folding landscape by interfacial confinement. *Biophys. J.*, 103:596–600, 2012.

[83] Michael Knott and Robert B. Best. A preformed binding interface in the unbound ensemble of an intrinsically disordered protein: evidence from molecular simulation. *PLoS Comp. Biol.*, 8:e1002605, 2012.

[84] Julius Schulz, Lennart Schmidt, Robert B. Best, Joachim Dzubiella, and Roland Netz. Peptide chain dynamics in light and heavy water: zooming in on internal friction. *J. Am. Chem. Soc.*, 134:6273–6279, 2012.

[85] Petra Kührová, Alfonso de Simone, Michal Otyepka, and Robert B. Best. Force-field dependence of chignolin folding and misfolding: comparison with experiment and redesign. *Biophys. J.*, 102:1897–1906, 2012.

[86] Robert B. Best, David de Sancho, and Jeetain Mittal. Residue-specific $\alpha$-helix propensities from molecular simulation. *Biophys. J.*, 102:1462–1467, 2012.

[87] Robert B. Best. Atomistic simulations of protein folding. *Curr. Opin. Struct. Biol.*, 22:52–61, 2012.

[88] Olga K. Dudko, Thomas G. W. Graham, and Robert B. Best. Locating the folding barrier for single molecules under an external force. *Phys. Rev. Lett.*, 107:208301, 2011.

[89] David de Sancho and Robert B. Best. Modulation of an IDP binding mechanism and rates by helix propensity and non-native interactions: association of Hif1$\alpha$ with CBP. *Mol. Biosyst.*, 8:256–267, 2011.

[90] Robert B. Best and Gerhard Hummer. Diffusion models of protein folding. *Phys. Chem. Chem. Phys.*, 13:16902–16911, 2011.

[91] Robert B. Best and Jeetain Mittal. Microscopic events in beta-hairpin folding from alternative unfolded ensembles. *Proc. Natl. Acad. Sci. U. S. A.*, 108:11087–11092, 2011.

[92] Madeleine B. Borgia, Alessandro Borgia, Robert B. Best, Annette Steward, Daniel Nettels, Bengt Wunderlich, Benjamin Schuler, and Jane Clarke. Single-molecule fluorescence reveals sequence-specific misfolding in multidomain proteins. *Nature*, 474:662–665, 2011.

[93] David de Sancho and Robert B. Best. What is the time scale for alpha-helix nucleation? *J. Am. Chem. Soc.*, 133:6809–6816, 2011.

[94] Po hung Wang, Robert B. Best, and Jochen Blumberger. A microscopic model for gas diffusion dynamics in a [NiFe]-hydrogenase. *Phys. Chem. Chem. Phys.*, 13:7708–7719, 2011.

[95] Po hung Wang, Robert B. Best, and Jochen Blumberger. Multiscale simulation reveals multiple pathways for $H_2$ and $O_2$ transport in a [NiFe]-hydrogenase. *J. Am. Chem. Soc.*, 133:3548–3556, 2011.

[96] Thomas G. W. Graham and Robert B. Best. Force-induced change in protein unfolding mechanism: discrete or continuous switch? *J. Phys. Chem. B*, 115:1546–1561, 2011.

[97] Robert B. Best and Jeetain Mittal. Free-energy landscape of the GB1 hairpin in all-atom explicit solvent simulations with different force fields: similarities and differences. *Proteins*, 79:1318–1328, 2011.

[98] Young C. Kim, Robert B. Best, and Jeetain Mittal. Macromolecular crowding effects on protein-protein binding affinity and specificity. *J. Chem. Phys.*, 133:205101, 2010.

[99] Robert B. Best and Jeetain Mittal. Protein simulations with an optimized water model: cooperative helix formation and temperature-induced unfolded state collapse. *J. Phys. Chem. B*, 114:14916–14923, 2010.

[100] Ian Tunbridge, Robert B. Best, James Gain, and Michelle M. Kuttel. Simulations of coarse-grained protein-protein interactions with graphics processing units. *J. Chem. Theor. Comput.*, 6:3588–3600, 2010.

[101] Jeetain Mittal and Robert B. Best. Tackling force field bias in protein folding simulations: folding of Villin HP35 and Pin WW domains in explicit water. *Biophys. J.*, 99:L26–L28, 2010.

[102] Robert B. Best and Jeetain Mittal. Balance between $\alpha$ and $\beta$ structures in *ab initio* protein folding. *J. Phys. Chem. B*, 114:8790–8798, 2010.

[103] Robert B. Best and Gerhard Hummer. Coordinate-dependent diffusion in protein folding. *Proc. Natl. Acad. Sci. U. S. A.*, 107:1088–1093, 2010.

[104] Jeetain Mittal and Robert B. Best. Dependence of protein folding stability and dynamics on the density and composition of macromolecular crowders. *Biophys. J.*, 98:315–320, 2010.

[105] Daniel Nettels, Sonja Müller-Spath, Frank Küster, Hagen Hofmann, Dominik Haenni, Stefan Rüegger, Luc Reymond, Armin Hoffmann, Jan Kubelka, Benjamin Heinz, Klaus Gast, Robert B. Best, and Benjamin Schuler. Single-molecule spectroscopy of the temperature-induced collapse of unfolded proteins. *Proc. Natl. Acad. Sci. U.S.A.*, 106:20740–20745, 2009.

