# Nicholas J. Mayhall


**Contact Information**

Department of Chemistry (0212)
480 Davidson Hall
Virginia Tech
900 W. Campus Drive
Blacksburg, VA 24061

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## Education

| | | | |
|---|---|---|---|
| Ph.D. | Indiana University, Bloomington, IN | Computational Chemistry | 2011 |
| B.S. | University of Southern Indiana, Evansville, IN | Chemistry | 2006 |

## Experience

Associate Professor — 2021 - Present
Virginia Tech

Assistant Professor — 2015 - 2021
Virginia Tech

Visiting Scientist — 2020, Jan-May
Simons Institute, University of CA - Berkeley

Post-Doctoral Associate — 2011 - 2015
University of CA – Berkeley
Research group of Prof. Martin Head-Gordon

Graduate Research Assistant — 2007 - 2011
Indiana University
Research group of Prof. Krishnan Raghavachari

Graduate Student Instructor — 2006 - 2007
Indiana University
General Chemistry I Lab with Prof. Todd Stone
General Chemistry II with Prof. Srinivasan Iyengar

Undergraduate Teaching Assistant — 2005 - 2006
University of Southern Indiana
Physical Chemistry I and II with Prof. Evan Millam

REU Undergraduate Researcher — 2005, May-July
University of Memphis
Research group of Prof. Ted Burkey

## Awards

| | | |
|---|---|---|
| John C. Schug Research Award | VT | 2023 |
| Alfred P. Sloan Research Fellow | VT | 2021 |
| NSF Career Award | VT | 2018 |
| ACS PHYS Division Postdoctoral Research Awards | UC Berkeley | 2014 |
| Richard Slagle Fellowship | Indiana University | 2010 |
| E.M. Kratz Fellowship | Indiana University | 2009 |
| Felix Haurowitz Award | Indiana University | 2009 |
| E. Campaigne C500 Award | Indiana University | 2008 |
| Academic Achievement Award for Chemistry | USI | 2006 |
| Outstanding Achievement Award in Physical Chemistry | USI | 2005 |
| Integra Bank Distinguished Professor Scholar | USI | 2005 |
| O. John Logsdon Chemistry Scholarship | USI | 2005 |
| CRC Freshman Chemistry Achievement Award | USI | 2003 |

## Publications

71 **TEPID-ADAPT: Adaptive variational method for simultaneous preparation of low-temperature Gibbs and low-lying eigenstates**
Bharath Sambasivam, Kyle Sherbert, Karunya Shirali, Nicholas J. Mayhall, Edwin Barnes, Sophia E. Economou
Submitted, (2025)

70 **Reducing the Resources Required by ADAPT-VQE Using Coupled Exchange Operators and Improved Subroutines**
Mafalda Ramôa, Panagiotis G. Anastasiou, Luis Paulo Santos, Nicholas J. Mayhall, Edwin Barnes, Sophia E. Economou
Submitted, (2024)

69 **How to really measure operator gradients in ADAPT-VQE**
Panagiotis G. Anastasiou, Nicholas J. Mayhall, Edwin Barnes, Sophia E. Economou
Submitted, (2024)

68 **Minimal evolution times for fast, pulse-based state preparation in silicon spin qubits**
Christopher K. Long, Nicholas J. Mayhall, Sophia E. Economou, Edwin Barnes, Crispin H. W. Barnes, Frederico Martins, David R. M. Arvidsson-Shukur, Normann Mertig
*npj Quantum Information*, Accepted (2025)

67 **How Much Entanglement Do Quantum Optimization Algorithms Require?**
Yanzhu Chen, Linghua Zhu, Chenxu Liu, Nicholas J. Mayhall, Edwin Barnes, Sophia E. Economou
Submitted, (2022)

66 **Adaptive variational algorithms for quantum Gibbs state preparation**
Ada Warren, Linghua Zhu, Nicholas J. Mayhall, Edwin Barnes, Sophia E. Economou
Submitted, (2022)

**Published**

65 **Parameterization and optimizability of pulse-level VQEs**
Kyle M Sherbert, Hisham Amer, Sophia E Economou, Edwin Barnes, Nicholas J. Mayhall
*Physical Review Applied*, Accepted (2025)

64 **Lewis Base Enhanced C–H Bond Functionalization Mediated by A Diiron Imido Complex**
Reilly K. Gwinn, Trevor P. Latendresse, Owen N. Beck, Carla Slebodnik, Nicholas J. Mayhall, Claire Casady, and Diana A. Thornton
*Inorganic Chemistry*, ASAP (2025)

63 **Reducing measurement costs by recycling the Hessian in adaptive variational quantum algorithms**
Mafalda Ramôa, Luis Paulo Santos, Nicholas J. Mayhall, Edwin Barnes, Sophia E. Economou
*Quantum Science and Technology*, 10, 015031 (2025)

