Lee-Ping Wang
Curriculum Vitae

ADDRESS

Chemistry Department, UC Davis
One Shields Ave, Chemistry Annex 4463
Davis, CA 95616

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E-mail: leeping@ucdavis.edu

EDUCATION AND POSTDOCTORAL EXPERIENCE

B.A. in Physics, UC Berkeley — May 2006

Ph.D. in Physical Chemistry, MIT — May 2011
Ph.D. Advisor: Prof. Troy Van Voorhis
Thesis: *Theoretical investigation of solar energy capture and water oxidation catalysis*

Postdoctoral Fellow, Stanford University — Sep 2011 – Jun 2015
Postdoctoral Advisor: Prof. Todd J. Martínez, Prof. Vijay S. Pande

ACADEMIC APPOINTMENTS

Assistant Professor — Jul 2015 – Jun 2020
Associate Professor — Jul 2020 – present
Department of Chemistry, University of California, Davis

PEER-REVIEWED PUBLICATIONS (* for corresponding author)

74. Reeves HL and Wang L-P.* (**2022**) "The impact of conformational sampling on first-principles calculations of vicinal COCH J-couplings in carbohydrates." *Glycobiology*, cwac073.

73. Yeo C, Nguyen M and Wang L-P.* (**2022**) "Benchmarking Density Functionals, Basis Sets, and Solvent Models in Predicting Thermodynamic Hydricities of Organic Hydrides." *J. Phys. Chem. A* 126, 7566–7577.

72. Nguyen QNN, Xia KT, Zhang Y, Chen N, Morimoto M, Pei X, Ha Y, Guo J, Yang W, Wang L-P, Bergman RG, Raymond KN, Toste FD and Tantillo DJ. (**2022**) "Source of Rate Acceleration for Carbocation Cyclization in Biomimetic Supramolecular Cages." *J. Am. Chem. Soc*. 144, 14413–11424.

71. Oh L, Varki A, Chen X and Wang L-P.* (**2022**) "SARS-CoV-2 and MERS-CoV Spike Protein Binding Studies Support Stable Mimic of Bound 9-O-Acetylated Sialic Acids." *Molecules* 2022, *27*, 5322.

70. Oh L, Ji Y, Li W, Varki A, Chen X and Wang L-P.* (**2022**) “O-Acetyl Migration within the Sialic Acid Side Chain: A Mechanistic Study Using the Ab Initio Nanoreactor.” *Biochemistry* 2022, 61, 2007–2013.

69. Xu Z, Federman SR, Jackson WM, Ng CY, Wang L-P and Crabtree KN. (**2022**) “Multireference configuration interaction study of the predissociation of C_2 via its $F\,^1\Pi_u$ state.” *J. Chem. Phys.* 157, 024302.

68. Lee J, Kind T, Tantillo DJ, Wang L-P and Fiehn O. (**2022**) “Evaluating the Accuracy of the QCEIMS Approach for Computational Prediction of Electron Ionization Mass Spectra of Purines and Pyrimidines.” *Metabolites* 12, 68.

67. Rao G, Chen N, Marchiori DA, Wang L-P and Britt RD. (**2022**) “Accumulation and Pulse Electron Paramagnetic Resonance Spectroscopic Investigation of the 4-Oxidobenzyl Radical Generated in the Radical S-Adenosyl-L-methionine Enzyme HydG”. *Biochemistry* 61, 107–116.

66. Britt RD, Tao L, Rao G, Chen N and Wang L-P. (**2022**) “Proposed Mechanism for the Biosynthesis of the [FeFe] Hydrogenase H-Cluster: Central Roles for the Radical SAM Enzymes HydG and HydE”, *ACS Bio. Med. Chem. Au* 2, 11–21.

65. Boothroyd S, Madin OC, Mobley DL, Wang L-P, Chodera JD, Shirts MR. (**2021**) “Improving Force Field Accuracy by Training against Condensed-Phase Mixture Properties.” J. Chem. Theory Comput. 18, 3577–3592.

64. Caceres-Delpiano J, Wang L-P* and Essex JW. (**2021**) “The automated optimisation of a coarse-grained force field using free energy data”, *Phys. Chem. Chem. Phys.* 23, 24842.

