Sandeep Sharma

Ekeley M321,
Boulder, Colorado 80309

Phone: 001-303-492-7907
Email: sandeep.sharma@colorado.edu

Education Background

Indian Institute of Technology	Chemical Engineering	B.Tech.	2003
Massachusetts Institute of Technology	Chemical Engineering	M.S.	2006
Massachusetts Institute of Technology	Chemical Engineering	Ph.D.	2009
Cornell University	Theoretical Chemistry	Postdoc	2011
Princeton University	Theoretical Chemistry	Postdoc	2014

Academic employment history

2016-present **Assistant Professor**, Chemistry and Biochemistry, University of Colorado
2014-2016 **Project leader**, Max Planck Institute for Solid State Research, Stuttgart

Awards and Appointments

2023 Visting fellow at Flatiron Insitute
2023 Visiting fellow at IQIM, Caltech
2022 Medal of the International Academy of Quantum Molecular Science
2022 Camille Dreyfus Teacher-Scholar Award
2022 NSF Career award
2020 JCP Best Paper by an Emerging Investigator Award
2019 Sloan research fellowship
2018 Quantum exploration in Science & Technology, QuEST award
2018 Kavli Fellow, honor given at Kavli symposia sponsored by the National Academy of Sciences
2014 Postdoctoral research award, from phys division of ACS
2009 Glenn Award, from the division of fuel chemistry of ACS
2007 Travel Grant, from catalysis and reaction engineering division of AIChE

Publications

62. Jo S. Kurian, Hong-Zhou Ye, Ankit Mahajan, Timothy C. Berkelbach, Sandeep Sharma, "Toward Linear Scaling Auxiliary Field Quantum Monte Carlo with Local Natural Orbitals", *Journal of Chemical Theory and Computations*, **20** (2024), 134.

61. Ankit Mahajan, Jo S. Kurian, Joonho Lee, David R. Reichman, Sandeep Sharma, "Response properties in phaseless auxiliary field quantum Monte Carlo", *Journal of Physical Chemistry*, **159** (2023), 184101. (***Editor's choice***).

60. Lacey J. Wayment, Xubo Wang, Shaofeng Huang, Matthew S. McCoy, Hongxuan Chen, Yiming Hu, Yinghua Jin, Sandeep Sharma, and Wei Zhang, "3D Covalent Organic Framework as a Metastable Intermediate in the Formation of a Double-Stranded Helical Covalent Polymer", *Journal of American Chemical Society* **144** (2023), 15547.

59. Qiucheng Xu, Xubo Wang, Shaofeng Huang, Dr. Yiming Hu, Dr. Simon J. Teat, Dr. Nicholas S. Settineri, Hongxuan Chen, Lacey J. Wayment, Dr. Yinghua Jin, Prof. Sandeep Sharma, Prof. Wei Zhang, "Dynamic Covalent Self-sorting in Molecular and Polymeric Architectures Enabled by Spiroborate Bond Exchange", *Angewandte Chemie International Edition* (2023), **62**, e202304279.

58. Alton, Mitchell; Johnson, Virginia; Sharma, Sandeep; Browne, Eleanor, "Volatile Methyl Siloxane Atmospheric Oxidation Mechanism from Theoretical and Experimental Perspectives – How is the Siloxanol Formed?", *The Journal of Physical Chemistry A*, **127** (2023), 10233.

57. Roland Wilcken, Jun Nishida, Johan F. Triana, Aurelian John-Herpin, Hatice Altug, Sandeep Sharma, Felipe Herrera, Markus Raschke, "Antenna-coupled infrared nanospectroscopy of intramolecular vibrational interaction", *Proceedings of the National Academy of Sciences*, **120** (2023), e2220852120.

56. Xubo Wang, Sandeep Sharma, "Relativistic semistochastic heat-bath configuration interaction", *Journal of Chemical Theory and Computation* **19** (2023), 848.

55. Alon Grinberg Dana, Matthew S Johnson, Joshua W Allen, Sandeep Sharma, Sumathy Raman, Mengjie Liu, Connie W Gao, Colin A Grambow, Mark J Goldman, Duminda S Ranasinghe, Ryan J Gillis, A Mark Payne, Yi-Pei Li, Xiaorui Dong, Kevin A Spiekermann, Haoyang Wu, Enoch E Dames, Zachary J Buras, Nick M Vandewiele, Nathan W Yee, Shamel S Merchant, Beat Buesser, Caleb A Class, Franklin Goldsmith, Richard H West, William H Green, "Automated reaction kinetics and network exploration (Arkane): A statistical mechanics, thermodynamics, transition state theory, and master equation software", *International Journal of Chemical Kinetics* **55** (2023), 300.

