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| Nathan Andrew Baker  Curriculum Vitae  7 August 2016 | PO Box 999, MSID K7-90  Richland, WA 99354  +1 509 375 3997  [nathan.baker@pnnl.gov](mailto:nathan.baker@pnnl.gov)  <http://go.usa.gov/czB5G> |

Nathan Baker, Ph.D. is the Director of the Advanced Computing, Mathematics, and Data Division at Pacific Northwest National Laboratory (PNNL) and a Visiting Faculty member at Brown University. His research interests include the development of new algorithms and mathematical methods in biophysics, nanotechnology, and informatics. Current research projects include [computational methods for modeling solvation in biomolecular systems](http://www.poissonboltzmann.org/), [mathematical methods for mesoscale materials modeling](http://www.pnnl.gov/computing/cm4), and [development of new methods for signature discovery](http://signatures.pnnl.gov). His research is primarily funded by the National Institutes of Health and the Department of Energy.

# Experience

2016–present **Director**, Advanced Computing, Mathematics, and Data Division, Pacific Northwest National Laboratory, Richland, WA.

2015–present **Visiting Professor**, Division of Applied Mathematics, Brown University, Providence, RI.

2012–2016 **Laboratory Fellow**, Computational and Statistical Analytics Division, Pacific Northwest National Laboratory, Richland, WA.

2013–2015 **Technical Group Manager**, Applied Statistics and Computational Modeling Group, Pacific Northwest National Laboratory, Richland, WA.

2010–2012 **Chief Scientist**, Computational and Statistical Analytics Division, Pacific Northwest National Laboratory, Richland, WA.

2006–2010 **Associate Professor** (tenured), Dept of Biochemistry and Molecular Biophysics, Washington University, St Louis, MO.

2002–2006 **Assistant Professor**, Dept of Biochemistry and Molecular Biophysics, Washington University, St Louis, MO.

# Education

2001–2002 **Postdoctoral Researcher**, Dept of Chemistry and Biochemistry, University of California San Diego, La Jolla, CA.

1997–2001 **PhD**, Physical Chemistry, University of California San Diego, La Jolla, CA.

1993–1997 **BS**, Chemistry, University of Iowa, Iowa City, IA, Honors and highest distinction.

# Selected honors and awards

2012 **Fellow**, American Association for the Advancement of Science.

2010 Cancer Biomedical Informatics Grid (caBIG) Connecting Collaborators Award, National Cancer Institute.

2007 Hewlett-Packard Junior Faculty Excellence Award, American Chemical Society.

2004 **Research Fellowship**, Alfred P Sloan Foundation.

2001 **All-hands Meeting Student Poster Award**, National Partnership Advanced Computational Infrastructure.

2001 Kamen Award for Outstanding Thesis in the Biological Sciences, Univ California San Diego.

2000 **IBM Student Award in Computational Chemistry**, First Place, American Chemical Society.

1999 **Predoctoral Fellowship**, Burroughs-Wellcome La Jolla Interfaces in Science Program.

1998-1999 **Letters of Commendation for Teaching**, Univ California San Diego.

1997 **Predoctoral Fellowship**, Howard Hughes Medical Institute.

1997 **Collegiate Scholar**, Univ Iowa.

1997 **Member**, Phi Beta Kappa, Univ Iowa.

1997 Undergraduate Liberal Arts Commencement Speaker, Univ Iowa.

1995 **Undergraduate Fellowship**, Barry M Goldwater Foundation.

# Service

## Selected extramural service

2014-2017 **Associate Editor**, Biophysical Journal, Biophysical Society.

2016-present **Executive Committee Member**, Carbon Capture Simulation Initiative, Department of Energy.

2015-2016 **External Advisory Board Member**, Visual Analytics for sense-making in Criminal Intelligence analysis (VALCRI) Project, European Commission.

2014-present **Editorial Board member**, Scientific Data, Nature Publishing Group.

2012-2016 **Member**, Macromolecular Structure and Function D Study Section, National Institutes of Health.

2016 **Reviewer**, MIT Sea Grants, Massachusetts Institute of Technology.

2014-2016 **Organizing committee member**, Conference on Data Analysis (CoDA).

2014-2015 **Reviewer**, INCITE Biological Sciences Review Panel, Advanced Scientific Computing Research, Dept of Energy.

2015 **Panelist**, National Strategic Computing Initiative Panel, HPC User Forum meeting.

2015 **Reviewer**, J9BA Life Sciences Red Team Review, Defense Threat Reduction Agency.

2015 **Advisory board member**, Data Management and Analysis Advisory Board, Novozymes.

2014 **Scientific Advisory Board member**, eNanoMapper Project, European Commission.

2012-2014 **Co-Chair**, Nanotechnology Databases and Ontologies, US-EU Communities of Research, OSTP National Nanotechnology Coordinating Office.

2011-2014 **Editor-in-Chief**, Computational Science and Discovery, Institute of Physics.

2009-2014 **Editorial Board member**, Computational Science and Discovery, Institute of Physics.