63. Stoppelman JP, Ng TT, Nerenberg PS and Wang L-P.* (**2021**) “Development and Validation of AMBER-FB15-compatible Force Field Parameters for Phosphorylated Amino Acids”, *J. Chem. Theory Comput.* 125, 11927-11942.

62. Chen N, Rao G, Britt RD and Wang L-P.* (**2021**) “Quantum Chemical Study of a Radical Relay Mechanism for the HydG-Catalyzed Synthesis of a Fe(II)$(CO)_2$(CN) cysteine Precursor to the H-Cluster of [FeFe] Hydrogenase”, *Biochemistry* 60, 3016-3026.

61. Qiu Y, Smith DGA, Boothroyd S, Jang H, Hahn DF, Wagner J, Bannan CC, Gokey T, Lim VT, Stern CD, Rizzi A, Tjanaka B, Tresadern G, Lucas X, Shirts MR, Gilson MK, Chodera JD, Bayly CI, Mobley DL and Wang L-P.* (**2021**) “Development and Benchmarking of Open Force Field v1.0.0 – the Parsley Small-Molecule Force Field”, *J. Chem. Theory Comput.* 17, 6262-6280.

60. Das M, Chen M, LiWang A and Wang L-P.* (**2021**) “Identification and characterization of metamorphic proteins: Current and future perspectives”, *Biopolymers* 112, e23473.

59. Borges RM, Colby SM, Das S, Edison AS, Fiehn O, Kind T, Lee J, Merrill AT, Merz KM, Metz TO, Nunez JR, Tantillo DJ, Wang L-P, Wang S and Renslow RS. (**2021**) "Quantum Chemistry Calculations for Metabolomics", *Chem. Rev.* 121, 5033–5670.

58. Ji Y, Sasmal A, Li W, Oh L, Srivastava S, Hargett AA, Wasik BR, Yu H, Diaz S, Choudhury B, Parrish CR, Freedberg DI, Wang L-P, Varki A and Chen X. (**2021**) "Reversible *O*-Acetyl Migration within the Sialic Acid Side Chain and Its Influence on Protein Recognition", *ACS Chem. Biol.* 16, 1951-1960.

57. Schauperl M, Kantonen SM, Wang L-P and Gilson MK. (**2020**) "Data-driven analysis of the number of Lennard-Jones types needed in a force field", *Commun. Chem.* 3, 173.

56. Seritan S, Bannwarth C, Fales BS, Hohenstein EG, Isborn CM, Kokkila-Schumacher SIL, Li X, Liu F, Luehr N, Snyder JW, Song CC, Titov AV, Ufimtsev IS, Wang L-P and Martinez TJ. (**2020**) "TeraChem: A graphical processing unit-accelerated electronic structure package for large-scale ab initio molecular dynamics", *WIREs Comput. Mol. Sci.* 10, e1494.

55. Chen N, Das M, LiWang A and Wang L-P.* (**2020**) "Sequence-Based Prediction of Metamorphic Behavior in Proteins", *Biophys. J.* 119, 1380–1390.

54. Li W, Battistel MD, Reeves H, Oh L, Yu H, Chen X, Wang L-P* and Freedberg DI. "A combined NMR, MD and DFT conformational analysis of 9-*O*-acetyl sialic acid-containing GM3 ganglioside glycan and its 9-*N*-acetyl mimic", *Glycobiology* 30, 787–801.

53. Qiu Y, Smith DGA, Stern CD, Feng M, Jang H, Wang L-P.* (**2020**) "Driving torsion scans with wavefront propagation", *J. Chem. Phys.* 152, 244116.

52. Liou S-H, Chuo S-W, Qiu Y, Wang L-P and Goodin DB. (**2020**) "Linkage between Proximal and Distal Movements of P450cam Induced by Putidaredoxin", *Biochemistry* 59, 2012–2021.

51. Schauperl MS, Nerenberg PS, Jang H, Wang L-P, Bayly CI, Mobley DM and Gilson MK. (**2020**) "Non-bonded force field model with advanced restrained electrostatic potential charges (RESP2)", *Commun. Chem.* 3, 44.

50. Hutchings ME, Johnson L, Qiu Y, Song CC and Wang L-P.* (**2020**) "Bond-Order Time Series Analysis for Detecting Reaction Events in Ab Initio Molecular Dynamics Simulations", *J. Chem. Theory Comput.* 16, 1606–1617.