54. Ji Yong Choi, Minyan Wang, Brianna Check, Michael Stodolka, Kyle Tayman, Sandeep Sharma, Jihye Park, "Linker-Based Bandgap Tuning in Conductive MOF Solid Solutions", *Small* **19** (2023), 2206988.

53. Ann Lii-Rosales, Virginia L. Johnson, Andrew S. Cavanagh, Andreas Fischer, Thorsten Lill, Sandeep Sharma and Steven M. George, "Effectiveness of Different Ligands on Silane Precursors for Ligand Exchange to Etch Metal Fluorides", *Chemistry of Materials* **34** (2022), 8641.

52. Sandeep Sharma, Alec White, Gregory Beylkin. "Fast exchange with Gaussian basis set using robust pseudospectral method" *Journal of Chemical Theory and Computations*, **18** (2022), 7306.

51. Zepeng Lei, Lacey J Wayment, Jackson R Cahn, Hongxuan Chen, Shaofeng Huang, Xubo Wang, Yinghua Jin, Sandeep Sharma, Wei Zhang. "Cyanurate-Linked Covalent Organic Frameworks Enabled by Dynamic Nucleophilic Aromatic Substitution" *Journal of American Chemical Society* **144** (2022), 17742.

50. Hoai Pham, Ji Yong Choi, Shaofeng Huang, Xubo Wang, Adam Claman, Michael Stodolka, Sadegh Yazdi, Sandeep Sharma, Wei Zhang, Jihye Park, "Imparting Functionality and Enhanced Surface Area to a 2D Electrically Conductive MOF via Macrocyclic Linker", *Journal of American Chemical Society* **144** (2022), 10615.

49. James ET Smith, Joonho Lee, Sandeep Sharma "Near-exact nuclear gradients of complete active space self-consistent field wave functions", *Journal of Chemical Physics* **157** (2022), 094104.

48. Ann Lii-Rosales, Virginia L. Johnson, Sandeep Sharma, Andreas Fischer, Thorsten Lill, and Steven M. George, "Volatile Products from Ligand Addition of P(CH3)3 to NiCl2, PdCl2, and PtCl2: Pathway for Metal Thermal Atomic Layer Etching", *Journal of Physical Chemistry C* **126** (2022), 8287.

47. Ankit Mahajan, Joonhoo Lee, Sandeep Sharma "Selected configuration interaction wave functions in phaseless auxiliary field quantum Monte Carlo", *Journal of Chemical Physics* **156** (2022), 174111 (**Editor's choice award**).

46. Nikolay Bogdanov, Giovanni Li Manni, Sandeep Sharma, Olle Gunnarsson, Ali Alavi "New superexchange paths due to breathing-enhanced hopping in corner-sharing cuprates", *Nature Physics* (accepted for publication).

45. Gregory Beylkin, Sandeep Sharma "A fast algorithm for computing the Boys function", https://arxiv.org/abs/2107.01488, (accepted for publication in Journal of Chemical Physics).

44. Ankit Mahajan, Sandeep Sharma "Taming the Sign Problem in Auxiliary-Field Quantum Monte Carlo Using Accurate Wave Functions", *Journal of Chemical Theory and Computations* **17**(2021), 4786.

43. Sandeep Sharma, Gregory Beylkin "Efficient evaluation of two-center Gaussian integrals in periodic systems", *Journal of Chemical Theory and Computations*, **17** (2021), 3916.

42. Seunghoon Lee, Huanchen Zhai, Sandeep Sharma, Cyrus J. Umrigar, Garnet Kin-Lic Chan "Externally corrected CCSD with renormalized perturbative triples (R-ecCCSD(T)) and density matrix renormalization group and selected configuration interaction external sources ", *Journal of Chemical Theory and Computations* (2021), **17**, 3414.

41. Xiye Yang, Yiming Hu, Nathan Dunlap, Xubo Wang, Shaofeng Huang, Zhiping Su, Sandeep Sharma, Yinghua Jin, Fei Huang, Xiaohui Wang, Se-hee Lee, and Wei Zhang, "Truxenone-based Covalent Organic Framework as All-Solid-State Li-ion Battery Cathode with High Capacity", *Angewandte Chemie International Edition* (2020), **59**, 20385.

