Jiahao Chen
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Work Experience

since 10/2013 **Staff Research Scientist**, *MIT Computer Science and Artificial Intelligence Laboratory*, Cambridge, Massachusetts.

Contributed to development of the Julia language, an open-source platform for scientific computing. Methods for computing statistics, distributions and random variates from random matrix theory and free probability theory, as well as wrappers for certain linear algebraic routines from the LAPACK library, have been implemented.

6—9/2013 **Visiting Scholar**, *Hirata Lab, Institute of Science and Engineering, Ritsumeikan University*, Kusatsu City, Shiga Prefecture, Japan.

Worked on computer code for reference interaction site model (RISM) calculations for studying the solvation of pharmaceutical drug candidates. Existing computer programs were refactored, rewritten and cleaned up for commercial distribution by Molecular Design Frontier, Inc. The new code can be used as a standalone program or integrated with Accelrys' Discovery Studio.

2009—13 **Postdoctoral Associate**, *MIT Department of Chemistry, ENI-MIT Solar Frontiers Center and Center for eXcitonics*, Cambridge, Massachusetts.

advisor Prof. Troy Van Voorhis

New models for disorder in organic solar cells

Assisted in writing a grant (NSF No. 1035400, $1.5m) that was responsible for bringing together an interdisciplinary group of materials scientists, mathematicians, computer scientists, and chemists to work on applications of random matrix theory to the chemistry and physics of organic photovoltaics. A reading group was organized to allow non-mathematicians to learn random matrix theory and free probability theory from the mathematicians. Several physics papers have been published in reputable journals, including one in *Physical Review Letters*, and a talk was presented at the national meeting of the American Physical Society in Boston, Massachusetts in 2012. The collaboration has also stimulated new developments in free probability theory, which were presented at a talk at the national meeting of the German Mathematical Society conference in Saarbrücken, Germany in 2012, and are being prepared for publication.

Automatic parameterization of force fields

Force field simulations are an important tool in computational chemistry, but their accuracy depends critically on the choice of parameters, whose appropriate values are not always clear. Force-matching methods were developed to improve systematically the agreement of force fields with data from quantum chemical calculations, and were furthermore extended to polarizable force fields. The results were published in *The Journal of Chemical Physics* and presented at the 14$^{\text{th}}$ American Computational and Theoretical Chemistry Conference in Telluride, Colorado, and the 241$^{\text{st}}$ National Meeting of the American Chemical Society in Salt Lake City, Utah, in 2011. The methods are available in the free ForceBalance software at `https://simtk.org/home/forcebalance`.

Excited states in force field simulations

Electronic excitations are difficult to model in conventional force fields. A new type, low cost model for charge-transfer excitations in particular was developed. A new physical definition of atomic charge from quantum chemical data was also proposed and studied. The results are currently being prepared for publication and were presented in a poster at the 244$^{\text{th}}$ National Meeting of the American Chemical Society in Philadelphia, Pennsylvania in 2012.

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Other collaborations

With the group of Stephen Buchwald, a study of an unusual dearomatization reaction in a platinum complex was launched. Density functional theory (DFT) calculations elucidated unusual changes in the electronic structure of the platinum ion which allowed this reaction to be thermodynamically feasible. The results were published in *The Journal of the American Chemical Society*.
With the group of JoAnne Stubbe, a study was initiated of a protein known as class III ribonucleotide reductase (RNR). Quantum chemical calculations suggested that the active conformation involves the formation of an unexpectedly weak sulfur-sulfur bond. The results are currently being prepared for publication.

2002—4 **Project Clerk/Member of Technical Staff**, *DSO National Laboratories*, Singapore.

New materials for optical power limiting applications, Advanced Materials Laboratory

To prevent being blinded by enemy lasers or by accident, the military have a need for materials that darken very quickly when exposed to laser radiation. Several new optically active compounds (porphyrins, phthalocyanines, and fullerene derivatives) were synthesized and characterized to increase the palette of available materials. To speed up the experiments, the Z-scan experimental setup was fully automated using new software written in LabVIEW G and Visual Basic for Applications, so that the optical activity of new materials can be studied at multiple wavelengths in the visible spectrum with a single mouse click. With this new software, the data can be analyzed immediately in Microsoft Excel, including nonlinear least-squares fitting tests to extract molecular optical cross-sections automatically.