49. Kantonen SM, Muddana HS, Schauperl M, Henriksen NM, Wang L-P and Gilson MK. (**2020**) "Data-Driven Mapping of Gas-Phase Quantum Calculations to General Force Field Lennard-Jones Parameters", *J. Chem. Theory Comput.* 16, 1115–1127.

48. Slochower DR, Henriksen NM, Wang L-P, Chodera JD, Mobley DL and Gilson MK. (**2019**) "Binding Thermodynamics of Host–Guest Systems with SMIRNOFF99Frosst 1.0.5 from the Open Force Field Initiative", *J. Chem. Theory Comput*. 15, 6225–6242.

47. Xu Z, Luo N, Federman SR, Jackson WM, Ng C-Y, Wang L-P & Crabtree KN. (**2019**) "Ab initio Study of Ground-State CS Photodissociation Via Highly Excited Electronic States", *Astrophys. J*. 882:86.

46. Chuo S-W, Liou S-H, Wang L-P, Britt RD, Poulos TL, Sevrioukova IR and Goodin DB. (**2019**) "Conformational Response of N-Terminally Truncated Cytochrome P450 3A4 to Ligand Binding in Solution", *Biochemistry* 58, 3903–3910.

45. Wang C-Y, Zhu A-Y, Liao X, Manga M & Wang L-P. (**2019**) "Capillary Effects on Groundwater Response to Earth Tides", *Water Resour. Res.* 55, 6886–6895.

44. Wang L-P* & Song CC. (**2019**) "Car–Parrinello Monitor for More Robust Born–Oppenheimer Molecular Dynamics", *J. Chem. Theory Comput*. 15, 4454–4467.

43. Qiu Y, Nerenberg PS, Head-Gordon T & Wang L-P.* (**2019**) "Systematic optimization of water models using liquid/vapor surface tension data", *J. Phys. Chem. B* 123, 7061–7073.

42. Chuo S-W, Wang L-P, Britt RD & Goodin DB. (**2019**) "An Intermediate Conformational State of Cytochrome P450cam-CN in Complex with Putidaredoxin", *Biochemistry* 58, 2353-2361.

41. Wade AD, Wang L-P* & Huggins DJ*. (**2018**) "Assimilating radial distribution functions to build water models with improved structural properties", *J. Chem. Inf. Model.* 58, 1766-1778.

40. Qiu Y, Schwegler BR & Wang L-P.* (**2018**) "Polarizable molecular simulations reveal how silicon-containing functional groups govern the desalination mechanism in nanoporous graphene", *J. Chem. Theory Comput.* 14*,* 4279-4290.

39. Jang H, Qiu Y, Hutchings ME, Nguyen M, Berben LA & Wang L-P.* (**2018**) "Quantum chemical studies of redox properties and conformational changes of a four-center iron CO_2 reduction electrocatalyst", *Chem. Sci.* 9, 2645-2654.

38. Demerdash O, Wang L-P & Head-Gordon T. (**2017**) "Advanced models for water simulations", *WIRES Comput. Mol. Sci.* 8, e1355.

37. Eastman P, Swails J, Chodera JD, McGibbon RT, Zhao Y, Beauchamp KA, Wang L-P, Simmonett AC, Harrigan MP, Stern CD, Wiewiora RP, Brooks BR & Pande VS. (**2017**) "OpenMM 7: Rapid development of high performance algorithms for molecular dynamics", *PLOS Comput. Biol.* 13, e1005659.

36. Huang J, Mei Y, König G, Simmonett AC, Pickard FC, Wu Q, Wang L-P, Mackerell AD, Brooks BR & Shao Y. (**2017**) "An estimation of hybrid quantum mechanical molecular mechanical polarization energies for small molecules using polarizable force-field approaches", *J. Chem. Theory Comput.* 13, 679-695.

35. Wang L-P, McKiernan KA, Gomes J, Beauchamp KA, Head-Gordon T, Rice JE, Swope WC, Martínez TJ & Pande VS. (**2017**) "Building a more predictive protein force field: A systematic and reproducible route to AMBER-FB15", *J. Phys. Chem. B* 121, 4023-4039.