40. Ankit Mahajan, Sandeep Sharma, "Efficient local energy evaluation for multi-Slater wave functions in orbital space quantum Monte Carlo", *Journal of Chemical Physics*, (2020), **153**, 194108 ***(Invited article)***

39. Janus J. Eriksen, Tyler A. Anderson, J. Emiliano Deustua, Khaldoon Ghanem, Diptarka Hait, Mark R. Hoffmann, Seunghoon Lee, Daniel S. Levine, Ilias Magoulas, Jun Shen, Norman M. Tubman, K. Birgitta Whaley, Enhua Xu, Yuan Yao, Ning Zhang, Ali Alavi, Garnet Kin-Lic Chan, Martin Head-Gordon, Wenjian Liu, Piotr Piecuch, Sandeep Sharma, Seiichiro L. Ten-no, C. J. Umrigar, Juergen Gauss, "The Ground State Electronic Energy of Benzene", *Journal of Chemical Physics Letters* (2020), **11**, 8922.

38. Nick Blunt, Ankit Mahajan, Sandeep Sharma, "Efficient multireference perturbation theory with high-order reduced density matrices", *Journal of Chemical Physics*, (2020), **153**, 164120.

37. Wyatt Zagorec-Marks, James E. T. Smith, Madison M Foreman, Sandeep Sharma and J. Mathias Weber, "Intrinsic Electronic Spectra of Cryogenically Prepared Protoporphyrin IX Ions inVacuo Deprotonation-Induced Stark Shifts", *Physical Chemistry Chemical Physics*, **22**, 20295. ***(2020 Hot article)***

36. Qiming Sun, Xing Zhang, Samragni Banerjee, Peng Bao, Marc Barbry, Nick S. Blunt, Nikolay A. Bogdanov, George H. Booth, Jia Chen, Zhi-Hao Cui, Janus J. Eriksen, Yang Gao, Sheng Guo, Jan Hermann, Matthew R. Hermes, Kevin Koh, Peter Koval, Susi Lehtola, Zhendong Li, Junzi Liu, Narbe Mardirossian, James D. McClain, Mario Motta, Bastien Mussard, Hung Q. Pham, Artem Pulkin, Wirawan Purwanto, Paul J. Robinson, Enrico Ronca, Elvira R. Sayfutyarova, Maximilian Scheurer, Henry F. Schurkus, James E. T. Smith, Chong Sun, Shi-Ning Sun, Shiv Upadhyay, Lucas K. Wagner, Xiao Wang, Alec White, James Daniel Whitfield, Mark J. Williamson, Sebastian Wouters, Jun Yang, Jason M. Yu, Tianyu Zhu, Timothy C. Berkelbach, Sandeep Sharma, Alexander Yu. Sokolov, and Garnet Kin-Lic Chan, "Recent developments in the PySCF program package", *Journal of Chemical Physics* (2020), **153**, 024109.

35. Kiel T. Williams, Yuan Yao, Jia Li, Li Chen, Hao Shi, Mario Motta, Chunyao Niu, Ushnish Ray, Sheng Guo, Robert J. Anderson, Junhao Li, Lan Nguyen Tran, Chia-Nan Yeh, Bastien Mussard, Sandeep Sharma, Fabien Bruneval, Mark van Schilfgaarde, George H. Booth, Garnet Chan, Shiwei Zhang, Emanuel Gull, Dominika Zgid, Andrew Millis, C. J. Umrigar, Lucas K. Wagner, "Direct comparison of many-body methods for realistic electronic Hamiltonians", *Physical Review X* (2020), **10**, 011041.

34. Junhao Li, Yuan Yao, Adam A Holmes, Matthew Otten, Qiming Sun, Sandeep Sharma, C. J. Umrigar, "Accurate many-body electronic structure near the basis set limit: application to the chromium dimer", *Physical Review Research* (2020), **2**, 012015.

33. Iliya Sabzevari, Ankit Mahajan, Sandeep Sharma, "An accelerated linear method for optimizing non-linear wavefunctions in variational Monte Carlo", *Journal of Chemical Physics* (2020), **152**, 024111.