[106] Sara Vaiana, Robert B. Best, Wai-Ming Yau, William A. Eaton, and James Hofrichter. Evidence for a partially structured state of the amylin monomer. *Biophys. J.*, 97:2948–2957, 2009.

[107] Robert B. Best and Gerhard Hummer. Optimized molecular dynamics force fields applied to the helix-coil transition of polypeptides. *J. Phys. Chem. B*, 113:9004–9015, 2009.

[108] Robert B. Best and Gerhard Hummer. Unfolding the secrets of calmodulin. *Science*, 323:593–594, 2009.

[109] Jeetain Mittal and Robert B. Best. Thermodynamics and kinetics of protein folding under confinement. *Proc. Natl. Acad. Sci. U. S. A.*, 105:20233–20238, 2008.

[110] Irina G. Tikhonova, Robert B. Best, Stanislav Engel, Marvin C. Gershengorn, Gerhard Hummer, and Stefano Costanzi. Atomic insights into rhodopsin activation from a dynamic model. *J. Am. Chem. Soc.,*, 130:10141–10149, 2008.

[111] Robert B. Best, Nicolae-Viorel Buchete, and Gerhard Hummer. Are current molecular dynamics force fields too helical? *Biophys. J.*, 95:L07–L09, 2008.

[112] Adrian Turjanski, Robert B. Best, J. Silvio Gutkind, and Gerhard Hummer. Binding-induced folding of a natively unstructured transcription factor. *PLoS Comp. Biol.*, 4(4):1000060, 2008.

[113] Robert B. Best and Gerhard Hummer. Protein folding kinetics under force from molecular simulation. *J. Am. Chem. Soc.*, 130:3706–3707, 2008.

[114] Robert B. Best, Emanuele Paci, Gerhard Hummer, and Olga K. Dudko. Pulling direction as a reaction coordinate for the mechanical unfolding of single molecules. *J. Phys. Chem. B*, 112:5968–5976, 2008.

[115] Kate S. Billings, Robert B. Best, Trevor J. Rutherford, and Jane Clarke. Crosstalk between the protein surface and hydrophobic core in a core-swapped fibronectin type III domain. *J. Mol. Biol.*, 375:560–571, 2008.

[116] Robert B. Best, Kusai A. Merchant, Irina V. Gopich, Benjamin Schuler, Ad Bax, and William A. Eaton. Effect of flexibility and cis residues in single-molecule FRET studies of polyproline. *Proc. Natl. Acad. Sci. U.S.A.*, 104:18964–18969, 2007.

[117] Sean P. Ng, Kate S. Billings, Tomoo Ohashi, Mark D. Allen, Robert B. Best, Lucy G. Randles, Harold P. Erickson, and Jane Clarke. Designing an extracellular matrix protein with enhanced mechanical stability. *Proc. Natl. Acad. Sci. U. S. A.*, 104:9633–9637, 2007.

[118] Kusai A. Merchant, Robert B. Best, John M. Louis, Irina V. Gopich, and William A. Eaton. Characterizing the unfolded states of proteins using single molecule FRET spectroscopy and molecular simulations. *Proc. Natl. Acad. Sci. U.S.A.*, 104:1528–1533, 2007.

[119] Robert B. Best, Kresten Lindorff-Larsen, Mark A. DePristo, and Michele Vendruscolo. Relation between native ensembles and experimental structures of proteins. *Proc. Natl. Acad. Sci. U.S.A.*, 103:10901–10906, 2006.

[120] Christian D. Geierhaas, Robert B. Best, Emanuele Paci, Michele Vendruscolo, and Jane Clarke. Structural comparison of the two alternative transition states for folding of TI I27. *Biophys. J.*, 91:263–275, 2006.

[121] Robert B. Best and Gerhard Hummer. Diffusive model of protein folding dynamics with Kramers turnover in rate. *Phys. Rev. Lett.*, 96:228104, 2006.

[122] Christopher J. Francis, Kresten Lindorff-Larsen, Robert B. Best, and Michele Vendruscolo. Characterization of the residual structure in the unfolded state of the $\Delta 131\Delta$ fragment of staphylococcal nuclease. *Proteins*, 65:145–152, 2006.

[123] Robert B. Best and Michele Vendruscolo. Structural interpretation of equilibrium hydrogen exchange protection factors in proteins: characterization of the large conformational fluctuations in the native state of CI2. *Structure*, 14:97–106, 2006.

[124] Kresten Lindorff-Larsen, Robert B. Best, and Michele Vendruscolo. Interpreting dynamically-averaged scalar couplings in proteins. *J. Biomol. NMR*, 32:273–280, 2005.

[125] Robert B. Best, Yng-Gwei Chen, and Gerhard Hummer. Slow protein conformational dynamics from multiple experimental structures: the helix/sheet transition of Arc repressor. *Structure*, 13:1755–1763, 2005.