2009-2014 **Chair**, E56.01 Nanotechnology Subcommittee on Informatics and Terminology, ASTM.

2008-2014 **Section Editor**, Annual Reports in Computational Chemistry, American Chemical Society.

2008-2014 **Editorial Board member**, Biophysical Journal, Biophysical Society.

2008-2014 **Member**, Faculty of 1000 Biology.

2005-2014 **Ad hoc member**, Various study sections, National Institutes of Health.

2013 **Reviewer**, Progress in Research on Environmental, Health, and Safety Aspects of Engineered Nanomaterials, National Academy of Sciences.

2012-2013 **Member**, Working Group 1, Nomenclature and Terminology, U.S. Technical Advisory Group, ANSI, ISO International Organization for Standardization.

2011-2013 **Organizing committee member**, Nanoinformatics Workshop.

2011-2013 **Organizing committee member**, Protein Electrostatics Workshop, Telluride Science Research Center.

2010-2013 **Advisory committee member**, Nanomaterial Registry, RTI International & National Institutes of Health.

2009-2013 **Working group lead**, Nanotechnology Working Group, caBIG Integrated Cancer Research Workspace, National Cancer Institute.

2008-2013 **Member**, Nanotechnology Working Group, caBIG Integrated Cancer Research Workspace, National Cancer Institute.

2007-2013 **Member**, Committee for Professional Opportunities for Women, Biophysical Society.

2006-2013 **Reviewer**, National Science Foundation.

2012 **Panelist**, National Academies Board on Environmental Studies and Toxicology Research Progress on Environmental, Health, and Safety Aspects of Nanotechnology Workshop, National Academies of Science.

2012 **Member**, Program Committee, caBIG Annual Meeting, National Cancer Institute.

2010-2012 **Member**, Public Affairs Committee, Biophysical Society.

2010 **Advisory board member**, Integrated Graduate Education and Research Training (IGERT) in Health-Assistive Smart Environments, Washington State Univ.

2008-2010 **Topic Page contributor**, Scirus.

2008 **Panelist**, “Transition from Postdoc to Faculty” Workshop, Biophysical Society.

2008-2009 **Co-organizer**, 23rd Annual Meeting, Gibbs Society for Biothermodynamics.

2006-2008 **Member**, Nanotechnology Alliance Informatics Working Group, National Cancer Institute.

2005-2008 **Member**, Program Committee, Biophysical Society.

2007 **Organizer and chair**, Early Careers Panel Discussion: Negotiating the Transition to Non-Traditional Careers, Biophysical Society.

2004-2007 **Member**, Early Careers Committee, Biophysical Society.

## Selected intramural service

2016-present **Member**, Compensation Manager search committee, Pacific Northwest Natl Lab.

2016-present **Member**, Scientist & Engineer Job Family review panel, Pacific Northwest Natl Lab.

2016-present **Executive secretary**, Integrated Plant, Atmosphere, & Soil System Initiative, Pacific Northwest Natl Lab.

2014-present **Lecturer and panelist**, Scientist & Engineer Development Program, Pacific Northwest Natl Lab

2015 **Panelist**, Council of Fellows “Increasing Scientific Impact” session, Pacific Northwest Natl Lab.

2015 **Member**, Interdisciplinary Applied Sciences Planning Committee, Washington State Univ Tri-Cities and Pacific Northwest Natl Lab.

2015-present **Advisory committee member**, Microbes in Transition Initiative Advisory Committee, Pacific Northwest Natl Lab.

2014-present **Executive secretary**, Analysis in Motion Initiative, Pacific Northwest Natl Lab.

2014-2016 **Chair**, PNNL Institutional Computing Steering Committee, Pacific Northwest Natl Lab.

2015 **Co-chair**, National Strategic Computing Initiative Planning Committee, co-chair, Pacific Northwest Natl Lab.

2014-present **Advisory committee member**, Analysis in Motion Initiative Advisory Committee, Pacific Northwest Natl Lab.

2013-present **Reviewer**, ASCR Early Career pre-proposals, Pacific Northwest Natl Lab.

2013-2016 **Member**, Council of Fellows Executive Committee, Pacific Northwest Natl Lab.

2012-2015 **Lead**, Signature Discovery Initiative, Pacific Northwest Natl Lab.

2011-present **Reviewer**, HHS LDRD proposals, Pacific Northwest Natl Lab.

2010-present **Chief Scientist**, Signature Discovery Initiative, Pacific Northwest Natl Lab.

2014-2015 **Judge**, Postdoc Symposium, Pacific Northwest Natl Lab.

2015 **Presenter**, Computing Assessment Committee, Pacific Northwest Natl Lab.

2015 **Member**, Physical and Computational Sciences Directorate Strategy Committee, Pacific Northwest Natl Lab.

2015 **Advocate**, Proposal-Writing Workshop development, Pacific Northwest Natl Lab.

2013-2015 **Presenter**, Publishing Workshop, National Security Directorate, Pacific Northwest Natl Lab.

2011-2015 **Lead**, Signatures Community of Interest Network, Pacific Northwest Natl Lab.