32. Ankit Mahajan, Nick Blunt, Iliya Sabzevari, Sandeep Sharma, "Multireference configuration interaction and perturbation theory without reduced density matrices", *Journal of Chemical Physics* (2019), **151**, 211102. ***(Invited article and Editor's choice)***

31. Joel W. Clancey, Andrew S. Cavanagh, James E. T. Smith, Sandeep Sharma, Steven M. George, "Volatile etch species produced during thermal Al2O3 atomic layer etching", *Journal of Physical Chemistry C* (2019), **124**, 287.

30. Ankit Mahajan, Sandeep Sharma, "Symmetry projected Jastrow mean field wavefunction in variational Monte Carlo", *Journal of Physical Chemistry A* (2019), **123**, 3911 ***(Invited article)***.

29. Iliya Sabzevari, Sandeep Sharma, "Improved Speed and Scaling in Orbital Space Variational Monte Carlo" *Journal of Chemical Theory and Computations* (2018), **14**, 6276.

28. Junhao Li, Matt Otten, Adam A Holmes, Sandeep Sharma, Cyrus J. Umrigar, "Fast Semistochastic Heat-Bath Configuration Interaction." *Journal of Chemical Physics* (2018), **149**, 214110.

27. B. Mussard, S. Sharma, "One-step treatment of spin-orbit coupling and electron correlation in large active spaces" *Journal of Chemical Theory and Computations* (2018), **14**, 154.

26. Alan D Chien, Adam A Holmes, Matthew Otten, Cyrus J Umrigar, Sandeep Sharma, Paul M Zimmerman, "Excited states of methylene, polyenes, and ozone from heat-bath configuration interaction" *Journal of Physical Chemistry A* (2018), **122**, 2714.

25. Q. Sun, T. C. Berkelbach, N. Blunt, G. H. Booth, J. McClain, S. Guo, Z. Li, J. Liu, S. Sharma, S. Wouters, G. K-L. Chan "The Python-based Simulations of Chemistry Framework (PySCF)." *WIREs Computational molecular science* (2018), **8**, e1340.

24. J. E. T. Smith, B. Mussard, A. A. Holmes, S. Sharma, "Cheap and near exact CASSCF with large active spaces" *Journal of Chemical Theory and Computations* (2017), **13**, 5468. ***(ACS Editors' Choice)***

23. A. A. Holmes, C. J. Umrigar, S. Sharma, "Excited states using semistochastic heat-bath configuration interaction" *Journal of Chemical Physics* (2017), **147**, 164111.

22. T. Yanai, M. Saitow, X.-G. Xiong, J. Chalupsky, Y. Kurashige, S. Guo, S. Sharma, "Multistate Complete-Active-Space Second-Order Perturbation Theory Based on Density Matrix Renormalization Group Reference States" *Journal of Chemical Theory and Computations* (2017), **13**, 4829. ***(ACS Editors' Choice)***

21. S. Sharma, A. A. Holmes, G. Jeanmairet, A. Alavi, C. J. Umrigar, "Semistochastic Heat-bath Configuration Interaction method: selected configuration interaction with semistochastic perturbation theory" *Journal of Chemical Theory and Computations* (2017), **13**, 1595.

20. T. Kawakami, T. Saito, S. Sharma, S. Yamanaka, S. Yamada, T. Nakajima, M. Okumura, K. Yamaguchi, "Full-valence density matrix renormalisation group calculations on meta-benzyne based on unrestricted natural orbitals. Revisit of seamless continuation from broken-symmetry to symmetry-adapted models for diradicals" *Molecular Physics* (2017), **115**, 2267.

19. T. Kawakami, T. Saito, S. Sharma, S. Mitsuo, S. Yamada, Y. Takano, S. Yamanaka, M. Okumura, T. Nakajima, K. Yamaguchi, "UNO DMRG CASCI calculations of effective exchange integrals for m-phenylene-bis-methylene spin clusters." *Molecular Physics* (2017), **115**, 2154.

18. G. Jeanmairet, S. Sharma, A. Alavi, "Stochastic multi-reference perturbation theory with application to linearized coupled cluster method." *Journal of Chemical Physics* (2017), **146**, 044107.

17. S. Sharma, G. Knizia, S. Guo, A. Alavi, "Combining Internally Contracted States and Matrix Product States To Perform Multireference Perturbation Theory." *Journal of Chemical Theory and Computations* (2017), **13**, 488.