62 **Restricted Open-shell cluster Mean-Field theory for Strongly Correlated Systems**
Arnab Bachhar, Nicholas J. Mayhall
*Journal of Physical Chemistry A*, 128, 41, 9015 (2024) "Gustavo Scuseria Festschrift "

61 **Physically motivated improvements of Variational Quantum Eigensolvers**
Nonia Vaquero-Sabater, Abel Carreras, Román Orús, Nicholas J. Mayhall, David Casanova
*Journal of Chemical Theory and Computation*, 20, 5133 (2024)

60 **Accurate and Interpretable Representation of Correlated Electronic Structure via Tensor Product Selected CI**
Nicole M. Braunscheidel, Arnab Bachhar, Nicholas J. Mayhall
*Faraday Discussions*, 254, 130-156 (2024)

59 **Tribute to Krishnan Raghavachari**
Hrant P. Hratchian, Amir Karton, Nicholas J. Mayhall
*Journal of Physical Chemistry A*, 13, 2523 (2024)

58 **Scaling adaptive quantum simulation algorithms via operator pool tiling**
John S. Van Dyke, Karunya Shirali, George S. Barron, Nicholas J. Mayhall, Edwin Barnes, Sophia E. Economou
*Phys. Rev. Res.* 6, 013254 (2024)

57 **TETRIS-ADAPT-VQE: An adaptive algorithm that yields shallower, denser circuit ansätze**
Panagiotis G. Anastasiou, Yanzhu Chen, Nicholas J. Mayhall, Edwin Barnes, Sophia E. Economou
*Phys. Rev. Res.* 6, 013254 (2024)

56 **Quantum simulation of molecular response properties**
Ashutosh Kumar, Ayush Asthana, Vibin Abraham, T. Daniel Crawford, Nicholas J. Mayhall, Yu Zhang, Lukasz Cincio, Sergei Tretiak, Pavel A. Dub
*Journal of Chemical Theory and Computation* 19, 24, 9136 (2023)

55 **Generalization of the tensor product selected CI method for molecular excited states**
Nicole M. Braunscheidel, Vibin Abraham, Nicholas J. Mayhall
*Journal of Physical Chemistry*, 39, 8179 (2023) "Krishnan Raghavachari Festschrift "

54 **Leakage Reduces Device Coherence Demands for Pulse-Level Molecular Simulation**
Ayush Asthana, Chenxu Liu, Oinam Romesh Meitei, Sophia E. Economou, Edwin Barnes, Nicholas J. Mayhall
*Physical Review Applied*, 19, 064071 (2023)

53 **Avoiding symmetry roadblocks and minimizing the measurement overhead of adaptive variational quantum eigensolvers**
V. O. Shkolnikov, Nicholas J. Mayhall, Sophia E. Economou, Edwin Barnes
*Quantum*, 7, 1040 (2023)

52 **Adaptive, problem-tailored variational quantum eigensolver mitigates rough parameter landscapes and barren plateaus**
Harper R. Grimsley, George S. Barron, Edwin Barnes, Sophia E. Economou, Nicholas J. Mayhall
*npj Quantum Information*, 19 (2023)

51 **Equation-of-motion variational quantum eigensolver method for computing molecular excitation energies, ionization potentials, and electron affinities**
Ayush Asthana, Ashutosh Kumar, Vibin Abraham, Harper Grimsley, Yu Zhang, Lukasz Cincio, Sergei Tretiak, Pavel A. Dub, Sophia E. Economou, Edwin Barnes, Nicholas J. Mayhall
*Chemical Science*, (2023)

50 **New Local Explorations of the Unitary Coupled Cluster Energy Landscape**
Harper R. Grimsley and Nicholas J. Mayhall
*Journal of Chemical Theory and Computation*, 18, 7350 (2022)

49 **Symmetry breaking slows convergence of the ADAPT Variational Quantum Eigensolver**
Luke W. Bertels, Harper R. Grimsley, Sophia E. Economou, Edwin Barnes, Nicholas J. Mayhall
*Journal of Chemical Theory and Computation*, 18, 6656 (2022)

48 **ONIOM Method with Charge Transfer Corrections (ONIOM-CT): Analytic Gradients and Benchmarking**
Vikrant Tripathy, Nicholas J. Mayhall, and Krishnan Raghavachari *Journal of Chemical Theory and Computation*, 18, 6052,(2022)

47 **Adaptive quantum approximate optimization algorithm for solving combinatorial problems on a quantum computer**
Linghua Zhu, Ho Lun Tang, George S. Barron, Nicholas J. Mayhall, Edwin Barnes, Sophia E. Economou
*Phys. Rev. Research*, 4, 033029 (2022)

46 **Coupled electron pair-type approximations for tensor product state wavefunctions**
Vibin Abraham and Nicholas J. Mayhall
*Journal of Chemical Theory and Computation* 18, 4856 (2022)