2015 **Member**, Diversity Internal Oversight Committee, Pacific Northwest Natl Lab.

2015 **Member**, Employee Time Reporting Reform Committee, Pacific Northwest Natl Lab.

2015 **Member**, Computational Materials Science Red Team, Pacific Northwest Natl Lab.

2011-2014 **Reviewer**, DHHS Sector LDRD Proposals, Pacific Northwest Natl Lab.

2012-2014 **Reviewer**, BES pre-proposals, Pacific Northwest Natl Lab.

2005-2010 **Director**, Siteman Center for Cancer Nanotechnology Excellence Biocomputing Core, Washington Univ St Louis

2007-2010 **Member**, Program and Student Affairs Committee, Division of Biology and Biomedical Sciences, Washington Univ St Louis.

2009-2010 **Member**, Nominating Committee, Biophysical Society.

2007-2010 **Director**, Computational and Molecular Biophysics graduate program, Washington Univ St Louis

2004-2010 **Steering committee member**, Computational and Molecular Biophysics graduate program, Washington Univ St Louis.

2008 **Chair**, Scientific Collaboration Panel Discussion, Annual Conference on Effective Research Management, Washington Univ St Louis.

2008 **Co-organizer**, Bridging Research and Teaching Workshop: Innovation at the Crossroads of Chemistry, Physics, and Biology, Washington Univ St Louis.

2003-2008 **Seminar co-organizer**, Center for Computational Biology, Washington Univ St Louis.

2007 **Member**, Education Planning Committee, Division of Biology and Biomedical Sciences, Washington Univ St Louis.

2004-2007 **Member**, Admissions Committee, Division of Biology and Biomedical Sciences, Washington Univ St Louis.

2004-2007 **Mentor**, Students and Teachers as Researchers (STARS) program, Univ Missouri St Louis.

2006-2007 **Member**, Faculty Search Committee, Dept of Mechanical and Aerospace Engineering, Washington Univ St Louis.

2006 **Member**, Liaison Committee on Medical Education and IT, School of Medicine, Washington Univ St Louis.

2006 **Co-organizer**, ICAM/Center for Computational Biology Multiscale Interactions and Dynamics in Biological Systems Workshop, Washington Univ St Louis.

2004 **Member**, Oversight Committee, Center for Scientific Parallel Computing, Washington Univ St Louis.

## Selected community service

2016 **Judge**, Mathematics, Engineering, Science Achievement (MESA) USA Engineering Design Competition, Pasco, WA.

2014-present **Communications representative**, Hansen Park Homeowners Association, Kennewick, WA.

2012-2014 **Webmaster**, Hansen Park Homeowners Association, Kennewick, WA.

2010-2011 **Den leader**, Cub Scouts, Kennewick, WA.

2006-2010 **Member**, Technology Committee, Our Lady of Lourdes School, St Louis, MO.

2005-2010 **Webmaster**, Ethical Society Nursery School, St Louis, MO.

## Selected manuscript review service

Acta Crystallographica, Annals of Biomedical Engineering, Biochemistry, Biochimica et Biophysica Acta - Biomembranes, Bioinformatics, Biomechanics and Modeling in Mechanobiology, Bioorganic and Medicinal Chemistry Letters, Biophysical Chemistry, Biophysical Journal, Biopolymers, BMC Biophysics, Cancer Biomarkers, Communications in Computational Physics, Computational Science and Discovery, Integrative Biology, Journal of Chemical Information and Modeling, Journal of Chemical Physics, Journal of Chemical Theory and Computation, Journal of Computational Chemistry, Journal of Computational Physics, Journal of Computer-Aided Molecular Design, Journal of Electrostatics, Journal of General Physiology, Journal of Lipid Research, Journal of Mathematical Analysis and Applications, Journal of Mathematical Biology, Journal of Molecular Biology, Journal of Molecular Graphics and Modeling, Journal of Neurophysiology, Journal of Physical Chemistry, Journal of Physical Chemistry B, Journal of Physical Chemistry C, Journal of Physical Chemistry Letters, Journal of Physics Condensed Matter, Journal of the American Chemical Society, Journal of Theoretical Biology, Molecular Informatics, Nature Nanotechnology, Nucleic Acids Research, Physical Biology, Physical Chemistry Chemical Physics, PLoS Computational Biology, PLoS ONE, PMC Biophysics, Proceedings of the National Academy of Sciences, Protein Engineering, Protein Science, Proteins, SIAM Journal on Applied Mathematics, SIAM Review, Soft Matter, Structure, Theoretical Chemistry Accounts.

## Selected grant proposal reviews

American Chemical Society Petroleum Research Fund, National Institutes of Health, National Science Foundation, United States Civilian Research and Development Foundation, United States-Israel Binational Science Foundation, Defense Threat Reduction Agency, United States Air Force Office of Science and Research, Dept of Energy Advanced Scientific Computing Research.

# Selected funding

2012-2016 **PNNL lead**, Collaboratory on Mathematics for Mesoscopic Modeling of Materials (FWP 63024), DOE ASCR.