PhD/Postdoc Publications

16. S. Sharma, G. Jeanmairet, A. Alavi, "Quasi-degenerate perturbation theory using matrix product states." *Journal of Chemical Physics* (2016), **144**, 034103.
15. S. Sharma, A. Alavi, "Multireference linearized coupled cluster theory for strongly correlated systems using matrix product states." *Journal of Chemical Physics* (2015), **143**, 102815.
14. S. Sharma, "A general non-Abelian density matrix renormalization group algorithm with application to the C2 dimer." *Journal of Chemical Physics* (2015), **142**, 024107.
13. R. Olivares-Amaya, W. Hu, N. Nakatani, S. Sharma, J. Yang, G. K.-L. Chan, "The *ab-initio* density matrix renormalization group in practice" *Journal of Chemical Physics* (2015), **142**, 034102.
12. S. Sharma, G. K.-L. Chan, "Communication: A flexible multi-reference perturbation theory by minimizing the Hylleraas functional with matrix product states." *Journal of Chemical Physics* (2014), **141**, 111101.
11. S. Sharma, K. Sivalingham, F. Neese, G. K.-L. Chan, "Low-energy spectrum of iron-sulfur clusters directly from many-particle quantum mechanics" *Nature Chemistry* (2014), **6**, 927.
10. Y. Shao, Z. Gan et al. "Advances in molecular quantum chemistry contained in the Q-Chem 4 program package." published online *Molecular Physics* (2014).
9. S. Sharma, C. Umrigar, T. Yanai, G. Booth, G. K.-L. Chan, "Spectroscopic accuracy directly from quantum chemistry: Application to ground and excited states of beryllium dimer." *Journal of Chemical Physics* (2014), **140**, 104112.
8. Q. Chen, G. H. Booth, S. Sharma, G. Knizia, G. K.-L. Chan, "Intermediate and spin-liquid phase of the half-filled honeycomb Hubbard model." *Physical Review B* (2014), **89**, 165134.
7. S. Sharma, G. K.-L. Chan, "Spin-adapted density matrix renormalization group algorithms for quantum chemistry." *Journal of Chemical Physics* (2012), **136**, 124121.
6. S. Sharma, S. Raman, W. H. Green, "Quantum calculations of important isomerization reaction rates." *ChemInform*, **43** (2012).
5. G. K.-L. Chan, S. Sharma, "The density matrix renormalization group in quantum chemistry." *Annual Review of Physical Chemistry* (2011), **62**, 465.
4. G. K.-L. Chan, S. Sharma, "Solving problems with strong correlation using the density matrix renormalization group (DMRG)", in: "Solving the Schrödinger equation: has everything been tried?", pp. 43-60, ed. P. Popelier, Imperial College Press, London (2011).
3. S. Sharma, W. H. Green, "Modeling of 1,3-hexadiene, 2,4-hexadiene and 1,4-hexadiene-doped methane flames: flame modeling, benzene and styrene formation." *Combustion and Flame* (2010), **157**, 1331.
2. S. Sharma, S. Raman, W. H. Green, "Intramolecular hydrogen migration in alkylperoxy and hydroperoxyalkylperoxy radicals: accurate treatment of hindered rotors." *Journal of Physical Chemistry A* (2010), **114**, 5689.
1. S. Sharma, W. H. Green, "Computed rate coefficients and product yields for $C_5H_5 + CH_3 \rightarrow$ products." *Journal of Physical Chemistry A* (2009), **113**, 8871.