34. Khedri Z, Xiao A, Yu H, Landig CS, Li W, Diaz S, Wasik BR, Parrish CR, Wang L-P, Varki A & Chen X. (**2017**) "A chemical biology solution to problems with studying biologically important but unstable 9-o-acetyl sialic acids", *ACS Chem. Biol.* 12, 214-224.

33. McKiernan KA, Wang L-P & Pande VS. (**2016**) "Training and validation of a liquid-crystalline phospholipid bilayer force field", *J. Chem. Theory Comput.* 12, 5960-5967

32. Albaugh A, Boateng HA, Bradshaw RT, Demerdash ON, Dziedzic J, Mao YZ, Margul DT, Swails J, Zeng Q, Case DA, Eastman P, Wang L-P, Essex JW, Head-Gordon M, Pande VS, Ponder JW, Shao YH, Skylaris CK, Todorov IT, Tuckerman ME & Head-Gordon T. (**2016**) "Advanced potential energy surfaces for molecular simulation", *J. Phys. Chem. B* 120, 9811-9832.

31. Wang C-Y, Liao X, Wang L-P, Wang C-H & Manga M. (**2016**) "Large earthquakes create vertical permeability by breaching aquitards", *Water Resour. Res.* 52, 5923-5937.

30. Wang L-P* & Song CC. (**2016**) "Geometry optimization made simple with translation and rotation coordinates", *J. Chem. Phys.* 144, 214108.

29. Song CC, Wang L-P & Martínez TJ. (**2016**) "Automated code engine for graphical processing units: Application to the effective core potential integrals and gradients", *J. Chem. Theory Comput.* 12, 92-106.

28. Wang L-P, McGibbon RT, Pande VS & Martínez TJ. (**2016**) "Automated discovery and refinement of reactive molecular dynamics pathways", *J. Chem. Theory Comput.* 12, 638-649.

27. McGibbon RT, Beauchamp KA, Harrigan MP, Klein C, Swails JM, Hernandez CX, Schwantes CR, Wang L-P, Lane TJ & Pande VS. (**2015**) "MDTraj: A modern open library for the analysis of molecular dynamics trajectories", *Biophys. J.* 109, 1528-1532.

26. Song CC, Wang L-P, Sachse T, Preiss J, Presselt M & Martínez TJ. (**2015**) "Efficient implementation of effective core potential integrals and gradients on graphical processing units", *J. Chem. Phys.* 143, 014114.

25. Qi R†, Wang L-P†, Wang QT, Pande VS & Ren PY. (**2015**) "United polarizable multipole water model for molecular mechanics simulation", *J. Chem. Phys.* 143, 014504. †*Equal contributions*.

Prior to current appointment at UC Davis:

24. Kokkila Schumacher SIL, Hohenstein EG, Parrish RM, Wang L-P & Martínez TJ. (**2015**) "Tensor hypercontraction second-order Moller-Plesset perturbation theory: Grid optimization and reaction energies", *J. Chem. Theory Comput.* 11, 3042-3052.

23. Welborn M, Chen JH, Wang L-P & Van Voorhis T. (**2015**) "Why many semiempirical molecular orbital theories fail for liquid water and how to fix them", *J. Comput. Chem*. 36, 934-939.

22. Laury ML†, Wang L-P†, Pande VS, Head-Gordon T & Ponder JW. (**2015**) "Revised parameters for the AMOEBA polarizable atomic multipole water model", *J. Phys. Chem. B* 119, 9423-9437. †*Equal contributions*.

21. Wang L-P, Titov A, Mcgibbon R, Liu F, Pande VS & Martínez TJ. (**2014**) "Discovering chemistry with an ab initio nanoreactor", *Nat. Chem.* 6, 1044-1048. *Highlighted in Nov. 10, 2014 issue of Chemical & Engineering News.*

20. Wang L-P, Martínez TJ & Pande VS. (**2014**) "Building force fields: An automatic, systematic, and reproducible approach", *J. Phys. Chem. Lett.* 5, 1885-1891.

19. Mavros MG, Tsuchimochi T, Kowalczyk T, Mcisaac A, Wang L-P & Van Voorhis T. (**2014**) "What can density functional theory tell us about artificial catalytic water splitting?", *Inorg. Chem.* 53, 6386-6397.