45 **Preparing Bethe Ansatz Eigenstates on a Quantum Computer**
John S. Van Dyke, George S. Barron, Nicholas J. Mayhall, Edwin Barnes, Sophia E. Economou
PRX Quantum, 2, 040329 (2021)

44 **Gate-free state preparation for fast variational quantum eigensolver simulations**
Oinam Romesh Meitei*, Bryan T. Gard*, George S. Barron, David P. Pappas, Sophia E. Economou, Edwin Barnes, Nicholas J. Mayhall
*npj Quantum Information*, 7, 155 (2021), *Co-first authors

43 **Revealing the Contest between Triplet–Triplet Exchange and Triplet-Triplet Energy Transfer Coupling in Correlated Triplet Pair States in Singlet Fission**
Vibin Abraham, Nicholas J. Mayhall
*Journal of Physical Chemistry Letters*, 12, 10505-10514 (2021)

42 **Preserving Symmetries for Variational Quantum Eigensolvers in the Presence of Noise**
George S. Barron, Bryan T. Gard, Orien J. Altman, Nicholas J. Mayhall, Edwin Barnes, and Sophia E. Economou
*Phys. Rev. Applied*, 16, 034003 (2021)

41 **Software for the frontiers of quantum chemistry: An overview of developments in the Q-Chem 5 package**
E. Epifanovsky, et al.
*Journal of Chemical Physics*, 155, 084801 (2021)

40 **Cluster many-body expansion: a many-body expansion of the electron correlation energy about a cluster mean-field reference**
Vibin Abraham, Nicholas J. Mayhall
*Journal of Chemical Physics*, 155, 054101 (2021) **Invited article** | **Editor's Pick**

39 **qubit-ADAPT-VQE: An adaptive algorithm for constructing hardware-efficient ansatze on a quantum processor**
Ho Lun Tang, Edwin Barnes, Harper R. Grimsley, Nicholas J. Mayhall, Sophia E. Economou
*PRX Quantum*, 2, 020310 (2021)

38 **Spin-flip pair-density functional theory: A practical approach to treat static and dynamical correlations in large molecules**
Oinam Romesh Meitei, Nicholas J. Mayhall
*Journal Chemical Theory and Computation*, 17, 2906–2916 (2021)

37 **Selected Configuration Interaction in a Basis of Cluster State Tensor Products**
Vibin Abraham and Nicholas J. Mayhall
*Journal Chemical Theory and Computation*, 16, 10, 6098–6113 (2020)

36 **Spin-Orbit Matrix Elements for a Combined Spin-Flip and IP/EA Approach**
Oinam Meitei, Shannon Houck, Nicholas J. Mayhall
*Journal Chemical Theory and Computation*, 16, 3597 (2020)

35 **Efficient Symmetry-Preserving State Preparation Circuits for the Variational Quantum Eigensolver Algorithm**
B. T. Gard, L. Zhu, G. S. Barron, N. J. Mayhall, S. E. Economou, E. Barnes
*npj Quantum Information*, 6, 10 (2020)

34 **Is the Trotterized UCCSD Ansatz usefully well-defined?**
Harper R. Grimsley, Daniel Claudino, Edwin Barnes, Sophia E. Economou, and N. J. Mayhall
*Journal Chemical Theory and Computation*, 16, 1-6 (2020)

33 **Simple and efficient truncation of virtual spaces in embedded wave functions via concentric localization**
D. Claudino and N. J. Mayhall
*Journal Chemical Theory and Computation*, 15, 6085 (2019)

32 **Multireference Ab Initio Studies of Magnetic Properties of Terbium-Based Single-Molecule Magnets**
R. Pederson, A. L. Wysocki, N. J. Mayhall, and K. Park
*Journal of Physical Chemistry A*, 123, 6996-7006 (2019)

31 **An adaptive variational algorithm for exact molecular simulations on a quantum computer**
H. R. Grimsley, S. E. Economou, Edwin Barnes, and N. J. Mayhall
*Nature Communications*, 10, 3007 (2019)

30 **A Combined Spin-Flip and IP/EA Approach for Handling Spin and Spatial Degeneracies: Application to Double Exchange Systems**
S. Houck and N. J. Mayhall
*Journal of Chemical Theory and Computation*, 15, 2278-2290 (2019)

29 **Automatic Partition of Orbital Spaces Based on Singular Value Decomposition in the Context of Embedding Theories**
D. Claudino and N. J. Mayhall
*Journal of Chemical Theory and Computation*, 15, 1053-1064 (2019)

28 **Negative exchange interactions in coupled few-electron quantum dots**
K. Deng, F. A. Calderon-Vargas, N. J. Mayhall, E. Barnes
*Phys. Rev. B*, 97, 245301, (2018)

27 **A Simple Rule to Predict Boundedness of Multi-Exciton States in Covalently-Linked Singlet Fission Dimers**
V. Abraham and N. J. Mayhall
*Journal of Physical Chemistry Letters*, 8, 5472-5478, (2017)