2004-2017 **PI**, APBS: Nanoscale biomolecular electrostatics software (R01 GM069702), NIH NIGMS.

2012-2016 **co-PI**, DNA-DNA interactions with atomic detail (R01 GM099450), NIH NIGMS.

2011-2014 **co-I**, Mechanism of oxysterol activation of membrane cholesterol (R01 HL067773), NIH NHLBI.

2012-2013 **PI**, ISA-TAB curation of electrostatic data, OpenEye Software.

2010-2013 **co-I**, Characterization/bioinformatics-modeling of nanoparticle-complement interactions (U01 NS073457), NIH NINDS.

2009-2013 **co-PI**, Collaborative research: Geometric flow approach to implicit solvation modeling (R01 GM090208-01), NIH NIGMS.

2004-2013 **co-I**, National Biomedical Computation Resource (P41 RR0860516), NIH NCRR.

2008-2011 **DBP PI**, Cancer Nanotechnology Knowledgebase for Nanoparticle Analysis and Design (U54 HG004028), NIH NHGRI.

2008-2011 **PI**, caBIG Integrative Cancer Research Workspace (GS-35F-0306J), NIH NCI subcontract.

2007-2010 **PI**, caNanoLab Data Submission Support (N01-CN-12400), NIH NCI subcontract.

2005-2010 **Core PI**, The Siteman Cancer Center Nanotechnology Excellence at Washington Univ Biocomputing Core (U54 CA11934205).

2008-2010 **co-I**, New Inhibitors of Acetylcholinesterase that Block Inactivation by Organophosphates (HDTRA1-08-C-0015), DoD DTRA.

2007-2009 **co-I**, Loss of Vascular Control in Pediatric Lung Injury: Disruption of NO Biotransport by Oxidative Stress, Children's Discovery Institute.

2006-2009 **co-PI**, Allosteric Regulation of the Nickel-dependent NikR Repressor (MCB-0520877), NSF MCB.

2005-2007 **PI**, Molecular Engineering of Thrombin-Based Nanocatalysts, National Academies Keck Futures Initiative.

# Mentoring

## Postdoctoral researchers

2013-2015 Huan Lei, Pacific Northwest Natl Lab.

2015 Xiu Yang, Pacific Northwest Natl Lab.

2011-2013 Mike Daily, Pacific Northwest Natl Lab.

2011-2013 Emilie Hogan, Pacific Northwest Natl Lab.

2008-2010 Marcelo Marucho, Washington Univ St Louis.

2006-2010 Dennis Thomas, Washington Univ St Louis.

2005-2007 Feng Dong, Washington Univ St Louis.

2002-2006 Yuhua Song, Washington Univ St Louis.

2002-2003 Seongeun Yang, Postdoc, Washington Univ St Louis.

## Graduate students

2015-2016 Mingge Deng, Brown Univ.

2010 Marc Sherman, Washington Univ St Louis.

2006-2010 Brett Olsen, Washington Univ St Louis.

2005-2010 Sunjoo Lee, Washington Univ St Louis.

2003-2009 Rachel Rice, Washington Univ St Louis.

2003-2009 Michael Bradley, Washington Univ St Louis.

## Undergraduate researchers

2009-2010 Arjun Bahl, Washington Univ St Louis.

2009 Aditya Nath, Washington Univ St Louis.

2009 Mark Rosenberg, Washington Univ St Louis.

2007-2009 Stephen Gradwohl, Washington Univ St Louis.

2008 Sechin Jain, Washington Univ St Louis.

2007-2008 Tom Richner, Washington Univ St Louis.

2005 Jeff Poskin, Washington Univ St Louis.

2002-2006 Jason Wagoner, Washington Univ St Louis.

## Other researchers

2015-present Ilke Arslan, Staff, Pacific Northwest Natl Lab.

2015-present Nathan Hodas, Staff, Pacific Northwest Natl Lab.

2015-present Juan Brandi, Postbac researcher, Pacific Northwest Natl Lab.

2015-2016 Maria Tartakovsky, High school researcher, Pacific Northwest Natl Lab.

2015-present Huan Lei, Staff, Pacific Northwest Natl Lab.

2015-present Xiu Yang, Staff, Pacific Northwest Natl Lab.

2014-2016 Luke Gosink, Staff, Pacific Northwest Natl Lab.

2014-2015 Peter Li, High school researcher, Pacific Northwest Natl Lab.

2015 Shadya Maldonado, Postbac researcher, Pacific Northwest Natl Lab.

2014-2015 Minju Chun, High school researcher, Pacific Northwest Natl Lab.

2013-present Landon Sego, Staff, Pacific Northwest Natl Lab.

2013-present Paul Bruillard, Staff, Pacific Northwest Natl Lab.

2013-present Courtney Corley, Staff, Pacific Northwest Natl Lab.

2012-2013 Max Li, High school researcher, Pacific Northwest Natl Lab.

2010-2011 Shy Brown, Postbac, Pacific Northwest Natl Lab.

2010-2011 Tyler Harmon, Postbac, Pacific Northwest Natl Lab.

