

# Nicholas J. Mayhall

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## CONTACT

### INFORMATION

Department of Chemistry (0212)  
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Virginia Tech  
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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

Assistant Professor Virginia Tech	2015 - Present
Visiting Scientist Simons Institute, University of CA - Berkeley	2020, Jan-May
Post-Doctoral Associate University of CA – Berkeley Research group of Prof. Martin Head-Gordon	2011 - 2015
Graduate Research Assistant Indiana University Research group of Prof. Krishnan Raghavachari	2007 - 2011
Graduate Student Instructor Indiana University General Chemistry I Lab with Prof. Todd Stone General Chemistry II with Prof. Srinivasan Iyengar	2006 - 2007
Undergraduate Teaching Assistant University of Southern Indiana Physical Chemistry I and II with Prof. Evan Millam	2005 - 2006
REU Undergraduate Researcher University of Memphis Research group of Prof. Ted Burkey	2005, May-July

## AWARDS

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

- 41 **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
  - 40 **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)
  - 39 **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)
  - 38 **qubit-ADAPT-VQE: An adaptive algorithm for constructing hardware-efficient ansatzes on a quantum processor**  
Ho Lun Tang, Edwin Barnes, Harper R. Grimsley, Nicholas J. Mayhall, Sophia E. Economou  
Submitted, (2020)
- 
- Published**
- 37 **Selected Configuration Interaction in a Basis of Cluster State Tensor Products**  
Vibin Abraham and Nicholas J. Mayhall  
*Journal Chemical Theory and Computation*, Accepted (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
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- 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<sub>2</sub>H<sub>2</sub>) 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<sub>3</sub>X<sub>y</sub><sup>-</sup> (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**

Daniel Claudino (postdoc, currently at Oakridge National Lab)  
Oinam Meitei (postdoc)  
Shannon Houck (grad student)  
Vibin Abraham (grad student)  
Harper Grimsley (grad student)  
Nicole Braunscheidel (grad student)  
Robert Smith (undergrad student)

**COURSES TAUGHT**

CHEM 6634: Quantum Chemistry and Spectroscopy  
CHEM 3616: Physical Chemistry

**PRESENTATIONS**

- **Invited Talk:** *Quasi-optimally compact ansatzes for quantum chemistry VQE simulations*  
Canadian Chemistry Conference and Exhibition, Winnipeg, 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<sub>2</sub> 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**

- 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)