26 **Using Higher-Order Singular Value Decomposition To Define Weakly Coupled and Strongly Correlated Clusters: The $n$-Body Tucker Approximation**
N. J. Mayhall
*Journal of Chemical Theory and Computation*, 13, 4818-4828, (2017)

25 **From model Hamiltonians to ab initio Hamiltonians and back again: Using single excitation quantum chemistry methods to find multiexciton states in singlet fission materials**
N. J. Mayhall
*Journal of Chemical Theory and Computation*, 12, 4263-4273, (2016)

**Prior To Virginia Tech**

24 **Computational Quantum Chemistry For Multiple Site Heisenberg Spin Couplings Made Simple: Still Only One Spin Flip Required**
N. J. Mayhall and M. Head-Gordon
*Journal of Physical Chemistry Letters*, 6, 1982-1988, (2015)

23 **Advances in molecular quantum chemistry contained in the Q-Chem 4 program package**
Y. Shao, et al.
*Molecular Physics*, 113, 184-215, (2014)

22 **Computational quantum chemistry for single Heisenberg spin couplings made simple: Just one spin flip required**
N. J. Mayhall and M. Head-Gordon
*Journal of Chemical Physics*, 141, 134111, (2014)

21 **Spin-Flip Non-Orthogonal Configuration Interaction: A variational and almost black-box method for describing strong correlation**
N. J. Mayhall, P. Horn, E. J. Sundstrom, and M. Head-Gordon
*Physical Chemistry Chemical Physics*, 16, 22694-22705, (2014)

20 **Increasing spin-flips and decreasing cost: Perturbative corrections for external singles to the complete active space spin flip model for low-lying excited states and strong correlation**
N. J. Mayhall and M. Head-Gordon
*The Journal of Chemical Physics*, 141, 044112, (2014)

19 **A Quasidegenerate Second-Order Perturbation Theory Approximation to RAS-*n*SF for Excited States and Strong Correlations**
N. J. Mayhall, M. Goldey, and M. Head-Gordon
*Journal of Chemical Theory and Computation*, 10, 589-599, (2014)

18 **On the Formation of Silacyclopropenylidene ($c$-$SiC_2H_2$) and its Role in the Organosilicon Chemistry in the Interstellar Medium**
D. S. N. Parker, A. V. Wilson, R. I. Kaiser, N. J. Mayhall, M. Head-Gordon, and A. G. G. M. Tielens
*The Astrophysical Journal*, 770, 33, (2013)

17 **A Composite Energy Treatment for Sterically Hindered Cluster Models for the Si(100) Surface**
B. C. Gamoke, N. J. Mayhall, and K. Raghavachari
*Journal of Chemical Theory and Computation*, 8, 5132-5136, (2012)

16 **Many-Overlapping-Body (MOB) Expansion: A Generalized Many Body Expansion for Nondisjoint Monomers in Molecular Fragmentation Calculations of Covalent Molecules**

N. J. Mayhall and K. Raghavachari
*Journal of Chemical Theory and Computation*, 8, 2669-2675, (2012)

15 **Modeling Nonperiodic Adsorption on Periodic Surfaces: A Composite Energy Approach for Low-Coverage Limits**
B. C. Gamoke, N. J. Mayhall, and K. Raghavachari
*Journal of Physical Chemistry C*, 116, 12048-12054, (2012)

14 **Properties of metal oxide clusters in non-traditional oxidation states**
J. E. Mann, N. J. Mayhall, and C. C. Jarrold
*Chemical Physics Letters*, 525-526, 1-12, (2012)

13 **Molecules-in-Molecules: A Hybrid-Energy Fragmentation Approach for Accurate Calculations on Large Molecules and Materials**
N. J. Mayhall and K. Raghavachari
*Journal of Chemical Theory and Computation*, 7, 1336-1343, (2011)

12 **Molybdenum Oxides vs. Molybdenum Sulfides: Geometric and Electronic Structures of $Mo_3X_y^-$ (X=O, S and y=6, 9) Clusters**
N. J. Mayhall, E. L. Becher, A. Chowdhury, K. Raghavachari
*Journal of Physical Chemistry A*, 115, 2291-2296, (2011)

11 **Charge transfer across ONIOM QM:QM boundaries: The impact of model system preparation**
N. J. Mayhall and K. Raghavachari
*Journal of Chemical Theory and Computation*, 6, 3131-3136 (2010)

10 **A Proton Hop Paves the Way for Hydroxyl Migration: Theoretical Elucidation of Fluxionality in Transition Metal Oxide Clusters**
R. Ramabhadran, N. J. Mayhall, K. Raghavachari
*Journal of Physical Chemistry Letters*, 1, 3066-3071 (2010)

9 **Multiple solutions to the single-reference CCSD equations for NiH**
N. J. Mayhall, K. Raghavachari
*Journal of Chemical Theory and Computation*, 6, 2714 (2010)