Remote sensing of chemical or biological threats, Applied Physics Laboratory

To combat terrorists and smugglers, the government desire technologies for rapid, minimally invasive screening of people and freight at border crossings and transportation hubs. The use of open-path Fourier-transform infrared spectroscopy to detect signatures of chemical and biological threats was studied and theoretical models were created to estimate the feasibility of deploying such technologies in various usage scenarios. A feasibility report was delivered to the government.

Other contributions

As part of a knowledge sharing initiative, lectures on quantum dynamics and photochemistry were prepared and delivered within DSO National Laboratories. A reading group on quantum information theory was organized and participated in. A review panel of international collaborations was also participated in.

Education

University of Illinois at Urbana-Champaign (UIUC)

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2004—9 **Doctor of Philosophy in Chemical Physics with Computational Science and Engineering Option**.

advisor Prof. Todd J. Martínez, Department of Chemistry (currently at Stanford University)

thesis Theory and applications of fluctuating-charge models

Fluctuating-charge models are a low cost method of modeling polarization and charge transfer processes in force field simulations. The problem of spurious long-distance charge transfer in previously existing models was addressed with a geometry-dependent attenuation of the potential difference between atoms. An equivalence between models expressed in pairwise charge transfer variables and atomic charge variables was established using graph matroid theory, thus allowing for significant savings in computational cost. The new model was found to improve the description of molecular polarizabilities in force field calculations. The results were published in several papers in *Chemical Physics Letters* and *The Journal of Chemical Physics*, as well as presented in several national conferences of the American Chemical Society and American Physical Society.

Reaction coordinates for nonequilibrium reactions

Diffusion maps, a type of nonlinear dimensionality reduction technique used in machine learning to summarize large data sets, were applied to the problem of find reaction coordinates for nonequilibrium reactions. The photochemistry and excited state dynamics of ethylene was found to identify correctly the two known reaction channels. The results were published in *The Journal of Chemical Physics* and a poster was presented at the CCP6 Workshop on Multidimensional Quantum Mechanics with Trajectories in Leeds, the United Kingdom in 2008.

2004—8 **Master of Science in Applied Mathematics With Applications to the Sciences**, GPA 3.91/4.00.

2000—2 **Bachelor of Science in Chemistry**, *magna cum laude with highest departmental distinction*, GPA 3.84/4.00.

advisor Prof. Nancy Makri, Department of Chemistry and Department of Physics

thesis Numerical simulations of the exciton coherence length in the photosynthetic light harvesting complex II (LHC-II) of higher plants

award C. S. Marvel Award for Best Thesis

To model experiments demonstrating coherence in photosynthetic proteins, the quantum statistics of excitons formed in LHC-II were studied. Using the quantum-classical isomorphism, the equilibrium density was found using path integral Monte Carlo (PIMC) to be largely localized between a coherent pair of chlorophyll molecules. Dynamical simulations using the quasi-adiabatic path integral (QUAPI) method showed that all the eigenstates of the chlorophyll aggregates decayed quickly to this equilibrium state.

2002 **Illinois Certificate in Business Administration for Scientists**.
Non-credit course for scientists on lab management.

Research Publications

Peer-reviewed publications

1 Matthew Welborn, Jiahao Chen, Lee-Ping Wang, and Troy Van Voorhis. Why many semiempirical molecular orbital theories fail for liquid water and how to fix them. *Journal of Computational Chemistry*, 36(12):934–939, 2015.

2 Yifeng Wei, Guinevere Mathies, Kenichi Yokoyama, **Chen, Jiahao**, Robert G. Griffin, and JoAnne Stubbe. A chemically competent thiosulfuranyl radical on the escherichia coli class III ribonucleotide reductase. *Journal of the American Chemical Society*, 136(25):9001–9013, 2014.

3 Jiahao Chen and Alan Edelman. Parallel prefix polymorphism permits parallelization, presentation & proof. In *HPTCDL'14 Proceedings of the 1st Workshop on High Performance Technical Computing in Dynamic Languages*, pages 47–56, New York, 2014. ACM.

4 Jeff Bezanson, Jiahao Chen, Stefan Karpinski, Viral Shah, and Alan Edelman. Array opera-

tors using multiple dispatch: a design methodology for array implementations in dynamic languages. In *ARRAY'14 Proceedings of ACM SIGPLAN International Workshop on Libraries, Languages, and Compilers for Array Programming*, pages 56–61, New York, NY, USA, 2014. ACM.