Invited Talks

Department Seminars and Colloquia

28. *Theoretical chemistry seminar*, Columbia University, New York, December 2023.
27. *Chemistry department seminar*, Yale University, New Haven, November 2023.
26. *Frontiers in chemistry*, California Institute of Technology, Pasadena, March 2023.
25. *Chemistry department seminar*, University of California Los Angeles, Los Angeles, October 2023.
24. *Theoretical Chemistry seminar*, Nagoya University, Nagoya, October 2023.
23. *Chemistry department seminar*, National University of Singapore, Singapore, October 2023.
22. *Theoretical Chemistry seminar*, Kobe University, Kobe, October 2023.
21. *Applied mathematics seminar*, University of California Berkeley, Berkeley, September 2023.
20. *Chemistry department seminar*, University of California Irvine, Irvine, September 2023.
19. *Chemistry department seminar*, University of California Santa Barbara, Santa Barbara, April 2023.
18. *Chemical Physics Seminar*, California Institute of Technology, Pasadena, March 2023.
17. *Chemistry department seminar*, University of Michigan, Ann Arbor, March 2023.
16. *Physical chemistry seminar*, University of Chicago, Chicago, February 2022.
15. *Theory Seminar*, University of Oxford, Virtual presentation, January 2022.
14. *Chemistry Colloquium*, Stanford University, Stanford, May 2021.
13. *Physical chemistry colloquium*, University of Pennsylvania, Philadelphia, May 2021.
12. *Chemistry Colloquium*, University of Southern California, Los Angeles, January 2020.
11. *Physical chemistry seminar*, Purdue University, West Lafayette, January 2020.
10. *Physics Colloquium*, Rutgers University, Newark, January 2020.
9. *Chemistry seminar*, University of Nevada, Reno, September 2019.
8. *Physics Colloquium*, Northeastern University, Boston, April 2019.
7. *Chemistry Seminar*, University of Missouri, September 2018.
6. *Condensed Matter Theory Seminar*, University of Colorado Boulder, April 2018.
5. *Analytical chemistry seminar*, University of Colorado, Boulder, October 2017.
4. *Chemistry Department Seminar*, University of Bochum, July 2016.
3. *Chemistry Department Seminar*, Cambridge University, May 2014.
2. *Theoretical Chemistry Seminar*, Kobe University, October 2014.
1. *Theoretical Chemistry Seminar*, Osaka University, September 2014.

Invited Conference Talks

43. *Quo Vadis Electronic Structure Theory*, Schloss Ringberg, Germany, October 2023.
42. *17th International Congress of Quantum Chemistry*, Bratislava, Slovakia, June 2023.
41. *Kavli Institute for Theoretical Chemistry, Nanoparticle assemblies*, Santa Barbara, April 2023.
40. *Emerging excited-state methods in electronic structure*, Toulouse France, April 2023.
39. *5th Anniversary of the Center for Computational Quantum Physics*, Flatiron Insitute, New York, December 2022.

38. *Quantum Monte Carlo in the Next Decade Workshop*, Flatiron Institute, New York, September 2022.
37. *Operators, Perturbations, Electrons, Relativity, and Multi-Scale Applications workshop*, Ingelheim am Rhein, Germany, September 2022.
36. *American Chemical Society Fall Meeting*, Chicago Illinois, August 2022.
35. *1st Annual PySCF Developers Meeting*, Pasadena California, July 2022.
34. *World Association of Theoretical and Computational Chemists conference*, Vacouver Canada, July 2022.
33. *Institute for Pure and Applied Mathematics: Monte Carlo and Machine Learning Approaches in Quantum Mechanics*, Los Angeles California, May 2022.
32. *Molecular chemistry meets materials science workshop*, Virtual meeting, March 2022.
31. *17th Theoretical Chemistry Symposium*, Virtual meeting, December 2021.
30. *57th Symposium on Theoretical Chemistry*, University of Wuerzburg, Germany, September 2021 (Virtual meeting).
29. *Electronic Structure workshop*, Flatiron Institute, New York city, July 2021 (Virtual meeting).
28. *Stochastic Methods in Electronic Structure Theory*, Telluride, Colorado, July 2021 (Virtual meeting).
27. *New frontiers in electron correlation*, Telluride, Colorado, June 2021 (Virtual meeting).
26. *Tensor product methods for strongly correlated molecular systems*, Dresden, Germany, March 2021 (Virtual meeting).
25. *Ab initio methods in quantum chemistry and nuclear physics*, Paris, France, February 2021 (Virtual meeting).
24. *8th OpenMolcas developer's meeting*, Stuttgart, Germany, June 2020 (Virtual meeting).
23. *Low-scaling and unconventional electronic structure theory*, Telluride, June 2020 (Virtual meeting).
22. *Workshop on strongly correlated electrons*, Qingdao, China, October 2019.
21. *International Society for Theoretical Chemical Physics*, Tromso, Norway, July 2019.
20. *Molecular quantum mechanics*, Heidelberg, Germany, July 2019.
19. *Emergent electronic structure*, Telluride, June 2019.
18. *International conference of quantum chemistry satellite meeting*, Strasbourg, June 2018.
17. *Low-scaling and unconventional electronic structure theory*, Telluride, June 2018.
16. *Auxiliary field quantum Monte Carlo Workshop*, New York city, February 2018.
15. *Stochastic methods in electronic structure theory*, Telluride, July 2017.
14. *European Seminar on Computational Methods in Quantum Chemistry*, Shropshire (UK), July 2017.
13. *New frontiers in electronic structure theory*, Telluride, June 2017.
12. *Canadian chemistry conference*, Toronto, May 2017.
11. *International workshop on massively parallel programming for quantum chemistry and physics*, Kobe, January 2017.
10. *Low scaling and unconventional electronic structure techniques*, Telluride, June 2016.
9. *ACS Spring meeting*, San Diego, March 2016
8. *University of Colorado, Boulder*, January 2016

