

Jeff R. Hammond
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Offices:	Chemistry (mail)	Computer Science
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	The University of Chicago	The University of Chicago
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Education and Research Positions

Pacific Northwest National Laboratory (June 2006 - present)

Supervisors: Drs. Wibe A. de Jong and Karol Kowalski

Description: developer of coupled-cluster molecular property codes in NWChem

University of Chicago (September 2003 to present)

Supervisors: Professors Karl F. Freed and L. Ridgway Scott

Thesis topic: parallel algorithms for coupled-cluster response theory and molecular properties

PhD in chemistry, expected June 2009

MS in Chemistry, August 2004

University of Washington (January 2001 to August 2003)

Supervisor: Professor Weston T. Borden

Thesis: *Evaluating the Bishomoaromatic Nature of Diaminodiformylsemibullvalene*

BS in Chemistry with Distinction, Minor in Applied Mathematics

BA in Mathematics

Whitman College (September 1999 to December 2000)

Honors and Awards

Chemical Computing Group Excellence Award - ACS Division of Computers in Chemistry (Spring 2008)

Department of Energy Computational Science Graduate Fellowship (2005 - 2009)

Harvey Fellow, The Mustard Seed Foundation (2006 - 2009)

Joan Shiu Award for Student Service, University of Chicago Chemistry Department (2006)

Freud Departmental Citizenship Award, University of Chicago Chemistry Department (2005)

McCormick Fellow, University of Chicago Physical Sciences Division (2003 - 2005)

Mary Gates Research Training Grant, University of Washington (2003)

William O. Douglas Scholar, Whitman College (1999)

Publications

(Corresponding author(s) underlined)

10. K. Kowalski, J. R. Hammond, W. A. de Jong and A. J. Sadlej, submitted. *Coupled cluster calculations for static and dynamic polarizabilities of C₆₀*.
9. R. K. Chaudhuri, J. R. Hammond, K. F. Freed, S. Chattopadhyay and U. S. Mahapatra, *J. Chem. Phys.* **129**, in press (2008). *Reappraisal of cis effect in 1,2-dihaloethenes: An improved virtual orbital (IVO) multi-reference approach*.
8. J. R. Hammond, W. A. de Jong and K. Kowalski, *J. Chem. Phys.* **128**, 224102 (2008). *Coupled cluster dynamic polarizabilities including triple excitations*.
7. K. Kowalski, J. R. Hammond and W. A. de Jong, *J. Chem. Phys.* **127**, 164105 (2007). *Linear response coupled cluster singles and doubles approach with modified spectral resolution of the similarity transformed Hamiltonian*.

6. J. R. Hammond, W. A. de Jong and K. Kowalski, *J. Chem. Phys.* **127**, 144105 (2007). *Dynamic polarizabilities of polyaromatic hydrocarbons using coupled-cluster linear response theory.*
5. J. R. Hammond, M. Valiev, W. A. de Jong and K. Kowalski, *J. Phys. Chem. A* **111**, 5492 (2007). *Calculations of properties using a hybrid coupled-cluster and molecular mechanics approach.*
4. J. R. Hammond and D. A. Mazziotti, *Physical Review A* **73**, 062505 (2006). *Variational reduced-density-matrix calculation of the one-dimensional Hubbard model.*
3. J. R. Hammond and D. A. Mazziotti, *Physical Review A* **73**, 012509 (2006). *Variational reduced-density-matrix calculations on small radicals: a new approach to open-shell ab initio quantum chemistry.*
2. M. Lingwood, J. R. Hammond, D. A. Hrovat, J. M. Mayer, and W. T. Borden, *Journal of Theory and Computation* **2**, 740 (2006). *MPW1K, rather than B3LYP, should be used as the functional for DFT calculations on reactions that proceed by proton-coupled electron transfer (PCET).*
1. J. R. Hammond and D. A. Mazziotti, *Physical Review A* **71**, 062503 (2005). *Variational two-electron reduced-density-matrix theory: Partial 3-positivity conditions for N-representability.*