5 Matthew G Welborn, **Chen**, **Jiahao**, and Troy Van Voorhis. Accurate approximations to Anderson models in two and three dimensions using free probability. *Physical Review B*, 88:205113, 2013.

6 Lee-Ping Wang, **Chen**, **Jiahao**, Daniel Tofan, Troy Van Voorhis, and Christopher Cummins. A pathway to diphosphorus from the dissociation of photoexcited tetraphosphorus. *RSC Advances*, 3:23166—23171, 2013.

7 Lee-Ping Wang, **Chen**, **Jiahao**, Todd J Martínez, and Troy Van Voorhis. Systematic parameterization of polarizable force fields from quantum chemistry data. *Journal of Chemical Theory and Computation*, 9:452—460, 2013.

8 Aaron M Virshup, **Chen**, **Jiahao**, and Todd J Martínez. Nonlinear dimensionality reduction for nonadiabatic dynamics: The influence of conical intersection topography on population transfer rates. *The Journal of Chemical Physics*, 137:22A519, 2012.

9 **Chen**, **Jiahao**, Eric Hontz, Jeremy Moix, Matthew Welborn, Troy Van Voorhis, Alberto Suárez, Ramis Movassagh, and Alan Edelman. Error analysis of free probability approximations to the density of states of disordered systems. *Physical Review Letters*, 109:036403, 2012.

10 Phillip J Milner, Thomas John Maimone, Mingjuan Su, **Chen**, **Jiahao**, Peter Müller, and Stephen L Buchwald. Investigating the dearomative rearrangment of biaryl monophosphine-ligated Pd(II) complexes. *Journal of the American Chemical Society*, 134:19922—19934, 2012.

11 **Chen**, **Jiahao** and Todd J Martínez. The dissociation catastrophe in fluctuating-charge models and its implications for the concept of atomic electronegativity. *Progress in Theoretical Chemistry and Physics*, 19:397–416, 2009.

12 **Chen**, **Jiahao** and Todd J Martínez. Charge conservation in electronegativity equalization and its implications for the electrostatic properties of fluctuating-charge models. *Journal of Chemical Physics*, 131(4):044114, 2009.

13 **Chen**, **Jiahao**, Dirk Hundertmark, and Todd J Martínez. A unified theoretical framework for fluctuating-charge models in atom-space and in bond-space. *Journal of Chemical Physics*, 129(21):214113, 2008.

14 **Chen**, **Jiahao** and Todd J Martínez. QTPIE: Charge transfer with polarization current equalization. A fluctuating charge model with correct asymptotics. *Chemical Physics Letters*, 438(4-6):315–320, 2007.

Articles submitted or in preparation

1 **Chen**, **Jiahao** and Alan Edelman. Partial freeness of random matrices. *submitted*, 2013. `arXiv:1204.2257`.

2 **Chen**, **Jiahao** and Troy Van Voorhis. An empirical fragment charge model for multiple electronic states. *submitted*, 2013.

3 **Chen**, **Jiahao** and Troy Van Voorhis. Sticky electrons: a physically motivated partitioning of charge densities. *submitted*, 2013.

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4 **Chen, Jiahao**, Matthew G Welborn, Shane Robert Yost, and Troy Van Voorhis. Excitonic bands in disordered phthalocynanines: a random matrix theoretic perspective. *submitted*, 2013.

Theses

1 Jiahao Chen. *Theory and applications of fluctuating-charge models.* PhD in Chemical Physics, University of Illinois at Urbana-Champaign, 2009.

2 Jiahao Chen. *Numerical simulations of the exciton coherence length in the photosynthetic light harvesting complex II (LHC-II) of higher plants.* BS in Chemistry, University of Illinois at Urbana-Champaign, 2002.

Non-peer-reviewed publications

1 **Chen, Jiahao**. Comments in general discussion. *Faraday Discussions*, 141:81–98, 309–345, 2008.

2 **Chen, Jiahao**, Audi Siu-Wah Fong, and Tzi-Sum Andy Hor. Synthesis of a mixed-metal {RuPt} complex from a ruthenium cluster'. In *Proceedings of the Science Research Congress Singapore*, 1998.

