# Research summary

My research interests include the development of new algorithms and mathematical methods in biophysics, nanotechnology, and informatics. Current research projects include new 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/). I am the author of over 80 peer-reviewed publications and lead developer of the [APBS and PDB2PQR software](http://www.poissonboltzmann.org/) with 26,000 registered users worldwide.

# Education

2001-2002 Postdoctoral researcher: University of California San Diego, J. Andrew McCammon research group (Department of Chemistry)

2001 PhD, Physical Chemistry: University of California San Diego, J. Andrew McCammon (Department of Chemistry) and Michael Holst (Department of Mathematics) research groups. Kamen award for best PhD thesis in the biological sciences.

1997 BS, Chemistry: University of Iowa, Daniel Quinn (Department of Chemistry) research group. Honors and highest distinction.

# Professional experience

2015-present Visiting Professor, Department of Applied Mathematics, Brown University

2012-present Laboratory Fellow, Computational and Statistical Analytics Division, Pacific Northwest National Laboratory

2010-2012 Chief Scientist, Computational and Statistical Analytics Division, Pacific Northwest National Laboratory

2006-2010 Associate Professor with tenure, Department of Biochemistry and Molecular Biophysics, Washington University in St. Louis School of Medicine

2002-2010 Assistant Professor, Department of Biochemistry and Molecular Biophysics, Washington University in St. Louis School of Medicine

# Selected honors

2012 Fellow, American Association for the Advancement of Science

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

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

2004-2006 Research Fellow, Alfred P. Sloan Foundation

1997-2001 Predoctoral fellowship, Howard Hughes Medical Institute

1995-1997 Undergraduate fellowship, Barry M. Goldwater fund

# Selected other activities

2014-2017 Associate Editor, Biophysical Journal.

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.

2013-present co-PI and Project Manager, CM4: Collaboration on Mathematics for Multiscale Modeling of Materials, DOE ASCR. $6M/5-year project. Provide scientific direction, working with PI Karniadakis, identifying application research priorities and staff hiring needs; manage budget, personnel, and project deliverables.

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

2012-2015 Lead, Signature Discovery Initiative, Pacific Northwest National Laboratory. $16M/6-year research portfolio. Provide scientific leadership, working with Lab leadership, identifying application research priorities and staff hiring needs; manage budget, personnel, and project deliverables; mentor junior staff on career growth and related activities; build scientific community and partnerships in the field of signature discovery; actively interact with potential sponsors for long-term external support.

2012-present Co-chair, United States-European Union Community of Research on Nanomaterial Databases and Ontology. Sponsored by US State Department, White House Office of Science and Technology Policy, and European Commission. Develop international research agenda to foster collaboration and growth of computational approaches to archiving, sharing, and analyzing nanotechnology data for safer nanomaterials; scientific diplomacy to build a community of interest while respecting multi-cultural research needs and collaboration perspectives.

2009-2013 Lead, National Cancer Informatics Program (formerly caBIG) Nanotechnology Working Group, National Cancer Institute. Grew a diverse international community of nanotechnology researchers from academia, industry, and government from an initial team of 5-10 to a current group of 20-30 participants; provided definitions and research priorities for the field of nanotechnology informatics; developed vocabulary and data-sharing standards for the nanotechnology community.

2007-2010 Director, Molecular Biophysics Graduate Program, Washington Univ. in St. Louis. Directed the PhD program in molecular biophysics: Supervised approximately 20 students and over 20 affiliated faculty; oversaw recruiting; provided admissions reviews; developed course curriculum; resolved faculty-student conflicts.

2005-2010 Director, Siteman Center for Cancer Nanotechnology Excellence Biocomputing Core, Washington Univ. in St. Louis. Create and sustain a computational core to support analysis and archival of data related to cancer imaging and nanomedicine development. Directly supervise systems administrators and work with them to select the best computational platforms for scientific mission.

# Publications

Please see [Google Scholar](https://scholar.google.com/citations?hl=en&user=L9dwKyUAAAAJ) for a complete publication list.