18. Mu XJ, Wang QT, Wang L-P, Fried SD, Piquemal JP, Dalby KN & Ren PY. (**2014**) "Modeling organochlorine compounds and the sigma-hole effect using a polarizable multipole force field", *J. Phys. Chem. B* 118, 6456-6465.

17. Fried SD, Wang L-P, Boxer SG, Ren PY & Pande VS. (**2013**) "Calculations of the electric fields in liquid solutions", *J. Phys. Chem. B* 117, 16236-16248.

16. Wang L-P, Tofan D, Chen JH, Van Voorhis T & Cummins CC. (**2013**) "A pathway to diphosphorus from the dissociation of photoexcited tetraphosphorus", *RSC Advances* 3, 23166-23171.

15. Wang L-P, Head-Gordon T, Ponder JW, Ren P, Chodera JD, Eastman PK, Martínez TJ & Pande VS. (**2013**) "Systematic improvement of a classical molecular model of water", *J. Phys. Chem. B* 117, 9956-9972.

14. Wang C-Y, Wang L-P, Manga M, Wang CH & Chen CH. (**2013**) "Basin-scale transport of heat and fluid induced by earthquakes", *Geophys. Res. Lett.* 40, 3893-3897.

13. Wang C-Y, Chen WP & Wang L-P. (**2013**) "Temperature beneath Tibet", *Earth Planet. Sci. Lett.* 375, 326-337.

12. Wang L-P, Chen JH & Van Voorhis T. (**2013**) "Systematic parametrization of polarizable force fields from quantum chemistry data", *J. Chem. Theory Comput.* 9, 452-460.

11. Eastman P, Friedrichs MS, Chodera JD, Radmer RJ, Bruns CM, Ku JP, Beauchamp KA, Lane TJ, Wang L-P, Shukla D, Tye T, Houston M, Stich T, Klein C, Shirts MR & Pande VS. (**2013**) "OpenMM 4: A reusable, extensible, hardware independent library for high performance molecular simulation", *J. Chem. Theory Comput.* 9, 461-469.

10. Wang L-P & Van Voorhis T. (**2012**) "A polarizable QM/MM explicit solvent model for computational electrochemistry in water", *J. Chem. Theory Comput.* 8, 610-617.

9. Kowalczyk T, Wang L-P & Van Voorhis T. (**2011**) "Simulation of solution phase electron transfer in a compact donor-acceptor dyad", *J. Phys. Chem. B* 115, 12135-12144.

8. Wang L-P & Van Voorhis T. (**2011**) "Direct-coupling O_2 bond forming a pathway in cobalt oxide water oxidation catalysts", *J. Phys. Chem. Lett.* 2, 2200-2204.

7. Yost SR, Wang L-P & Van Voorhis T. (**2011**) "Molecular insight into the energy levels at the organic donor/acceptor interface: A quantum mechanics/molecular mechanics study", *J. Phys. Chem. C* 115, 14431-14436.

6. Wang L-P, Wu Q & Van Voorhis T. (**2010**) "Acid-base mechanism for ruthenium water oxidation catalysts", *Inorg. Chem.* 49, 4543-4553.

5. Wang L-P & Van Voorhis T. (**2010**) "Communication: Hybrid ensembles for improved force matching", *J. Chem. Phys.* 133, 231101.

4. Difley S, Wang L-P, Yeganeh S, Yost SR & Van Voorhis T. (**2010**) "Electronic properties of disordered organic semiconductors via QM/MM simulations", *Accounts Chem. Res.* 43, 995-1004 and front cover.

3. Van Voorhis T, Kowalczyk T, Kaduk B, Wang L-P, Cheng CL & Wu Q. (**2010**) "The diabatic picture of electron transfer, reaction barriers, and molecular dynamics", *Ann. Rev. Phys. Chem.* 61 (eds S. R. Leone *et al*.), 149-170.

2. Khine M, Ionescu-Zanetti C, Blatz A, Wang L-P & Lee LP. (**2007**) "Single-cell electroporation arrays with real-time monitoring and feedback control", *Lab on a Chip* 7, 457-462.

1. Ionescu-Zanetti C, Wang L-P, Di Carlo D, Hung P, Di Blas A, Hughey R & Lee LP. (**2005**) "Alkaline hemolysis fragility is dependent on cell shape: Results from a morphology tracker", *Cytom. Part A* 65, 116-123.

