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, IN	Computational Chemistry	2011
B.S.	University of Southern Indiana, Evansville, IN	Chemistry	2006

Experience

Assistant Professor — 2015 - Present
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

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

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 **Cluster many-body expansion: a many-body expansion of the electron correlation energy about a cluster mean-field reference**
Vibin Abraham, Nicholas J. Mayhall
Submitted, (2021)

43 **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)

42 **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

41 **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)

40 **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

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

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

- **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-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

- 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: 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)

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)