

# 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](mailto: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 Virginia Tech	2015 - Present
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 - 2005

## 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

- 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*, ASAP, (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)
- 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> (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)

#### 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)

#### JOURNALS REFEREED

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

#### ORAL PRESENTATIONS

- **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, March 21 (2018)
- *A generalized Ovchinnikov's rule can predict the biexciton boundedness in covalently linked singlet fission chromophores*  
255th ACS National Meeting, 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)

**POSTER  
PRESENTATIONS**

- *Active space-based spin-flip methods for strongly correlated systems: Method development and phenomenological extensions*  
SciDAC-3 PI Meeting, Washington DC (2014)
- *A perturbative approximation to RAS-*n*SF for excited states and strong correlations*  
SciDAC-3 PI Meeting, Rockville, MD (2013)
- *Is Coupled Cluster a Black Box?*  
42st Midwest Theoretical Chemistry Conference, Purdue University, West Lafayette, IN (2010)
- *H<sub>2</sub> Production and Kinetic Traps: Water Reactivity with Tungsten Oxides*  
41st Midwest Theoretical Chemistry Conference, University of Southern Illinois, Carbon-dale, Ill (2009)
- *Transition Metal Thermochemistry with Composite Methods: Application and Assessment of Current Methods*  
40th Midwest Theoretical Chemistry Conference, University of Michigan, Ann Arbor, MI (2008)
- *Two Methanes are Better than One: A Density Functional Theory Study of the Reactions of Mo<sub>2</sub>O<sub>*y*</sub><sup>-</sup> (*y* = 2-5) with Methane*  
39th Midwest Theoretical Chemistry Conference, Indiana University, Bloomington, IN (2007)