Presentations

11. National Center for Supercomputing Applications, University of Illinois at Urbana-Champaign; Urbana, Illinois (July 30, 2008). *Accurate molecular property calculations using supercomputers: algorithms and applications.*
10. American Chemical Society National Meeting; New Orleans, LA (April 7, 2008). *Nonlinear optical spectroscopy of conjugated molecules using coupled-cluster theory.* (with K. Kowalski)
9. Department of Energy Computational Science Graduate Fellowship Annual Fellows' Conference; Washington, DC (June 19, 2007). *E Pluribus Duo* (old title, new talk).
8. Department of Chemistry, Cornell University; Ithaca, NY (June 14, 2007). *Quantum many-body theory without so many bodies.*
7. The Twelfth Annual James Franck Institute Symposium, The University of Chicago; Chicago, IL (May 17, 2007). *E Pluribus Duo.*
6. American Chemical Society National Meeting; Chicago, IL (March 27, 2007). *Coupled-cluster property calculations of aromatic molecules.* (with W. A. de Jong and K. Kowalski)
5. American Physical Society National Meeting; Denver, CO (March 7, 2007). *Variational reduced-density-matrix theory applied to the Hubbard model.* (with D. A. Mazziotti)
4. Computer Science and Mathematics Division, Oak Ridge National Laboratory; Oak Ridge, TN (February 8, 2007). *Massively Parallel Many-Body Methods for Hard Systems.*
3. Chemistry Department Tiger Talk, The University of Chicago; Chicago, IL (April 26, 2006). *Solving hard problems with RDM theory: from radical chemistry to ultracold atoms and high- T_c superconductivity.*
2. Mathematics and Computer Science Division, Argonne National Laboratory; Argonne, IL (July 29, 2005). *Quantum chemistry without wavefunctions: the role of semidefinite programming and some new results for radicals.*
1. Mary Gates Undergraduate Research Symposium, The University of Washington; Seattle, WA (May 16, 2003). *Bishomoaromaticity in the Cope rearrangement of semibullvalene.*

Posters

8. American Conference on Theoretical Chemistry, Northwestern University; Evanston, IL (July 21, 2008). *Accurate spectroscopic properties of molecules using coupled-cluster response theory and supercomputers.*
7. Department of Energy Computational Science Graduate Fellowship Annual Fellows' Conference; Washington, DC (June 18, 2008). *Coupled-cluster theory on supercomputers.* (with K. Kowalski)
6. American Chemical Society National Meeting, New Orleans, LA (April 8, 2008). *Coupled-cluster theory on supercomputers.* (with K. Kowalski)
5. NWChem Meeting on Science Driven Petascale Computing and Capability Development, Pacific Northwest National Laboratory; Richland, WA (January 25, 2007). *Coupled-cluster linear response properties for very large systems using new functionality within NWChem.* (with K. Kowalski and W. A. de Jong)
4. Department of Energy Computational Science Graduate Fellowship Annual Fellows' Conference; Washington, DC (June 21, 2006). *New frontiers in quantum many-body theory using state-of-the-art semidefinite programming algorithms.* (with D. A. Mazziotti)
3. American Conference on Theoretical Chemistry, UCLA; Los Angeles, CA (July 18, 2005). *Variational reduced-density-matrix calculations on open-shell systems.* (with D. A. Mazziotti)
2. 30th Reaction Mechanisms Conference, Northwestern University; Evanston, IL (June 25, 2004). *A DFT study of hydrogen transfer in ribonucleotide reductase: mechanisms and the role of mediating water molecules.* (with D. A. Hrovat and W. T. Borden)
1. European Summer School in Quantum Chemistry, Lund University; Lund, Sweden (August 24, 2003). *PCET vs. HAT in ribonucleotide reductase: a DFT study.* (with D. A. Hrovat and W. T. Borden)

External Support (Proposal author(s) underlined)

Testing and tuning NWChem for BlueGene/P and studies of nonlinear optical properties of conjugated chromophores

Investigators: Jeff R. Hammond, Donyou Wang, Manojkumar Krishnan, Sriram Krishnamoorthy
Sponsor: Argonne Leadership Computing Facility (ALCF)
Amount: 1,000,000 hours for July-December 2008.

QM/MM simulation of nonlinear optical and Raman spectroscopy of molecules in solution using coupled-cluster response theory

Investigators: Jeff R. Hammond, Karol Kowalski and Marat Valiev
Sponsor: National Energy Research Scientific Computing Center (NERSC)
Amount: 250,000 units for FY2008.

High Accuracy Modeling of Frequency Dependent Polarizabilities: Exploring the Cutting Edge Limits of NWChem

Investigators: Wibe A. de Jong, Jeff R. Hammond, Karol Kowalski and Marat Valiev
Sponsor: Environmental Molecules Sciences Laboratory (EMSL), Pacific Northwest National Laboratory
Amount: 250,000 hours for FY2007; 350,000 hours for FY2008.