8 **ONIOM-based QM:QM electronic embedding method using Löwdin atomic charges: Energies and analytic gradients**
N. J. Mayhall, K. Raghavachari, H. P. Hratchian
*Journal of Chemical Physics*, 132, 114107 (2010)

7 **Termination of the $W_2O_y^-$ + $H_2O/D_2O \rightarrow W_2O_{y+1}^-$+$H_2/D_2$ sequential oxidation reaction: An exploration of kinetic versus thermodynamic effects**
D. W. Rothgeb, E. Hossain, N. J. Mayhall, K. Raghavachari, C. C. Jarrold
*Journal of Chemical Physics*, 131, 144306 (2009)

6 **Water Reactivity with Tungsten Oxides: $H_2$ Production and Kinetic Traps**
N. J. Mayhall, D. W. Rothgeb, E. Hossain, C. C. Jarrold, K. Raghavachari
*Journal of Chemical Physics*, 131, 144302 (2009)

5 **Electronic structures of $MoWO_y^-$ and $MoWO_y$ determined by anion photoelectron spectroscopy and DFT calculations**
N. J. Mayhall, D. W. Rothgeb, E. Hossain, K. Raghavachari, C. C. Jarrold
*Journal of Chemical Physics*, 130, 124313 (2009)

4 **Investigation of G4 Theory for Transition Metal Thermochemistry**
N. J. Mayhall, K. Raghavachari, P. C. Redfern, L. A. Curtiss
*Journal of Physical Chemistry A*, 113 5170-5175 (2009)

3 **Unusual products observed in gas-phase $W_xO_y^-$ + $H_2O$ and $D_2O$ reactions**
D. W. Rothgeb, E. Hossain, A. T. Kuo, J. L. Troyer, C. C. Jarrold, N. J. Mayhall, K. Raghavachari
*Journal of Chemical Physics*, 130, 124314 (2009)

2 **Toward accurate thermochemical models for transition metals: G3Large basis sets for atoms Sc-Zn**
N. J. Mayhall, K. Raghavachari, P. C. Redfern, L. A. Curtiss, V. Rassolov
*Journal of Chemical Physics*, 128, 144122 (2008)

1 **Two Methanes are Better than One: A Density Functional Theory Study of the Reactions of $Mo_2O_y^-$ (y = 2-5) with Methane**
N. J. Mayhall, K. Raghavachari
*Journal of Physical Chemistry A*, 111, 8211-8217 (2007)

## Project Funding

- **Quantum Utility with hardware- and application- Informed Near-Term Algorithms (QUINTA)**

| | |
|---|---|
| PI | Edwin Barnes |
| co-PIs | Mayhall, Sophia Economou, Sumeet Khatri, Lex Kemper, Murphy Niu |
| Source of Support | Department of Energy |
| Total award amount | $4,800,000 (Mayhall's budget $800,000) |
| Total award period | 2024 - 2029 |

- **EAGER: Quantum-inspired Electronic Structure**

| | |
|---|---|
| PI | Mayhall |
| co-PIs | – |
| Source of Support | National Science Foundation |
| Total award amount | $300,000 |
| Total award period | 07/24 - 07/26 |

- **Exploiting sparsity and locality in ab initio open quantum systems**

| | |
|---|---|
| PI | Mayhall |
| co-PIs | Edwin Barnes |
| Source of Support | Dept. of Energy |
| Total award amount | $570,000 |
| Total award period | 08/23 - 07/26 |

- **Alfred P. Sloan Research Fellow**

| | |
|---|---|
| PI | Mayhall |
| co-PIs | – |
| Source of Support | Alfred P. Sloan Foundation |
| Total award amount | $75,000 |
| Total award period | Sept. 2021 - Sept. 2023 |

- **CAREER: Many-body expansions for strongly correlated systems**

| | |
|---|---|
| PI | Mayhall |
| co-PIs | – |
| Source of Support | National Science Foundation |
| Total award amount | $575,305 |
| Total award period | Apr.1, 2018 - Dec. 2024 |
| Award Number | 1752612 |

- **Simulating strongly correlated molecules with a superconducting processor**

| | |
|---|---|
| PI | Mayhall |
| co-PIs | Sophia Economou, Edwin Barnes, David Pappas |
| Source of Support | Department of Energy |
| Total award amount | $1,875,000 (Mayhall's budget $308,871) |
| Total award period | Sept. 15, 2018 - Sep. 14, 2021 |
| Award Number | DE-SC0019199 |

- **Ab initio design of quantum molecular magnets for information applications**

| | |
|---|---|
| PI | Edwin Barnes |
| co-PIs | Mayhall, Sophia Economou, Kyunghwa Park |
| Source of Support | Department of energy |
| Total award amount | $1,800,000 (Mayhall's budget $610,526 ) |
| Total award period | Sept.1, 2017 - Aug. 31, 2021 |
| Award Number | DE-SC0018326 |

