Biographical Sketch: Nicholas J. Mayhall

Contact Information

Department of Chemistry (0212)
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Virginia Tech
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Education and Training

Postdoc	University of CA, Berkeley		2011-2015
Ph.D.	Indiana University	Computational Chemistry	2011
B.S.	University of Southern Indiana	Chemistry	2006

Experience

Assistant Professor	Virginia Tech	Chemistry	2015-Present

Selected Relevant Publications

1. **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)

2. **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)

3. **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)

4. **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)

5. **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)

6. **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)

7. **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)

8. **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)

9. **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. **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)

Synergistic Activities

Supervising 3 PhD students (Houck,Abraham,Shaikh)

Taught undergraduate Physical Chemistry second semester (quantum) CHEM 3616 (01/17-05/17), and graduate Quantum Chemistry CHEM 6634 (08/15-12/15 and 08/16-08/16).

5 invited talks since 2015

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

Collaborators and other affiliations

Martin Head-Gordon (UC Berkeley), Amanda Morris (Virginia Tech) P. Horn (Google), E. J. Sundstrom (Zenefits), M. Goldey (Univ. of Chicago),

Graduate and Postdoctoral Advisors and Advisees

PhD Advisor: Krishnan Raghavachari (Indiana University)

Postdoc Advisor: Martin Head-Gordon (UC Berkeley)

Graduate student Advisees: Vibin Abraham (current), Shannon Houck (current)