[126] Robert B. Best and Gerhard Hummer. Comment on "Force-clamp spectroscopy monitors the folding trajectory of a single protein". *Science*, 308:498b, 2005.

[127] Robert B. Best and Gerhard Hummer. Reaction coordinates and rates from transition paths. *Proc. Natl. Acad. Sci. U. S. A.*, 102(19):6732–6737, 2005.

[128] Robert B. Best, Jane Clarke, and Martin Karplus. What contributions to protein sidechain dynamics are probed by NMR experiments? A molecular dynamics simulation analysis. *J. Mol. Biol.*, 349:185–203, 2005.

[129] Kresten Lindorff-Larsen, Robert B. Best, Mark A. DePristo, Christopher M. Dobson, and Michele Vendruscolo. Simultaneous determination of protein structure and dynamics. *Nature*, 433:128–132, 2005.

[130] B. Trevor Sewell, Robert B. Best, Shaoxia Chen, Alan M. Roseman, George W. Farr, Arthur L. Horwich, and Helen R. Saibil. A mutant chaperonin with rearranged inter-ring electrostatic contacts and temperature-sensitive dissociation. *Nat. Struct. Mol. Biol.*, 11(11):1128–1133, 2004.

[131] Robert B. Best and Michele Vendruscolo. Determination of ensembles of protein structures consistent with NMR order parameters. *J. Am. Chem. Soc.*, 126(26):8090–8091, 2004.

[132] Robert B. Best, Jane Clarke, and Martin Karplus. The origin of protein sidechain order parameter distributions. *J. Am. Chem. Soc.*, 126(25):7734–7735, 2004.

[133] Robert B. Best, Trevor J. Rutherford, Stefan M. V. Freund, and Jane Clarke. Hydrophobic core fluidity of homologous protein domains: relation of side-chain dynamics to core composition and packing. *Biochemistry*, 43(5):1145–1155, 2004.

[134] Robert B. Best, Susan B. Fowler, José Luis Toca-Herrera, Annette Steward, Emanuele Paci, and Jane Clarke. Mechanical unfolding of a titin Ig domain: (2) Structure of transition state revealed by combining AFM, protein engineering and molecular dynamics simulations. *J. Mol. Biol*, 330(4):867–877, 2003.

[135] Philip M. Williams, Susan B. Fowler, Robert B. Best, José Luis Toca-Herrera, Kathryn Scott, Annette Steward, and Jane Clarke. Hidden complexity in the mechanical properties of titin. *Nature*, 422:446–449, 27 March 2003.

[136] Robert B. Best, David J. Brockwell, José L. Toca-Herrera, Anthony W. Blake, D. Alistair Smith, Sheena E. Radford, and Jane Clarke. Force mode AFM as a tool for protein folding studies. *Anal. Chim. Acta.*, 479(1):87–105, 2003.

[137] Robert B. Best, Graham E. Jackson, and Kevin J. Naidoo. An NMR investigation into the dynamics of panose, an alpha(1→4) and alpha(1→6)-linked trisaccharide. *Spec. Lett.*, 5:625–632, 2002.

[138] Susan B. Fowler, Robert B. Best, José L. Toca-Herrera, Trevor J. Rutherford, Annette Steward, Emanuele Paci, Martin Karplus, and Jane Clarke. Mechanical unfolding of a titin Ig domain: (1) Structure of unfolding intermediate revealed by combining AFM, molecular dynamics simulations, NMR and protein engineering. *J. Mol. Biol.*, 322:841–849, 2002.

[139] Robert B. Best, Susan B. Fowler, José L. Toca-Herrera, and Jane Clarke. A simple method for probing the mechanical unfolding pathway of proteins in detail. *Proc. Natl. Acad. Sci. U.S.A.*, 99(19):12143–12148, 2002.

[140] Robert B. Best and Jane Clarke. What can atomic force microscopy tell us about protein folding? *Chem. Comm.*, (3):183–192, 2002.

[141] Robert B. Best, Bin Li, Annette Steward, Valerie Daggett, and Jane Clarke. Can non-mechanical proteins withstand force? Stretching barnase by atomic force microscopy and molecular dynamics simulation. *Biophys. J.*, 81(4):2344–2356, 2001.

[142] Robert B. Best, Graham E. Jackson, and Kevin J. Naidoo. Modelling the $\alpha(1 \rightarrow 6)$ branch point of amylopectin. *J. Phys. Chem. B*, 106(19):5091–5098, 2002.

[143] Robert B. Best, Graham E. Jackson, and Kevin J. Naidoo. Molecular dynamics and NMR study of the $\alpha(1 \rightarrow 4)$ and $\alpha(1 \rightarrow 6)$ glycosidic linkages: maltose and isomaltose. *J. Phys. Chem. B*, 105(20):4742–4751, 2001.

## Book Chapters

Atomistic force fields for proteins. In "Biomolecular Simulations", Springer, 2019 (Editors: Massimiliano Bonomi and Carlo Camilloni)

Coarse-grained simulations of intrinsically disordered proteins. In "Computational Approaches to Protein Dynamics From Quantum to Coarse-Grained Methods", Taylor and Francies, 2015 (Editor: Monika Fuxreiter).