- **RAISE: TAQS: Fast multiqubit control of high-coherence transmons for efficient quantum chemistry simulations**

| | |
|---|---|
| PI | Sophia Economou |
| co-PIs | Mayhall, Edwin Barnes, David Pappas |
| Source of Support | National Science Foundation |
| Total award amount | $1,000,000 (Mayhall's budget $226,316) |
| Total award period | Oct.1, 2018 - Sep. 31, 2022 |
| Award Number | 1839136 |

- **QLCI-CG: Center for Interdisciplinary Research in Quantum Information Theory and Simulation**

| | |
|---|---|
| PI | Sophia Economou |
| co-PIs | Mayhall, Edwin Barnes, Kyunghwa Park |
| Source of Support | National Science Foundation |
| Total award amount | $118,125 (Mayhall's budget 25%) |
| Total award period | Sept. 1, 2019 - Aug 31, 2020 |
| Award Number | 1936726 |

## Service

- Editorial Advisory Board

  Journal of Physical Chemistry Letters

- Reviewer

  Journal of Chemical Physics
  Journal of Chemical Theory and Computation
  Journal of Physical Chemistry
  Physical Chemistry Chemical Physics
  Chemical Science
  Journal of Physical Chemistry Letters
  Molecular Physics
  Chemical Physics Letters
  Nature Communications
  Advanced Quantum Technologies
  Quantum

- Guest editing

  *Krishnan Raghavachari Festschrift*, J. Phys. Chem. A (2024)

- Symposium Organization

  *Exploring Transition Metal Chemistry & Spectroscopy with Quantum Chemistry*, National ACS Meeting in San Diego (2019)
  *COMP: Krishnan Raghavachari Tribute*, National ACS Meeting in New Orleans (2024)

- Conference Organization

  *Virginia Tech Quantum Swiss Summer Workshop (2023)*

## Book Chapters

- *Projection-Based Molecular Quantum Embedding via Singular-Value-Informed Orbital Partitioning*
  D. Claudino, R. Smith, & N. J. Mayhall
  in *Comprehensive Computational Chemistry*
  Editor(s): Manuel Yáñez, Russell J. Boyd,
  Comprehensive Computational Chemistry (First Edition),
  Elsevier,
  Pages 111-120 (2024)

- *Energy Transfer in Metal Organic Frameworks*
  J. Zhu, S. Shaikh, N. J. Mayhall, & A. Morris
  in *Elaboration and Applications of Metal-Organic Frameworks*
  Editor: S. Ma
  World Scientific Publishers/Imperial College Press (2017)

## Students/Postdocs Mentored

Kyle Sherbert (postdoc)

Harjeet Singh (grad student)

Arnab Bachhar (grad student)

Riley Porteus (grad student)

Chinmay Shrikhande (grad student)

Ayush Asthana (postdoc, now Assist. Prof. at U. of North Dakota)

Luke Bertels (postdoc, now Wigner Fellow at ORNL)

Diksha Dhawan (postdoc, now at Xanadu)

Nicole Braunscheidel (grad student)

Robert Smith (grad student)

Harper Grimsley (grad student, now postdoc at Emory - Evangelista group)

Shannon Houck (grad student, now at QChem)

Vibin Abraham (grad student, now at U. of Michigan - Zgid group)

Daniel Claudino (postdoc, now Staff at Oakridge National Lab)

Oinam Meitei (postdoc, now at MIT - Van Voorhis group)

## Courses Taught

CHEM/PHYS 3684: Quantum Software I (Developed)

CHEM/PHYS 4684: Quantum Software II (Developed)

CHEM 4616: Physical Chemistry for Life Sciences (Thermo)