2008-2010 Michal Lijowksi, Bioinformatics curator, Washington Univ St Louis.

2007-2010 Yong Huang, Programmer, Washington Univ St Louis.

2007-2010 Samir Unni, High school and undergraduate researcher, Washington Univ St Louis.

2006-2010 Dave Gohara, Programmer, Washington Univ St Louis.

2006-2008 Peter Jones, Programmer, Washington Univ St Louis.

2005 Eric Mintun, High school researcher, Washington Univ St Louis.

2004 Prachi Mayenkar, High school researcher, Washington Univ St Louis.

2002-2006 Todd Dolinsky, Programmer, Washington Univ St Louis.

# Current Professional memberships

American Chemical Society, Association for Computing Machinery, Biophysical Society, IEEE, Society for Industrial and Applied Mathematics.

# Selected presentations

2016 N Baker. Univ Illinois Computational Science and Engineering Annual Symposium, Keynote talk.

2015 NA Baker\*, H Lei, X Yang, B Zheng, G Lin. Brown Univ, Division of Applied Mathematics Seminar, Invited talk.

2015 NA Baker\*, H Lei, X Yang, B Zheng, G Lin. Multiple faces of biomolecular electrostatics workshop, Mathematical Biosciences Institute, Invited talk.

2015 NA Baker. IDC HPC User Forum NSCI Panel Discussion, Panelist.

2015 C Dowling, T Pulsipher, L Gosink, S-A Sansone, NA Baker\*. Biophysical Society Annual Meeting, Invited talk.

2014 NA Baker. VALCRI seminar, Linköping Univ, Invited talk.

2014 NA Baker. Materials Frontiers to Empower Quantum Computing, LANL workshop, Invited talk.

2014 NA Baker. SCIX Conference, Reno, NV, Keynote.

2014 NA Baker. Univ Pittsburgh, Computational & Systems Biology Seminar, Invited talk.

2014 NA Baker. Univ Maryland Baltimore County Seminar, Invited talk.

2014 NA Baker. Conference on Data Analysis (CoDA 2014), Invited talk.

2014 NA Baker. Lawrence Livermore Natl Lab Lab Days, Invited talk.

2013 J Chun, DG Thomas, M Daily, L Gosink, E Hogan, GW Wei, NA Baker\*. Univ Washington Nanotechnology Seminar, Invited talk.

2013 J Chun, DG Thomas, M Daily, L Gosink, E Hogan, GW Wei, NA Baker\*. Third Biological Diffusion and Brownian Dynamics Brainstorm: BDBDB3, Invited talk.

2013 C Dowling, S-A Sansone, NA Baker\*. Gordon Research Conference Computer-Aided Drug Design, Invited talk.

2013 L Gosink, E Hogan, T Pulsipher, NA Baker\*. Telluride Science Research Center Protein Electrostatics Workshop, Invited talk.

2013 J Chun, DG Thomas, M Daily, L Gosink, E Hogan, GW Wei, NA Baker\*. Tsinghua Univ Chemistry Seminar, Invited talk.

2013 J Chun, DG Thomas, M Daily, L Gosink, E Hogan, GW Wei, NA Baker\*. Wuhan Univ Physics Seminar, Invited talk.

2013 J Chun, DG Thomas, M Daily, L Gosink, E Hogan, GW Wei, NA Baker\*. International Conference on Mathematical Modeling and Computation, Invited talk.

2013 J Chun, DG Thomas, M Daily, L Gosink, E Hogan, GW Wei, NA Baker\*. Chinese Academy of Sciences Applied Mathematics Seminar, Invited talk.

2013 NA Baker. Arizona State Univ Biophysics Seminar, Invited talk.

2013 NA Baker, H Rauscher. Society of Toxicology Annual Meeting presentation, Invited talk.

2013 NA Baker. Acoustics Dept, Univ Washington Applied Physics Laboratory, Invited talk.

2013 NA Baker. Microproducts Breakthrough Institute Seminar, Oregon State Univ, Invited talk.

2012 NA Baker. EU-US: Bridging NanoEHS Research Efforts, Invited talk.

2012 NA Baker. National Academies Research Progress on Environmental, Health, and Safety Aspects of Nanotechnology, Invited talk.

2012 NA Baker. Science of Multi-INT Workshop, Contributed talk.

2012 J Chun, DG Thomas, GW Wei, NA Baker\*. American Chemical Society National Meeting, Invited talk.

2012 DG Thomas, J Chun, GW Wei, NA Baker\*. Georgia Tech Mathematics Seminar, Invited talk.

2012 NA Baker. EU-US Communities of Research in Nanotechnology Databases and Ontology, Invited talk.

2012 DG Thomas, A Chappell, E Freund, S Gaheen, S Harper, JD Klemm, DS Paik, NA Baker\*. ICSU-CODATA Paris Meeting on Nanotechnology Informatics, Invited talk.

2012 NA Baker. National Geospatial-Intelligence Agency Technical Exchange, Invited talk.

2011 DG Thomas, A Chappell, E Freund, S Gaheen, S Harper, JD Klemm, DS Paik, NA Baker\*. Nanoinformatics 2011, Invited talk.