Teaching experience

Fall 2015 **Guest lecturer**, *18.337/6.338*, Massachusetts Institute of Technology, Cambridge, MA.
Gave guest lectures on parallel computing in Julia for the course 18.337/6.338, "Numerical computing in Julia", taught by Prof. Alan Edelman. `http://courses.csail.mit.edu/18.337/2015`

since 2012 **Technical consultant**, *Ask-An-Engineer Project*, School of Engineering, Massachusetts Institute of Technology, Cambridge, MA.
Contributed content to questions about physics and chemistry asked by the public through the Ask-an-Engineer website. `http://engineering.mit.edu/ask`

2011–2013 **Technical consultant**, *K-12 Videos Project*, School of Engineering, Massachusetts Institute of Technology, Cambridge, MA.
The Project is a collaboration with the Khan Academy to make videos with experimental demonstrations of scientific concepts to complement teaching in K-12 schools. Consultation sessions were held for student teams to discuss the science behind their video projects. The student-produced videos were reviewed for technical accuracy before public release. Worked with 14 student teams over 5 seasons of video making. The videos can be viewed for free at `http://k12videos.mit.edu`.

since 2007 **Informal mentoring of graduate students**.

2004—5 **Teaching Assistant**, *University of Illinois at Urbana-Champaign.*
Graded homework and examinations, held office hours, and delivered substitute lecturers when the main instructor was unavailable.

CHEM 444	Physical Chemistry II (Nancy Makri, Fall 2004)
	Thermodynamics and statistical mechanics at the senior undergraduate level
CHEM 550	Advanced Quantum Dynamics (Nancy Makri, Spring 2005)
	Graduate special topics course in theoretical and computational chemistry
CHEM 442	Physical Chemistry I (Todd J. Martínez, Fall 2005)
	Quantum mechanics and spectroscopy at the senior undergraduate level

2002 **Teacher**, *Gan Eng Seng Secondary School*, Singapore.
Taught chemistry at the Secondary 3 (Grade 9 equivalent) level.

2001 **Tutor**, *Florida Avenue Residence Hall, University of Illinois*, Urbana, IL.
Volunteered to tutor fellow undergraduate students in general chemistry, general physics and calculus.

Other work experience

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2001—2 **Administrative Assistant**, *Makri group, UIUC Department of Chemistry*, Urbana, Illinois.
Digitized, filed and retrieved papers and other academic documents

2000 **Logistics supply assistant**, *Third Signals Battalion, Singapore Armed Forces*, Singapore, military service.

Professional Service

6/2015 **Program Chair**, *JuliaCon 2015*, Cambridge, Massachusetts.
Issued call for participation. Reviewed and shortlisted contributed talks in conjunction with program committee. Handled local and technical logistics for conference with about 200 participants.

6/2015 **Workshop organizer**, *High Performance Computing with Julia and OpenTuner*, Singapore-MIT Alliance for Research and Technology, Singapore.
Organized workshop and coordinated logistics for a workshop with 150 participants. Presented material introducing Julia and its applications to high performance computing and data science.

2/2015 **Minisymposium organizer**, *High-level Technical Computing with Julia Minisymposium*, SIAM Conference on Computational Science and Engineering 2015, Salt Lake City, Utah.
Organized minisymposium consisting of four talks showcasing applications of Julia in computational mathematics and sciences, which was attended by about 76 participants.

11/2014 **Program Chair**, *First Workshop in High Performance Technical Computing in Dynamic Languages*, in conjunction with Supercomputing 2014, New Orleans, Louisiana.
Wrote proposal for workshop, issued call for participation, handled the reviews for 10 submitted papers, and organized the actual workshop, attended by about 50 participants.

6/2014 **Program Chair**, *JuliaCon 2014*, Chicago, Illinois.
Issued call for participation. Reviewed and shortlisted contributed talks in conjunction with program committee. Handled technical logistics for conference with 75 participants.

11/2012 **Participant**, *Visiting Committee Meeting*, MIT Department of Chemistry, Cambridge, Massachusetts.
Participated in department review by a visiting committee comprised of faculty from other schools, members of the MIT corporation, business leaders and alumni. The committee assessed the strength of the department's educational and research programs. Feedback was provided on the research environment and quality of graduate student education in the Department.