OTHER PUBLICATIONS

2. LiWang PJ, Wang L-P, LiWang A. (**2021**) "Resurrected Ancestors Reveal Origin of Metamorphism in XCL1." Spotlight in *Trends in Biomolecular Sciences*, 46, 433-434.

1. "Force Field Development and Nanoreactor Chemistry", Wang L-P*, in Computational Approaches for Chemistry under Extreme Conditions, ed. N. Goldman, Springer, **2019**.

RESEARCH FUNDING (Only Wang Lab funds are shown)

National Institute of General Medical Sciences (NIGMS), 2020-2024 $85,000
Open data-driven infrastructure for building biomolecular force fields for predictive

biophysics and drug design
(as Co-I; PI is Michael Shirts at CU Boulder)

Gift from Relay Therapeutics, 2019-2020 $50,000
Systematic optimization of small molecule force fields using graph-based automatic differentiation and crystal structure databases

National Institute of Environmental Health Sciences (NIEHS), 2018-2022 $70,160
West Coast Metabolomics Center for Compound Identification
(as Co-I; PI is Oliver Fiehn at UC Davis)

Gift from XtalPi Inc., 2018-2019 $50,000
Developing molecular simulation methods for industrial clean energy catalysis

NASA Astrophysics Research and Analysis, 2018-2021 $45,168
Vacuum UV laboratory study of the photodissociation of CS, C_2, and CH
(as Co-PI; PI is Kyle Crabtree at UC Davis)

National Institute of Allergy and Infectious Diseases (NIAID), 2017-2021 $185,023
Exploring the biology of O-acetyl sialic acids using stable synthetic mimics
(as Co-I; PI is Xi Chen at UC Davis)

Army Research Office, 2017-2021 $279,666
Birth of the Metamorphome, Life Sciences
(as PI of multicampus agreement; contact PI is Andy LiWang at UC Merced)

American Chemical Society Petroleum Research Fund, 2017-2019 $110,000
Computational design of deep eutectic solvents for natural gas sweetening applications

Gift from Walt Disney Imagineering, 2015-2017 $150,000
Engineering the Solution Interface in Membrane Distillation

AWARDS AND FELLOWSHIPS

Postdoctoral Fellow, NIH SimBios Center for Biomedical Computation 2011-2014
Graduate Student Poster Award, ACS 238th National Meeting 2009
Outstanding Teaching Assistant Award, MIT Chemistry Department 2007
High Distinction in Scholarship, U.C. Berkeley 2006
Isidore Pomerantz Scholarship, U.C. Berkeley Physics Department 2005
Guidant Summer Research Scholarship, U.C. Berkeley 2004

PROFESSIONAL ACTIVITIES AND AFFILIATIONS

Peer Reviewer
Nature Communications
Journal of the American Chemical Society
Journal of Chemical Theory and Computation
Journal of Physical Chemistry
Journal of Chemical Physics

Inorganic Chemistry

Member of American Physical Society Since 2019
Member of American Institute of Chemical Engineers Since 2014
Member of Biophysical Society Since 2012
Member of American Chemical Society Since 2007
Member of Phi Beta Kappa Since 2005

INVITED TALKS

28. "*Systematic parameter optimization in an open small molecule force field*."
Extreme-scale Mathematics for Computational Chemistry workshop. February 2021

27. "*Computational prediction of metamorphism in protein sequences*."
Chemistry Seminar, Western Washington University. January 2021

26. "*Computational prediction of metamorphism in protein sequences*."
Physics Colloquium, University of Houston. January 2021

25. "*Systematic parameter optimization in an open small molecule force field*."
Vertex Pharmaceuticals virtual lecture. September 2020

24. "*New capabilities of ForceBalance and its role in the Open Force Field Initiative*."
Free Energy Workshop, Santa Fe, NM. June 2019

23. "*Car-Parrinello Monitor for more robust Born-Oppenheimer molecular dynamics*."
Northern California Theoretical Chemistry Meeting, Berkeley, CA. May 2019

22. "*Quantum chemical studies of redox properties and catalytic mechanism of a four-center iron CO_2 reduction electrocatalyst*."
Chemistry Seminar, University of the Pacific, Stockton, CA. February 2019

21. "*Quantum chemical studies of redox properties and catalytic mechanism of a four-center iron CO_2 reduction electrocatalyst*."
CECAM Workshop: Computational Electrochemistry, Helsinki, Finland. July 2018

