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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, mathematical methods for mesoscale materials modeling, and development of new methods for signature discovery. I am the author of over 80 peer-reviewed publications and lead developer of the APBS and PDB2PQR software 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 for a complete publication list.