04/2008 **Participant**, *Calculus and* Mathematica *Review Meeting*, Department of Mathematics, UIUC, Urbana, Illinois.
The mathematics department offers innovative courses using *Mathematica* to teach calculus, differential equations and linear algebra. Feedback was provided on how well the courses prepared undergraduate students for mathematically demanding courses in other departments, e.g. the physical chemistry sequence.

since 2008 ***Ad hoc* reviewer for scientific journals**.
Peer reviewer for scientific manuscripts submitted to *The Journal of Chemical Education*, *The Journal of Chemical Physics*, *The Journal of Physical Chemistry B*, *The Journal of Photochemistry and Photobiology A*,and the *International Journal of Molecular Sciences*.

08/2006 **Laboratory teaching assistant for the 2006 Summer School, "*Ab Initio* Molecular Dynamics Simulation Methods in Chemistry"** , *Materials Computation Center, Frederick Seitz Materials Research Laboratory, UIUC*, Urbana, Illinois.
Assisted in the setup and installation of software for computer laboratory sessions, including troubleshooting software and hardware errors.

Other professional activities

since 2013 **Open source software developer**, *Julia Project*, `http://julialang.org`, since version 0.1.
Implemented methods for computing statistics, distributions and random variates from random matrix theory and free probability theory in the Julia platform for scientific computing.

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since 2010 **Advisor**, *Mendeley*.
Volunteer for community outreach at MIT for Mendeley, a startup focused on collaborative scientific document management and discovery.

since 2010 **Software developer**, *Q-Chem, Inc.*, `http://q-chem.com`.
Currently implementing new wavefunction analyses for the computation of physically-motivated atomic charges in the Q-Chem quantum chemistry software package.

since 2010 **Open source software developer**, *Open Babel Project*, `http://openbabel.org`, since version 2.3.0.
Implemented models for partial charge calculations in Open Babel, a popular chemical toolbox for interconversion of chemical data and cheminformatics.

since 2006 **Wikipedia contributor**.
Occasional contributor to Wikiproject Chemistry, particularly on topics in quantum chemistry and computational chemistry.

2001 Attended UIUC Illinois Leadership programs

Oral Presentations

Invited talks

7/2015 **Analyzing high frequency trading data for suspicious financial activity in Julia**, *DARPA*, Arlington, Virginia.
Invited by Mr. Wade Shen

6/2015 **Introduction to Julia**, *SAP Research and Innovation*, Singapore.
Invited by Dr. Daniel Dahlmeier

6/2015 **Workshop on High Performance Computing with Julia and OpenTuner**, *Singapore-MIT Alliance for Research and Technology*, Singapore.
Workshop organized with Prof. Alan Edelman and Prof. Saman Amarasinghe

5/2015 **Analyzing electrocardiogram data from the MIMIC II data set in Julia**, *MIT Big Data to Insights Workshop*, Singapore.
Invited by Dr. Daniel Dahlmeier

5/2015 **Analyzing electrocardiogram data from the MIMIC II data set in Julia**, *MIT Big Data to Insights Workshop*, Singapore.
Invited by Dr. Daniel Dahlmeier

4/2015 **Computational random matrix theory in Julia**, *Stanford University*, Palo Alto, California, ICME Departmental Colloquium.
Invited by Prof. Jack Poulson

4/2015 **What does computer science have to offer computational science?**, *Stanford University*, Palo Alto, California, ICME 401 Seminar Series.
Invited by Prof. Jack Poulson

2/2015 **Julia - a Fast New Language for Technical Computing**, *SIAM Conference on Computational Science and Engineering 2015*, Salt Lake City, Utah, Featured Minisymposium MS 182: CSE Software.
Invited by Prof. Hans Petter Langtangen, session organizer

9/2014 **Julia: compiler and community**, *Schlumberger, Inc.*, Cambridge, Massachusetts.
Invited by Dr. Roberta Mazzoli

8/2014 **Big Data analytics in Julia**, *Intel Science and Technology Center for Big Data*, Hillboro, Oregon.
Invited by Prof. Sam Madden and Dr. Tim Mattson

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7/2014 **Julia: compiler and community**, *Intel, Inc.*, Santa Clara, California.
Invited by Dr. Shameem Akhter

8/2013 **Disorder and excitonic structure in organic semiconductors**, *Osaka University*, Osaka, Japan.
Invited by Prof. Shigeta Yasutera.

6/2013 **Disorder and excitonic structure in organic semiconductors**, *Nagoya University*, Nagoya, Japan.
Invited by Prof. Dr. Stephan Irle.

