Nicholas J. Mayhall

CONTACT INFORMATION	Department of Chemistry (0212) 480 Davidson Hall Virginia Tech 900 W. Campus Drive Blacksburg, VA 24061	Voice: (540) 231-3298 E-mail: nmayhall@vt.edu
EDUCATION	Ph.D. Indiana University, Bloomington B.S. University of Southern Indiana,	· · · · · · · · · · · · · · · · · · ·
Experience	Assistant Professor Virginia Tech	2015 - Present
	Visiting Scientist Simons Institute, University of CA	2020, Jan-May - Berkeley
	Post-Doctoral Associate University of CA – Berkeley Research group of Prof. Martin He	2011 - 2015 ad-Gordon
	Graduate Research Assistant Indiana University Research group of Prof. Krishnan F	2007 - 2011 aghavachari
	Graduate Student Instructor Indiana University General Chemistry I Lab with Prof General Chemistry II with Prof. Sri	
	Undergraduate Teaching Assistant University of Southern Indiana Physical Chemistry I and II with Pi	2005 - 2006 rof. Evan Millam
	REU Undergraduate Researcher University of Memphis Research group of Prof. Ted Burkey	2005, May-July
Awards	Alfred P. Sloan Research Fellow NSF Career Award ACS PHYS Division Postdoctoral Resea Richard Slagle Fellowship E.M. Kratz Fellowship Felix Haurowitz Award E. Campaigne C500 Award Academic Achievement Award for Cher Outstanding Achievement Award in Ph Integra Bank Distinguished Professor S O. John Logsdon Chemistry Scholarship CRC Freshman Chemistry Achievemen	Indiana University 2010 Indiana University 2009 Indiana University 2009 Indiana University 2008 Indiana University 2009 Indiana University 2008 Indiana University 2006 Indian

PUBLICATIONS

45 Biexciton Hamiltonian for the correlated triplet pair states in singlet fission: Revealing the contest between triplet-triplet exchange and triplet-triplet energy transfer coupling

Vibin Abraham, Nicholas J. Mayhall Submitted, (2021)

44 Preparing Bethe Ansatz Eigenstates on a Quantum Computer

John S. Van Dyke, George S. Barron, Nicholas J. Mayhall, Edwin Barnes, Sophia E. Economou Submitted, (2021)

43 Gate-free state preparation for fast variational quantum eigensolver simulations: ctrl-VQE

Oinam Romesh Meitei*, Bryan T. Gard*, George S. Barron, David P. Pappas, Sophia E. Economou, Edwin Barnes, Nicholas J. Mayhall Submitted, (2020), *Co-first authors

42 An 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 Submitted, (2020)

41 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 Submitted, (2020)

Published -

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)

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)

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 RASnSF 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-SiC₂H₂) 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 $Mo_3X_v^-$ (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: H₂ 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 $W_xO_v^- + H_2O$ 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 $Mo_2O_v^-$ (y = 2-5) with Methane

N. J. Mayhall, K. Raghavachari Journal of Physical Chemistry A, 111, 8211-8217 (2007)

PROJECT FUNDING

Total Amount \$5,368,430
Total Budget for Mayhall lab
Number of grants \$1,750,549

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 - Mar. 31, 2023

Award Number 1752612

· Simulating strongly correlated molecules with a superconducting processor

PI Mayhall

co-Pls 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-Pls 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-Pls 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

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

· Symposium Organization

Exploring Transition Metal Chemistry & Spectroscopy with Quantum Chemistry, National ACS Meeting in San Diego (2019)

BOOK CHAPTERS

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

Luke Bertels (postdoc)

Vibin Abraham (grad student)
Harper Grimsley (grad student)
Nicole Braunscheidel (grad student)

Robert Smith (grad student)

Shannon Houck (grad student, currently at QChem)

Daniel Claudino (postdoc, currently at Oakridge National Lab) Oinam Meitei (postdoc, currently at MIT - Van Voorhis group)

Courses Taught

CHEM 6634: Quantum Chemistry and Spectroscopy

CHEM 3616: Physical Chemistry

PRESENTATIONS

• 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: spinflip 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)
- H₂ 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)

STUDENT/POSTDOC TALKS

- (Invited) Meitei*, Mayhall, Gate-free state preparation for fast variational quantum eigensolver simulations, MIT, Van Voorhis Group, Oct. 29 (2020)
- Oinam Meitei; Gate-free state preparation for fast variational quantum eigensolver simulations: ctrl-VQE; Quantum computing for quantum chemistry; Cambridge Quantum Computing, 25th Sept. 2020

- Vibin Abraham; Tensor Product Selected CI: Compact wave function for strongly correlated clusterable systems; Virtual Conference on Theoretical Chemistry June 27-29 2020
- Oinam Meitei; Optimal control in variational quantum simulation for molecules; Virtual Conference on Theoretical Chemistry 2020, 29th July 2020
- Claudino*, Mayhall, Compact and optimal representation of embedded wave functions via concentric localization, Sanibel Symposium, St. George, GA, Feb. 16-21 (2020)
- (Invited) Shannon Houck*, Combining spin-flip and IP/EA approaches for handling spin and spatial degeneracies: Application to double exchange systems, 255th ACS Meeting Orlando, FL (2019)
- Daniel Claudino*, Automatic partition of orbital spaces based on singular value decomposition in the context of embedding, 255th ACS Meeting Orlando, FL (2019)