2011 DG Thomas, A Chappell, E Freund, S Gaheen, S Harper, JD Klemm, DS Paik, NA Baker\*. American Society for Nanomedicine Annual Meeting, Invited talk.

2011 DG Thomas, A Chappell, E Freund, S Gaheen, S Harper, JD Klemm, DS Paik, NA Baker\*. SRC-SEMATECH Environmental Research Center, Invited talk.

2011 DS Thomas, J Chun, Z Chen, G Wei, NA Baker\*. MBI Modeling and Computation of Biomolecular Structure and Dynamics, Invited talk.

2011 DS Thomas, J Chun, Z Chen, G Wei, NA Baker\*. Univ Washington Applied Mathematics Seminar, Invited talk.

2011 BN Olsen, Schlesinger PH, DS Ory, NA Baker\*. American Chemical Society National Meeting, Invited talk.

2011 DS Paik, NA Baker\*. National Center for Biomedical Ontology Annual Meeting, Invited talk.

2010 NA Baker. Nanoinformatics 2010, Invited talk.

2010 N Baker\*, others. caBIG Annual Meeting, Contributed poster.

2010 S Gaheen\*, others. caBIG Annual Meeting, Contributed poster.

2010 NA Baker. Univ North Carolina Chapel Hill Physical Chemistry Seminar, Invited talk.

2010 NA Baker. Washington Univ School of Medicine Dept. of Genetics Seminar, Invited talk.

2010 NA Baker. Pacific Northwest Natl Lab seminar, Invited talk.

2009 NA Baker. National Cancer Institute Nanotechnology Alliance Meeting, Co-chair and invited talk.

2009 NA Baker. Univ California Davis, Dept of Chemistry Seminar, Invited talk.

2009 SJ Lee\*, BN Olsen, Schlesinger PH, NA Baker. Gibbs Conference on Biothermodynamics, Invited talk.

2009 B Olsen\*, P Schlesinger, N Baker. Gibbs Conference on Biothermodynamics, Contributed poster.

2009 MJ Bradley, RL Rice, NA Baker\*. Biomolecular Modeling and Simulations, Israel Science Foundation Workshop, Invited talk.

2009 BN Olsen, NA Baker\*. Anesthesiology Research Unit Seminar, Washington Univ St Louis, Invited talk.

2009 NA Baker. caBIG Integrative Cancer Research Workspace Meeting, Invited talk.

2009 SJ Lee\*, NA Baker. National Biomedical Computation Resource Summer Institute, Invited talk.

2009 DG Thomas, RV Pappu, NA Baker\*. International Conference on Biomedical Ontology, Contributed poster.

2009 DG Thomas, RV Pappu, NA Baker\*. caBIG Annual Meeting, Contributed poster.

2009 Baker\* NA\*, others. caBIG Annual Meeting, Contributed poster.

2009 T Carstensen, JE Nielsen, Y Huang, NA Baker. TSRC Protein Electrostatics Workshop, Invited talk.

2009 NA Baker. National Center for Biomedical Ontology Seminar, Stanford Univ, Invited talk.

2009 NA Baker. Bioinformatics Institute, Agency for Science, Technology, and Research (A\*STAR Biopolis), Singapore, Visiting scientist lecture series and workshop.

2009 NA Baker. Univ Texas at Austin ICES Seminar, Invited talk.

2009 NA Baker\*, K Tai. Specialised Training Workshop on Electrostatics Calculations, Collaborative Computational Project for Biomolecular Simulation, Invited workshop.

2009 JA Wagoner, F Dong, NA Baker\*. Biomolecular simulation 2009, Collaborative Computational Project for Biomolecular Simulation, Plenary talk.

2008 JA Wagoner, F Dong, NA Baker\*. Solvation Workshop, Institute for Mathematics and its Applications, Invited talk.

2008 NA Baker. Univ Illinois Materials Science and Engineering Seminar, Invited talk.

2008 NA Baker. Rensselaer Polytechnic Institute Seminar, Invited talk.

2008 D Paik\*, others. Radiological Society of North America 94th Scientific Sessions, Contributed poster.

2008 RL Rice, NA Baker\*. Gibbs Conference on Biothermodynamics, Contributed poster.

2008 NA Baker. Univ Iowa Physical Chemistry Seminar, Invited talk.

2008 NA Baker, D Sept\*. Center for Theoretical Biological Physics Summer Workshop, Univ California San Diego, Invited talk.

2008 NA Baker. Seminar, Dept of Biological Science, Florida State Univ, Invited talk.

2008 J Wagoner, F Dong, NA Baker\*. Protein Electrostatics Workshop, Telluride Science Research Center, Invited talk.

2008 J Wagoner, F Dong, NA Baker\*. Computational Chemistry Gordon Research Conference, Invited talk.

2008 DG Thomas, PL Jones, RV Pappu, NA Baker. caBIG Annual Meeting, Invited talk.

2008 J Wagoner, F Dong, NA Baker\*. Biopolymers Gordon Research Conference, Invited talk.

2008 EA Hahn-Dantona\*, MJ Fritts, AK Patri, NA Baker, DG Thomas, FW Hartel. Nanobiology Think Tank Meeting, Contributed poster.

