Sandeep Sharma

Ekeley M321,
Boulder, Colorado 80309

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

1. 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

2. 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

3. Awards

2023 Visting 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

4. Research

Publications

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* (2022), 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, Jonhoo 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* **18** (2022), 190.

45. Gregory Beylkin, Sandeep Sharma "A fast algorithm for computing the Boys function", *Journal of Chemical Physics* **155** (2021), 174117.

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 nonlinear 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.
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.

Colloquia

16. *Chemistry Colloquium*, University of Chicago, Chicago, Feb 2022.
15. *Chemistry Colloquium*, Stanford University, Stanford, May 2021.
14. *Physical chemistry colloquium*, University of Pennsylvania, Philadelphia, May 2021.
13. *Chemistry Colloquium*, University of Southern California, Los Angeles, January 2021.
12. *Physical chemistry seminar*, Purdue University, West Lafayette, January 2021.

11. *Theory Seminar*, University of California, Berkeley, June 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 Physics Thursday Seminar*, University of Colorado Boulder, April 2018.
5. *Analytical chemistry seminar*, University of Colorado, Boulder, October 2017.
4. *Seminar*, University of Bochum, July 2016.
3. *Seminar*, Cambridge University, May 2014.
2. *Seminar*, Kobe University, October 2014.
1. *Seminar*, Osaka University, September 2014.

Invited Talks

41. *CCQ Anniversary conference*, Flatiron Institute New York, December 2022.
40. *QMC workshop*, Flatiron Insitute New York, September 2022.
39. *OPERA-2020*, Ingelheim am Rhein Germany, August 2022.
38. *ACS meeting*, Chicago Illinios, August 2022.
37. *PySCF conference*, Pasadena California, July 2022.
36. *Watocc 2022*, Vancouver Canada, July 2022.
35. *IPAM meeting*, University of California at Los Angeles, May 2022.
34. *Molecular chemistry meets materials science*, Organized by Molssi NSF, March 2022 (Virtual meeting).
33. *Simons Collaboration on the many electron problem*, Organized by CCQ at the Flatiron institute, February 2022.
32. *Theoretical chemistry symposium*, Kolkata, India, December 2021 (Virtual meeting).
31. *57th Symposium on Theoretical Chemistry*, University of Wuerzburg, Germany, September 2021 (Virtual meeting).
30. *Electronic Structure workshop*, Flatiron Institute, New York city, July 2021 (Virtual meeting).
29. *Stochastic Methods in Electronic Structure Theory*, Telluride, Colorado, July 2021 (Virtual meeting).
28. *New frontiers in electron correlation*, Telluride, Colorado, June 2021 (Virtual meeting).
27. *Tensor product methods for strongly correlated molecular systems*, Dresden, Germany, March 2021 (Virtual meeting).
26. *Ab initio methods in quantum chemistry and nuclear physics*, Paris, France, February 2021 (Virtual meeting).
25. *8th OpenMolcas developer's meeting*, Stuttgart, Germany, June 2020 (Virtual meeting).
24. *Low-scaling and unconventional electronic structure theory*, Telluride, June 2020 (Virtual meeting).
23. *Sanibel meeting*, St. Simons Island, February 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. *ICQC satellite meeting*, Strasbourg, June 2018.
17. *Low-scaling and unconventional electronic structure theory*, Telluride, June 2018.

16. *AFQMC 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. *LUEST*, 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. *ICQC 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.