7. *New frontiers in electron correlation*, Telluride, July 2015.
6. *International conference of quantum chemistry satellite symposium*, Kobe, June 2015.
5. *University of Bristol*, Bristol, May 2015.
4. *Riken Advanced Institute for Computational Science* (Kobe, Japan), October 2014.
3. *European Seminar on Computational Methods in Quantum Chemistry* (Houffalize, Belgium), September 2014.
2. *Watoc satellite conference* (La Coruna, Spain), July 2011.
1. *Pacifichem Conference* (Honolulu, USA) , December 2010.

Conference organization

2. **New Frontiers in Electronic Structure workshop**, June 2021. Organizers: Dominika Zgid (U. Michigan) and Sandeep Sharma (CU Boulder). Organized through Telluride science research center (TSRC). Venue: Virtual meeting.
1. **1st Annual PySCF Developers Meeting**, Juny 2022. Organizers: Garnet Chan (Caltech), Mario Motta (IBM), Nicholas Rubin (Google) and Sandeep Sharma (CU Boulder). Organized with sponsership from IBM, Google Quantum AI and Microsoft Research. Venue: Caltech, Pasadena.

Professional activities and Services

2023 Appointed to the Journal of Chemical Physics Advisory Board, December 2023.
NSF Site review for "The Molecular Sciences Software Institute" in Blacksburg, VA.
Physical chemistry Admissions committee

2022 Hosted Prof. Denis Magero from Apule University in Nigeria by participating in the U.S.-Africa Initiative in Electronic Structure
Chemical physics, graduate student advisor
Organized the conference "1st Annual PySCF Developers Meeting" in Pasadena.
NSF CTMC Panel
NSF Career awards Panel

2021 Chemical physics, graduate student advisor
Organized an international workshop "New frontiers in electronic correlation" in Telluride
DOE reviewer

2020 Physical chemistry Admissions Committee
NSF CTMC Panel
Chemical physics, graduate student advisor
DOE reviewer

2019 Physical chemistry Admissions Committee
Theory search committee
NSF reviewer for two Panels
Chemical Physics executive committee

2018 Physical chemistry Admissions Committee
NSF reviewer for two Panels
Chemical Physics executive committee

2017 Physical chemistry Admissions Committee

Grants

Industry

Lam Research	**co-PI** Machine learning models for atomic layer etching (2016-2022, $600 K).
Qsimulate	**PI** Consultant (2020-2022, $54 K).

Federal

NSF Career Award	**PI** High accuracy methods for electronic structure of molecules and materials (2022-2027, $647 K)
NSF	**PI** Accurate treatment of strong electron correlation in relativistic systems (2018-2022, $405 K)
DOE	**co-PI** Cloud-based Low-Scaling Quantum Chemistry Simulations (2022-2023, $350K)

Philanthropy and non-profit

Camille and Henry Dreyfus Foundation	**PI** Camille dreyfus teacher-scholar award (2022-2024, $100 K)
Caltech University (IQIM)	**PI** Support for sabbatical stay (2023, $50 K)
Sloan Foundation	**PI** Sloan Research Fellowship (2018, $70 K)

Internal

Seed grant CU Boulder	**co-PI** Thinning to Nothing control of decoherence from microscale to molecular quantum opto-mechanics by atomic layer etching (2020, $50 K)
Quest Award (RIO)	**co-PI** Quantum Entanglement in Strongly Spin-Orbit Coupled Matter (2018, $ 50 K)

Teaching accomplishments

University courses taught

Course	Course Name	Semester
CHEM-5581	Introductory Quantum Chemistry	Fall 2016 Fall 2017 Fall 2019
CHEM-4531	Physical Chemistry-2	Spring 2018 Spring 2019 Spring 2021
CHEM-6401	Seminar:Physical Chemistry	Fall 2019 Spring 2020
CHEM-4511	Physical Chemistry-1	Fall 2020
CHEM-5531	Statistical Mechanics	Spring 2022 Spring 2024
CHEM-5501	Advanced topics in PChem	Fall 2022

Non-university courses taught

1. Summer school on electronic structure, Sao Paulo Brazil, 2019.
2. European summer school in quantum chemistry, Pisa Italy, 2023.