CHEM 6634: Quantum Chemistry and Spectroscopy

CHEM 3616: Physical Chemistry

## Presentations

- **Invited Talk:** *Intro to modeling chemistry with VQE's*
  APS March Meeting, Anaheim, CA, March 16 (2025)
- **Invited Talk:** *Fast state preparation for electronic structure theory on quantum computers*
  Sanibel Symposium, St. Augustine, FL, February 27 (2025)
- **Invited Talk:** *Outrunning decoherence: Fast state preparation for studying molecules with quantum computers*
  Indiana University, Bloomington, IN, (2025)
- **Invited Talk:** *Chemistry via Quantum Computing*
  University of Southern Indiana, Evansville, IN, Oct 11 (2024)
- **Invited Talk:** *Accurate and Interpretable Representation of Correlated Electronic Structure via Tensor Product Selected CI*
  Faraday Discussions, London, UK, July 17 (2024)
- **Invited Talk:** *Outrunning Decoherence: Fast state preparation for studying molecules with quantum computers*
  MIT, GBA Theochem Seminar, Boston, MA, April 17 (2024)
- **Invited Talk:** *Accurate and interpretive electronic structure via Tensor Product State methods*
  ACS National Meeting, New Orleans, LA, March 19 (2024)
- **Invited Talk:** *Outrunning Decoherence: Fast state preparation for studying molecules with quantum computers*
  UNC Charlotte, Nanoscale Science Seminar, Jan 25 (2024)
- **Invited Talk:** *Electronic structure theory via Classical and Quantum Computation*
  UCLA, IPAM, Nov 6 (2023)
- **Invited Talk:** *Outrunning decoherence: Fast state preparation for studying molecules with quantum computers*
  University of Memphis, Chemistry Seminar, Oct 6 (2023)
- **Invited Talk:** *Fast state preparation for variational quantum algorithms*
  ACS National Meeting, San Francisco, CA, August 16 (2023)
- **Invited Talk:** *New tensor product state approximations for strongly correlated molecules*
  ICQC Satellite Meeting on Strong Correlation in Molecules, Znojmo, Czech Republic, June 21 (2023)
- **Invited Talk:** *Fast state preparation for variational quantum algorithms*
  Hitachi Cambridge Laboratory, University of Cambridge, Cambridge UK, March 16 (2023)
- **Invited Talk:** *Fast state preparation for variational quantum algorithms to outrace decoherence*
  New Trends in Computational Chemistry, iqtc, Barcelona, Spain, August 24 (2022)
- **Invited Talk:** *Fast state preparation for variational quantum algorithms*
  Psi-k 2022, Lausanne, Switzerland, August 24 (2022)
- **Invited Talk:** *Outrunning quantum decoherence: Fast state preparation for variational quantum algorithms*
  ACS National Meeting, Chicago, IL, August 21 (2022)
- **Invited Plenary Talk:** *Fast state preparation for variational quantum algorithms to outrace decoherence on near term quantum computers*
  MQM 2022, Blacksburg, VA, June 28 (2022)

- **Invited Talk:** *Fast state preparation for variational quantum algorithms to outrace decoherence on near term quantum computers*
  CCCE 2022, Calgary, Canada, June 17 (2022)
- **Invited Talk:** *Outrunning Quantum Decoherence: Fast State Preparation for Variational Quantum Algorithms*
  Optica Quantum 2.0, Boston, MA, June 13 (2022)
- *Course-grained electronic structure for modeling molecular qubits*
  ACS National Meeting, San Diego, CA, March 23 (2022)
- *Fast state preparation for variational quantum algorithms to outrace decoherence*
  ACS National Meeting, San Diego, CA, March 20 (2022)
- *Gate-free state preparation for fast variational quantum eigensolver simulations: ctrl-VQE*
  APS March Meeting, Chicago, IL, March 15 (2022)
- **Invited Talk:** *Towards discovery in chemistry with quantum computers*
  APS March Meeting, Chicago, IL, March 14 (2022)
- **Invited Talk:** *Outrunning decoherence: fast state preparation for accurate, near-ish-term variational quantum computing*
  University of Michigan, Ann Arbor, MI, Dec 9 (2021)
- **Invited Talk:** *Outrunning decoherence: fast state preparation for accurate, near-ish-term variational quantum computing*
  Theory and Simulation of Electronic and Optical Processes in Molecules and Materials, Dec 1 (2021)
- **Invited Talk:** *Gate-free state preparation for fast variational quantum eigensolver simulations: ctrl-VQE*
  Practical Intermediate Representation for Quantum (PIRQ) Workshop, QED-C, July 30 (2021)
- **Invited Talk:** *Selected Configuration Interaction in a Basis of Cluster State Tensor Products*
  Virtual New Frontiers in Electron Correlation, Telluride, CO, June 17 (2021)
- **Invited Talk:** *Selected Configuration Interaction in a Basis of Cluster State Tensor Products*
  Tensor Methods and their Applications in the Physical and Data Sciences, IPAM, UCLA, April 1 (2021)
- **Invited Talk:** *Selected Configuration Interaction in a Basis of Cluster State Tensor Products*
  TPMSCM21, Dresden, Germany, March 10 (2021)
- **Invited Talk:** *Outrunning decoherence: Fast state preparation for studying molecules with quantum computers*
  University of South Dakota, Chemistry Seminar, Nov. 9 (2020)
- **Invited Talk:** *Outrunning decoherence: Fast state preparation to increase the accuracy of near-term variational quantum computing*
  Ohio State University, Physical Chemistry Seminar, Oct. 5 (2020)
- **Invited Talk:** *Quasi-optimally compact ansatze for quantum chemistry VQE simulations*
  Psi-k 2020, EPFL, Lausanne, Switzerland, Sept 14-17 (2020) (Cancelled for COV-19)
- **Invited Talk:** *Using quantum computers to solve quantum chemistry problems*
  Virginia Tech, Highlands Chemistry Colloquium, Sept. 4 (2020)