12/2012 **Disorder and excitonic structure in organic semiconductors**, *Boston University*, Boston, MA.
Invited by Prof. David Coker.

9/2012 **Disorder and excitonic structure in organic semiconductors**, *Harvard University*, Cambridge, MA.
Invited by Prof. Alán Aspuru-Guzik.

8/2012 **Disorder in organic semiconductors: a random matrix perspective**, *Stanford University*, Stanford, CA.
Invited by Prof. Todd Martínez.

6/2012 **Partial freeness of random matrices**, *Institute for Mathematical Sciences, National University of Singapore*, American Mathematics Society Summer School: Random Matrix Theory and its Applications II.
Invited by Prof. Alan Edelman, organizer.

6/2012 **Error analysis of free probability approximations to the density of states of disordered systems**, *Institute for Mathematical Sciences, National University of Singapore*, American Mathematics Society Summer School: Random Matrix Theory and its Applications II.
Invited by Prof. Alan Edelman, organizer.

1/2012 **Calculating the density of states in disordered organic semiconductors using free probability theory**, *Harvard University*, Cambridge, MA, Synergy Between Experiment and Computation in Energy-Looking to 2030 (ENCON1).
Invited by Prof. Michael Stopa, organizer.

9/2011 **Numerical and scientific computing in Python**, *Boston Python User Group*, Cambridge, MA.
Invited by Mr. Ned Batchelder, organizer.

7/2010 **The description of polarization and charge transfer effects in force fields using fluctuating charges**, *The University of Chicago*, Chicago, IL.
Invited by Dr. Jeff Hammond, Argonne National Laboratory. Jointly presented also to the groups of Prof. Benoît Roux and Prof. Gregory A. Voth.

3/2003 **Short-range exciton coherence in light harvesting complex II (LHC-II)**, *Kumamoto University*, Kumamoto, Japan.
Invited by Prof. Manabu Sugimoto

Presentations at Conferences

9/2012 **Partial freeness of random matrices**, *Minisymposium on Free Probability and Random Matrices, Annual Meeting of the German Mathematical Society (Minisymposium über Freie Wahrscheinlichkeitstheorie und Zufallsmatrizen, Jahrestagung der Deutschen Mathematiker-Vereinigung)*, Saarbrücken, Germany.

8/2007 **QTPIE: A new charge model for arbitrary geometries and systems**, *American Chemical Society, Division of Computers in Chemistry, 234th National Meeting*, Boston, MA.

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8/2007 **Representing molecules as atomic-scale electrical circuits with fluctuating-charge models**, *American Physical Society, Division of Chemical Physics, National Meeting*, Denver, CO.
Received Graduate Student Travel Award.

Internal Presentations

3/2010 **Theoretical investigation of the water oxidation mechanism in a cobalt phosphate water splitting catalyst**, *ENI-MIT Solar Frontiers Center*, Cambridge, MA.

3/2010 **Looking into the black box: computing molecular excited states with time-dependent density functional theory**, *MIT Center for eXcitonics*, Cambridge, MA.
Briefly introduced the calculations performed in quantum chemistry software for experimental quantities of interest for Frenkel excitons and other molecular excited states.

12/2002 **Theories on the biological origins of porphyrins**, *Advanced Materials Laboratory, DSO National Laboratories*, Singapore.
Departmental level literature review.

11/2002 **Operating principles of charge-coupled devices**, *Advanced Materials Laboratory, DSO National Laboratories*, Singapore.
Group level literature review.

Poster Presentations

8/2012 **Quantum mechanical charge equilibration model for open fragments: Extending force fields to handle molecular excited states**, *Division of Physical Chemistry, American Chemical Society, 244th National Meeting*, Philadelphia, PA.

3/2012 **Calculating the density of states in disordered systems using free probability**, *American Physical Society National Meeting*, Boston, MA.

7/2011 **An empirical potential for electronic excitations using charge equilibration**, *14th American Conference on Theoretical Chemistry*, Telluride, CO.

3/2009 **Fluctuating-charge models in bond space and their exact reformulation in atomic space**, *Division of Physical Chemistry, American Chemical Society, 237th National Meeting*, Salt Lake City, UT.

3/2009 **Investigating the properties of new water models capable of polarization and intermolecular charge transfer**, *Division of Computers in Chemistry, American Chemical Society, 237th National Meeting*, Salt Lake City, UT.
Received Chemical Computing Group Excellence Award.