20. "*Systematic development of accurate empirical model potentials (force fields) for water and proteins*."
Physics Colloquium, University of Vermont, Burlington, VT. April 2018

19. "*Car-Parrinello monitor for treating self-consistent field convergence failures in Born-Oppenheimer molecular dynamics*."
Free Energy Workshop, Telluride, CO. July 2017

18. "*The CO_2 reduction mechanism of multi-center iron carbonyl catalysts as revealed by an ab initio nanoreactor*."
Chemistry Seminar, University of Missouri, Columbia, MO. April 2017

17. "*The CO_2 reduction mechanism of multi-center iron carbonyl catalysts as revealed by an ab initio nanoreactor*."
Chemistry Seminar, UC Merced, Merced, CA. February 2017

16. "*Geometry optimization made simple with translation and rotation coordinates*."
Chemistry Seminar, San Jose State University, San Jose, CA. September 2016

15. "*Geometry optimization made simple with translation and rotation coordinates*."
Theory and Applications of Computational Chemistry, Seattle, WA. August 2016

14. "Lessons learned in building polarizable and fixed-charge water models."
CECAM Workshop: "Beyond Point Charges", Lausanne, Switzerland. April 2016

13. "Software for force field optimization and application to a protein force field."
Workshop on Advanced Potential Energy Surfaces, Telluride, CO. June 2015

12. "*Ab initio* discovery of energy conversion pathways: Theory and applications."
Quarterly Research Seminar, Disney Research, Shanghai, China. April 2015

11. "*Ab initio* discovery of energy conversion pathways: Theory and applications."
Chemistry Department Seminar, UC Davis, Davis, CA. January 2015

10. "*Ab initio* discovery of energy conversion pathways."
Statistical Mechanics Seminar Series, UC Berkeley, Berkeley, CA. November 2014

9. "Automatic development of effective potentials in the condensed phase."
National Institutes of Health, Rockville, MD. September 2014

8. "Making compromises between theory and experiment with effective potentials."
Workshop on Many-Body Interactions, Telluride, CO. May 2014

7. "Systematic improvement of a classical molecular model of water."
ACS 246th National Meeting, Indianapolis, IN. September 2013

6. "Systematic optimization of a direct polarization water model."
UC Davis, Davis, CA. June 2013

5. "Simple and systematic optimization of polarizable water models."
Uppsala University, Uppsala, Sweden. December 2012

4. "Grid computing methods for systematic force field optimization."
Cooperative Computing Workshop, Notre Dame University, IN. June 2012

3. "Automatic force field parameterization methods for molecular simulation."
Quantitative Analysis Seminar, Imperial College, London, UK. April 2012

2. "Development and application of an automatic force field parameterization method." IBM Almaden Research Center, San Jose, CA. December 2011

1. "Theoretical Investigation of Water Oxidation Catalysis."
Chemical Synthesis Symposium, Columbia University, New York, NY. May 2011

TEACHING EXPERIENCE

Instructor for CHE 155 (Scientific Programming for Chemistry), 2 times UC Davis
Evaluations: Course 4.8/5.0; Instructor 4.8/5.0 Spring 2022 – Fall 2022

Instructor for CHE 110A (Quantum Mechanics), 2 times — UC Davis
Evaluations: Course 4.2/5.0; Instructor 4.5/5.0 — Spring 2020 – Spring 2021

Instructor for CHE 211A (Statistical Thermodynamics), 8 times — UC Davis
Evaluations: Course 4.7/5.0; Instructor 4.7/5.0 — Winter 2016 – Fall 2022

Instructor for CHE 2AH (Honors General Chemistry), 6 times — UC Davis
Evaluations: Course 4.8/5.0; Instructor 4.7/5.0 — Fall 2015 – Fall 2020

Instructor for BIOS 203 (Atomistic Simulations) — Stanford University
Co-taught with Heather J. Kulik — Spring 2013

TA for 5.61 (Quantum Mechanics) — MIT
Instructor: Prof. Troy Van Voorhis — Fall 2007

TA for 5.112 (Principles of Chemical Science) — MIT
Instructors: Prof. Christopher C. Cummins, Prof. Moungi G. Bawendi — Fall 2006