

Nicholas J. Mayhall

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
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

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

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*-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_y ($\text{X}=\text{O}, \text{S}$ 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 $\text{W}_2\text{O}_y^- + \text{H}_2\text{O}/\text{D}_2\text{O} \rightarrow \text{W}_2\text{O}_{y+1}^- + \text{H}_2/\text{D}_2$ 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 $\text{W}_x\text{O}_y^- + \text{H}_2\text{O}$ 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)

**JOURNALS
REFEREED**

Journal of Chemical Physics
Journal of Chemical Theory and Computation
Journal of Physical Chemistry
Molecular Physics
Chemical Physics Letters

**ORAL
PRESENTATIONS**

- **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)
- *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)

**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)

- *H₂ 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
Mo₂O_y⁻ (y = 2-5) with Methane*
39th Midwest Theoretical Chemistry Conference, Indiana University, Bloomington, IN
(2007)