2008 M Bradley, R Rice, E Di Cera, N Baker\*. American Chemical Society National Meeting, Invited talk.

2008 J Wagoner, F Dong, D Cerutti, JA McCammon, NA Baker. American Chemical Society National Meeting, Invited talk.

2008 NA Baker. Seminar, Conway Institute, Univ College Dublin, Invited talk.

2008 NA Baker. Mechanical Engineering Seminar, Washington Univ, Invited talk.

2008 NA Baker. Protein Folding Workshop, Institute for Mathematics and its Applications, Invited talk.

2007 NA Baker. Quantitative Biology and Modeling/Dept. of Mathematics Seminar, Michigan State Univ, Invited talk.

2007 NA Baker. Seminar, Univ Kansas, Invited talk.

2007 DG Thomas, H Sim, P Jones, D Sept, R Pappu, NA Baker. National Cancer Institute Nanotechnology Alliance Meeting, Invited talk.

2007 NA Baker\*, others. National Cancer Institute Nanotechnology Alliance Meeting, Invited talk.

2007 B Olsen\*, Y Song, DP Tieleman, Baker N. Gibbs Conference on Biothermodynamics, Contributed poster.

2007 M Bradley\*, P Chivers, Baker N. Gibbs Conference on Biothermodynamics, Contributed poster.

2007 P-C Li\*, MJ Bradley, NA Baker, D Sept. Gibbs Conference on Biothermodynamics, Contributed poster.

2007 NA Baker. Mathematics of DNA Structure, Function, and Interactions, Institute for Mathematics and its Applications, Invited talk.

2007 NA Baker. National Biomedical Computation Resource Summer Institute Mini-Symposium, Invited talk.

2007 NA Baker. Seminar, Integrated DNA Technologies, Invited talk.

2007 NA Baker. Biophysical Evenings, Washington Univ St Louis, Invited talk.

2007 D Thomas, P Jones, R Pappu, D Sept, N Baker\*. Trans-NIH Nano Task Force Meeting, Invited talk.

2007 RL Rice\*, NA Baker. Biophysical Society Meeting, Contributed poster.

2007 SJ Lee, Y Song, NA Baker. Biophysical Society Meeting, Contributed poster.

2007 D Thomas, H Sim, P Jones, R Pappu, D Sept, N Baker\*. Nanotechnology and the Life Sciences Symposium, Talk and poster.

2007 F Dong, JA Wagoner, NA Baker\*. American Chemical Society National Meeting, Invited talk.

2007 B Olsen, Y Song, SJ Lee, Tieleman DP, NA Baker\*. American Chemical Society National Meeting, Invited talk.

2006 NA Baker. Future of Biomolecular Simulations: From Ab Initio to Nano-molecular Machines, National Center for Computational Sciences, Oak Ridge National Lab, Invited talk.

2006 JA Wagoner, F Dong, NA Baker\*. Gibbs Conference on Biothermodynamics, Invited talk.

2006 B Olsen\*, SJ Lee, Y Song, NA Baker. Gibbs Conference on Biothermodynamics, Contributed poster.

2006 F Dong\*, J Wagoner, NA Baker. Gibbs Conference on Biothermodynamics, Contributed poster.

2006 M Bradley\*, Baker N P Chivers. Gibbs Conference on Biothermodynamics, Contributed poster.

2006 NA Baker. National Biomedical Computation Resource Summer Institute, Invited workshop.

2006 NA Baker. Bioinformatics Institute, Agency for Science, Technology, and Research (A\*STAR Biopolis), Singapore, Visiting scientist lecture series.

2006 NA Baker. Computer Science and Engineering Seminar Series, Univ Notre Dame, Invited talk.

2006 Y Song\*, NA Baker. Biophysical Society Meeting, Contributed poster.

2006 JA Wagoner\*, NA Baker. Biophysical Society Meeting, Contributed poster.

2006 NA Baker. Theoretical and Computational Biophysics Seminar, Univ Illinois Urbana-Champaign, Invited talk.

2006 NA Baker. Biocomplexity Institute Seminar, Univ Indiana, Invited talk.

2005 NA Baker. Japan Society for the Promotion of Science, U.S. National Academy of Sciences: Eighth Annual Japanese-American Frontiers of Science Symposium, Invited poster.