- **Invited Talk:** *Quasi-optimally compact ansatze for quantum chemistry VQE simulations*
  Canadian Chemistry Conference and Exhibition, Winnepeg, Canada, May 24-28 (2020) (Cancelled for COV-19)
- **Invited Talk:** *Tensor product methods for strongly correlated molecular systems*
  TPMSCM, Dresden, Germany, March 9 (2020) (Cancelled for COV-19)
- **Invited Talk:** *Tensor product states for more compact electronic state descriptions*
  Sanibel Symposium, February 16 (2020)
- **Invited Talk:** *Picking the right gates at the right time: an adaptive quantum algorithm for simulating molecular systems on quantum computers*
  University of Southern California, Physical Chemistry Seminar, November 4 (2019)
- **Invited Talk:** *ADAPT-VQE: Quasi-optimally compact wavefunctions for simulating molecules on a quantum computer*
  ACS National Meeting, San Diego, CA, August 28 (2019)
- **Invited Talk:** *Using Quantum Computers to Solve Quantum Chemistry Problems*
  MERCURY Conference, Greenville, SC, July 19 (2019)
- **Invited Talk:** *ADAPT-VQE: Adaptive variational algorithm for fermionic QC-simulations*
  DOE PI Meeting, Gaithersburg, MD, May 22 (2019)
- **Invited Talk:** *Picking the right gates at the right time: an adaptive quantum algorithm for simulating molecular systems on quantum computers*
  SETCA, Knoxville, TN, May 17 (2019)
- **Invited Talk:** *Higher order singular-value decomposition for strongly correlated systems*
  ACS National Meeting, Orlando, FL. April 03 (2019)
- **Invited Talk:** *Modeling singlet-fission biexciton states as an ab initio spin model: Justifications and applications*
  ACS National Meeting, Orlando, FL. April 02 (2019)
- **Invited Talk:** *Using quantum chemistry to simulate SMM qubits to (someday) simulate quantum chemistry*
  Gordon Research Conference, Computational Chemistry, West Dover, VT (2018)
- **Invited Talk:** *Using single-excitation wavefunctions to compute exciton-binding energies in singlet fission materials*
  East Tennessee State University, Johnson City, TN April 13 (2018)
- *Using higher-order singular value decomposition to define weakly coupled and strongly correlated clusters: the n-body Tucker approximation*
  255th ACS National Meeting, New Orleans, LA, March 21 (2018)
- *A generalized Ovchinnikov's rule can predict the biexciton boundedness in covalently linked singlet fission chromophores*
  255th ACS National Meeting, New Orleans, LA, March 19 (2018)
- *Multiexcitons and strong correlation via single-excitation wavefunctions: applications and future directions*
  2017 WATOC, Munich, Germany, August 31 (2017)
- **Invited Talk:** *Spin flip methods for Spin Hamiltonians*
  New Frontiers in Electron Correlation, Telluride TSRC, CO, June 23 (2017)

- *Using single-excitation wavefunctions to compute exciton-binding energies in singlet fission materials*
  253rd ACS National Meeting, San Francisco, CA, April 4 (2017)

- **Invited Talk:** *Using simple ab initio methods to construct even simpler Hamiltonians: applying spin-flip methods for strong correlation and excited states*
  Joint Condensed Matter and Center for Soft Matter and Biological Physics Seminar, Virginia Tech, Nov. 14 (2016)

- **Invited Talk:** *Using single-excitation wavefunctions to compute exciton-binding energies in singlet fission materials*
  Department Seminar, James Madison University, Nov. 11 (2016)

- **Invited Talk:** *Using simple ab initio methods to construct even simpler Hamiltonians: spin-flip methods for strong correlation and excited states*
  SETCA, Tallahassee, FL (2016)

- **Invited Talk:** *Ab initio Quantum Chemistry for multiradical molecules: A spin-flip approach*
  251st ACS National Meeting, San Diego, CA (2016)

- **Invited Talk:** *Heisenberg spin couplings are difficult but not impossible: Ab initio Quantum Chemistry for multiradical molecule*
  UC Merced, Merced, CA (2015)

- **Invited Talk:** *Toward accurate single-reference descriptions of strongly correlated systems: Spin-flip methods for several coupled electrons*
  248st ACS National Meeting, San Francisco, CA (2014)

- *Cost effective modeling of spin-coupled molecules: A 2nd order perturbative treatment of orbital relaxation in complete active space spin-flip CI*
  246st ACS National Meeting, Indianapolis, IN (2013)

- *Improving hybrid energy schemes for large molecules: Inclusion of charge-redistribution across regional boundaries*
  241st ACS National Meeting, Anaheim, CA (2011)

- **Invited Talk:** *Composite Energy Models in Quantum Chemistry*
  UC Berkeley, CA (2011)

- *$H_2$ Production and Kinetic Traps: Water Reactivity with Tungsten Oxides*
  65th International Symposium on Molecular Spectroscopy, The Ohio State University, Columbus, OH (2010)

- *First Principles Determination of the Acetyl Anion Photoelectron Spectrum*
  Undergraduate Research Conference, Butler University, Indianapolis, IN (2006)