Effective teaching workshops attended

Name	Description
Faculty Teaching and Excellence Program	In Spring 2019 Dr. Angela R Bielefeldt conducted a "Classroom Learning Interview Process" for my physical chemistry-2 course.
ASSETT's Gamification	on May 5th I attended a workshop organized by Jacie Moriyama that talked about using games in the classroom.
Center for Teaching and Learning	Inclusive Community of Practice
Center for Teaching and Learning	Overview of what micro-credentials and badges are
Center for Teaching and Learning	Active Listening and Teaching
Center for Teaching and Learning	The 4 C's of Effective Learning

Postdoctoral advising

Adam Holmes	(2016-2017)	Currently a postdoc in Virginia Tech.
Bastien Mussard	(2016-2019)	Currently working in company called "MyScript" developing software for Natural language processing.
Kori Smyser	(2021-present)	

Graduate student advising

Student	Department	Year	Fellowships
James Smith (graduated with PhD in 2020)	Chemistry	2017	GAANN fellowship (2017) MolSSI Phase 1 (2018) MolSSI Phase 2 (fall 2018 to fall 2020) Flatiron Institute Fellowship (2019)
Matthew Mulligan (graduated with MS in 2020)	Chemistry	2017	
Ankit Mahajan (graduated with PhD in 2022)	Chemistry	2017	Sharrah Graduate Fellowship (2019)
Iliya Sabzevari (graduated with PhD in 2022)	Chemistry	2017	Sharrah Graduate Fellowship (2019) GAANN Fellowship (2019) MolSSI Phase 1 (2020)
Xubo Wang (graduated with PhD in 2023)	Chemistry	2017	
Tri Le Hyun (graduated with MS in 2021)	Chemistry	2018	
Virginia Johnson	Chemistry	2019	NSF Graduate Student Fellowship
Minyan Wang	Material Science and Engineering	2019	
Robert Voinescu (graduated with MS in 2021)	Physics	2019	
Ethan Anderson	Physics	2019	
Yichi Zhang	Physics	2021	
Baljit Singh	Chemical Engineering	2023	

Graduate student advisees from other universities

Student	Visit duration
Chaoqun Zhang	Summer 2018 (undergraduate from Zhejiang University)
Olajumoke D Adeyiga	Summer 2019 (graduate student from the University of Nevada, Reno)
Nina Glaser	Spring 2020 (undergraduate from ETH Zurich)
Natalie LeMessurier	Summer 2020 (undergraduate from McGill University)
Sabari Nath Kumar	Summer 2020 (engineer at Rule4)

Other Service

1. I have been on qualifying exams and/or thesis defense of the following students (not including my own)

Department	**Students**
Chemistry	Steve Strong, Peyton Cline, Yisrael Lattke, Laura Maurer, Tri Le, Hayden Hamby, Jessica Murdzek, Marla Devault, Kori Smyser, Joel Clancy, Rebecca Hirsch, Andrew Jensen Robert Wells, Jonathan Partridge, Wyatt Zagorec-Marks, Garrett Evenson, Ryal Dill, Anastasia Jeffreys, Henning Finkenzeller, Austin Mitchell Cano, Mitchell Alton, Liang-chun Lin
Physics	Han Ma, Kyle Gordon, Hao Zheng, Shriya Ramachandran Pai, Thomas Gray, Yu Ping, Garrison Linn, Ty Gardner, Pepei Hao, Pete Johnson, Raythe Owens, Tzu-chi Hseih, Koushik Ganesh, Michael Perlins, Thomas Gray
Chemical Engineering	Jacob Clary, Ryan Tottier
Chemistry (Columbia University)	Sam Greene, Jack Weber

2. I have been a reviewer of article in Joural of chemical theory and computation, Journal of chemical physics, Journal of physical chemistry A, Molecular Physics, Journal of physical chemistry letters, Journal of of computational chemistry, Physical Review B, Physical review letters, International journal of quantum chemistry, Quantum, Nature, Nature quantum information.