2005 NA Baker. Contemporary Biochemistry Seminar Series, Univ Wisconsin at Madison, Invited talk.

2005 Y Song\*, V Guallar, NA Baker. Gibbs Conference on Biothermodynamics, Invited talk.

2005 JA Wagoner\*, NA Baker. Gibbs Conference on Biothermodynamics, Contributed poster.

2005 M Bradley\*, P Chivers, N Baker. Gibbs Conference on Biothermodynamics, Contributed poster.

2005 NA Baker. Institute for Computational Engineering and Sciences, Univ Texas at Austin, Invited talk.

2005 NA Baker. IPAM Workshop: Bridging Time and Length Scales in Materials Science and Bio-Physics, Invited talk.

2005 NA Baker\*, T Dolinsky, J Wagoner, Y Song. QBMI Computational Structural Biology Workshop, Invited talk.

2005 NA Baker. Univ Iowa Dept of Chemistry Seminar, Invited talk.

2005 Y Song\*, NA Baker. Biophysical Society Meeting, Contributed poster.

2005 NA Baker. St Louis RCGA Bioinformatics Network Seminar, Invited talk.

2004 NA Baker. 2nd Annual National Academies Keck Futures Initiative, Invited poster.

2004 J Wagoner\*, A Melnykov, NA Baker. Gibbs Conference on Biothermodynamics, Contributed poster.

2004 NA Baker. Algorithms for Multiscale Modeling IV, Invited talk.

2004 NA Baker. JASON Summer Study 2004 Computation for Biology and Medicine, JASON group (Mitre Corporation), Invited briefing.

2004 NA Baker. Multiscale Computational Models for Biomolecular Research, National Biomedical Computation Resource, Invited talk.

2004 Y Song\*, Y Zhang, T Shen, CL Bajaj, JA McCammon, NA Baker. Biophysical Society Meeting, Contributed poster.

2003 NA Baker\*, X Zhang, Z Xu, CL Bajaj. Digital Biology: The Emerging Paradigm (NIH BISTIC), Contributed poster.

2003 Y Song\*, Y Zhang, T Shen, C Bajaj, JA McCammon, NA Baker. Gibbs Conference on Biothermodynamics, Contributed poster.

2003 M Bradley\*, E Schreiter, C Drennan, P Chivers, Baker N. Gibbs Conference on Biothermodynamics, Contributed poster.

2003 NA Baker. The Third Virtual Conference on Genomics and Bioinformatics, Invited talk.

2003 NA Baker. Rush Medical College, Dept of Molecular Biophysics and Physiology Seminar, Invited talk.

2003 NA Baker. Univ Texas at Austin, Center for Computational Visualization Seminar, Invited talk.

2003 NA Baker, C Bajaj\*, JA McCammon, Sanner M, Olson A. NPACI All-Hands Meeting, Invited talk.

2003 NA Baker\*, D Sept, S Joseph, MJ Holst, JA McCammon. SIAM Computation Science and Engineering meeting, Contributed talk.

2002 NA Baker. Univ Illinois Urbana-Champaign, Theoretical Biophysics Seminar, Invited talk.

2002 NA\* Baker, D Sept, S Joseph, MJ Holst, JA McCammon. Gibbs Conference on Biothermodynamics, Contributed poster.

2002 NA Baker. NPACI All-Hands Meeting, Invited talk.

2002 NA Baker\*, D Sept, MJ Holst, JA McCammon. NPACI All-Hands Meeting, Contributed poster, first place student award.

2002 NA Baker\*, D Sept, S Joseph, MJ Holst, JA McCammon. Biophysical Society Annual Meeting, Contributed poster.

2002 NA Baker. The Salk Institute, Young Investigator Symposium, Invited talk.

2002 D Sept\*, NA Baker, JA McCammon. Biophysical Society Annual Meeting, Contributed poster.

2001 NA Baker. Univ Chicago, Computations in Science Seminar, Invited talk.

2001 Baker,NA. Washington Univ School of Medicine, Dept of Biochemistry and Molecular Biophysics Special Seminar, Invited talk.

2001 NA Baker. Univ Michigan, Bioinformatics Program Seminar, Invited talk.

2001 NA Baker. Seminar, The Burnham Institute, Invited talk.

2001 NA Baker. Univ California San Diego, Biochemistry Seminar, Invited talk.

2001 NA Baker\*, D Sept, M Holst, JA McCammon. American Chemical Society National Meeting, Invited talk.

2000 NA Baker\*. The First SIAM Conference on Computational Science and Engineering, Contributed talk.

2000 NA Baker\*, MJ Holst, JA McCammon. La Jolla Interfaces in Science 2000 Symposium: Quantitative Challenges in the Post-genomic Sequence, Contributed poster.

1998 NA Baker\*, G Huber, JA McCammon. The Sixth International Meeting on Cholinesterases, Contributed poster.

1997 N Baker, W Kearney, D Quinn\*. Experimental Nuclear Magnetic Resonance Conference, Contributed poster.

1996 N Baker, S Feaster, D Quinn\*. Gordon Conference: Enzymes, Coenzymes, Metabolic Pathways, Contributed poster.

# Selected publications

A full publication list with bibliometrics is available from [Google Scholar](https://scholar.google.com/citations?user=L9dwKyUAAAAJ&hl=en).

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Lei, H., Yang, X., Zheng, B., Lin, G., & Baker, N. A. (2015). Constructing Surrogate Models of Complex Systems with Enhanced Sparsity: Quantifying the Influence of Conformational Uncertainty in Biomolecular Solvation. *Multiscale Modeling and Simulation*, *13*(4), 1327–1353. <http://doi.org/10.1137/140981587>

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