8/2008 **A flexible water model capable of polarization and charge-transfer**, *Faraday Discussion 141: Water - from interfaces to the bulk*, Edinburgh, United Kingdom.

7/2008 **Toward a flexible water model capable of polarization and charge-transfer**, *13th American Conference in Theoretical Chemistry*, Evanston, IL.

7/2008 **Toward a flexible water model capable of polarization and charge-transfer**, *XIIIth International Workshop on Quantum Systems in Chemistry and Physics*, East Lansing, MI.

8/2007 **QTPIE: A minimal extension of Goddard's QEq model with correct dissociation**, *Division of Computers in Chemistry, American Chemical Society, 233rd National Meeting*, Boston, MA.

5/2006 **A fluctuating-charge model with charge-transfer and correct asymptotics**, *XIIth International Congress on Quantum Chemistry*, Kyoto, Japan.

3/2006 **A fluctuating-charge model with correct asymptotics**, *Physical Chemistry Recruiting Weekend, UIUC*, Urbana, IL.

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11/2005 **A New Model for Charge Distributions in Molecular Systems**, *NSF DMR-03 25939 ITR Review Meeting, UIUC Materials Computation Center*, Urbana, IL.

10/2005 **A New Model for Charge Distributions in Molecular Systems**, *The Eighteenth Annual Cell & Molecular Biology/ Molecular Biophysics Training Grant Research Symposium, UIUC Beckman Institute*, Urbana, IL.
Received Best Poster Award.

Other participation in meetings & short courses

8/2012 **Attendee**, *Q-Chem Developers' Workshop*, University of Pennsylvania.

9/2010 **Short course attendee**, *Introduction to Immunology for Physical Scientists and Engineers*, Boston University.
Taught by Prof. Arup Chakraborty, MIT Chemistry & the Ragon Institute.

7/2005 **Attendee**, *12th American Conference in Theoretical Chemistry*, University of California at Los Angeles.
Received Travel Award.

12/2004 **Attendee**, *Hot Topics: "Mathematical and Statistical Methods for Visualization and Analysis of High Dimensional Data" Workshop*, Mathematical Sciences Research Institute, Berkeley, CA.

10/2001 **Attendee**, *34th Midwest Theoretical Chemistry Conference*, University of Minnesota at Minneapolis-St. Paul.

Awards

4/2010 Nominated into the Sigma Xi, The Scientific Research Society

3/2009 Chemical Computing Group Excellence Award, Division of Computers in Chemistry, American Chemical Society

8/2008 Conference Travel Award, UIUC Graduate College

4/2008 Phi Kappa Phi Honors Society

8/2007 Lester E. & Kathleen A. Coleman Predoctoral Fellow

3/2007 Graduate Student Travel Award, Division of Chemical Physics, American Physical Society

8/2006 Robert F. Carr Predoctoral Fellow

6/2006 Travel Award, UIUC Center for Advanced Theory and Molecular Simulation

4/2006 Conference Travel Award, UIUC Graduate College

8/2005 Travel Award for the 12th American Conference on Theoretical Chemistry, UCLA

12/2004 Travel Grant to attend "Hot Topics Workshop: Mathematical and Statistical Methods for Visualization and Analysis of High-Dimensional Data", Mathematical Sciences Research Institute, Berkeley, CA

8/2004 Roger Adams Predoctoral Fellow

5/2002 C. S. Marvel Award, UIUC Department of Chemistry

5/2002 Phi Lambda Upsilon/Arthur R. Sloan Award, UIUC Department of Chemistry

5/2002 Dean's List (all semesters), UIUC College of Liberal Arts and Sciences

5/2002 Edmund W. James Scholar (all semesters), UIUC College of Liberal Arts and Sciences

4/2001 Arthur W. Sloan Prize, UIUC Department of Chemistry

12/2000 Mothers'Association Book Award, UIUC

8/2000 Singapore Government Scholarship, Public Service Commission, Singapore

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1995-9 Multiple awards in the National Olympiad for Informatics, National Chemistry Olympiad and National Physics Olympiad in Singapore

Affiliations

- American Chemical Society
- American Physical Society
- Royal Society of Chemistry
- Society for Industrial and Applied Mathematics
- Erdős number: 4

Languages

Native speaker of English and Mandarin Chinese. Beginner in American Spanish, German and Japanese.