Large-Scale Semidefinite Programming Calculations for Molecular Electronic Structure

Investigators: Jeff R. Hammond and David A. Mazziotti
Facility: National Energy Research Scientific Computing Center (NERSC)
Amount: 20,000 hours for FY2006; 20,000 hours for FY2007.

Software

SPAGHETTY (Self-optimizing Python Automatic Generator of Hierarchically blockEd Tensor Transpose library), GNU General Public License v3 (2008). Contribution: I am the exclusive author of this program.

NWChem, A Computational Chemistry Package for Parallel Computers, Version 5.1 (2007), Pacific Northwest National Laboratory, Richland, Washington 99352-0999, USA. Contribution: linear response dynamic polarizabilities at the CCSD and CCSDT levels of theory.

NWChem, A Computational Chemistry Package for Parallel Computers, Version 5.1.1 (2008), Pacific Northwest National Laboratory, Richland, Washington 99352-0999, USA. Contribution: linear response dynamic polarizabilities at the CCSDTQ levels of theory, hybrid out-of-core integral transformation algorithms, undocumented features (pending publication).

Professional Memberships

American Chemical Society (since 2004)

American Physical Society (since 2006)

Mathematical Programming Society (since 2007)

OpenFPGA (since 2008)

Workshops and Summer Schools

Accelerators for Science and Engineering Applications: GPUs and Multicores
National Center for Supercomputing Applications — Urbana, IL (August 18-22, 2008)

Leap to Petascale BlueGene/P workshop
Argonne National Laboratory — Argonne, IL (July 29-31, 2008)

Workshop on Programming Massively Parallel Processors
National Center for Supercomputing Applications — Urbana, IL (July 10, 2008)

PSI developer's workshop
Virginia Tech — Blacksburg, GA (February 22-23, 2007)

Eighth Workshop on the DOE Advanced Computational Software (ACTS) Collection
Lawrence Berkeley National Laboratory — Berkeley, CA (August 21-24, 2007)

NWChem Meeting on Science Driven Petascale Computing and Capability Development
Pacific Northwest National Laboratory — Richland, WA (January 24-25, 2007)

European Summer School in Quantum Chemistry
Lund University — Lund, Sweden (August 17-30, 2003).

Computer Skills

Programming Languages: Fortran 77, Python, C, Cuda, C++, Java (varying levels of proficiency)

Programming Tools: Eclipse, KDevelop, versioning software (CVS/Subversion/Mercurial)

Parallel Tools: MPI, OpenMP, Global Arrays

Other Languages: Matlab, Mathematica, \LaTeX , HTML

Chemistry Software: NWChem, Dalton, Aces II, PSI, Gaussian, GAMESS, MPQC

Departmental Service

Co-Chair, Safety and Security Committee (2006 - 2007)
Member, Web Committee (2005 - 2007)
Member, Graduate Student Recruiting Committee (2003 - 2005)
Member, Departmental Brochure Committee (2003 - 2004)

Other Service

Referee for *Theoretical Chemistry Accounts* and *Journal of Chemical Physics*.
Science fair judge for Chicago Public Schools.
Member of student committee for the redesign of the University of Chicago home page.
Member of student committee for the selection of the Dean of Rockefeller Chapel.

Teaching Experience

The University of Chicago - Teaching Assistant

CHEM122 *Honors General Chemistry* - Fall 2003
Supervisors: Professor David A. Mazziotti and Dr. Meishan Zhao
CHEM112 *General Chemistry* - Winter 2004
Supervisors: Professor Takeshi Oka and Dr. Meishan Zhao
CHEM113 *General Chemistry* - Spring 2004
Supervisors: Professor Gregory L. Hillhouse and Dr. Meishan Zhao

The University of Chicago - Graduate Teaching Assistant

CHEM361 *Wave Mechanics and Spectroscopy* - Fall 2004
Supervisor: Professor Donald H. Levy
CHEM362 *Quantum Chemistry* - Winter 2005
Supervisor: Professor David A. Mazziotti
CHEM361 *Wave Mechanics and Spectroscopy* - Fall 2006
Supervisor: Professor Karl F. Freed

The University of Chicago - The College

Harper Tutor in chemistry and mathematics - Fall 2004 to Spring 2005