Hrant Patrick Hratchian

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EMPLOYMENT

- 2008-Present Research Scientist
  Gaussian, Inc., Wallingford, CT
- 2005-2008 Post-Doctoral Fellow with Prof. K. Raghavachari
  Indiana University, Bloomington, IN

EDUCATION

- 2001-2005 Ph. D. (Theoretical Chemistry) with Prof. H. B. Schlegel
  Wayne State University, Detroit, MI
- 1997-2001 B. S. Cum Laude (Professional Chemistry) with Prof. M. C. Milletti
  Eastern Michigan University, Ypsilanti, MI

CURRENT RESEARCH INTERESTS

- QM/QM and QM/MM hybrid energy models
- *Ab initio* molecular dynamics
- Electronic structure studies of spin-coupled complexes
- Reactivity and rational design of transition metal catalysts

HONORS AND AWARDS

- 2005-2008 Ernest R. Davidson Postdoctoral Fellow, Indiana University
- 2005 Dan Trivich Memorial Award, Wayne State University
- 2001-2005 NSF-IGERT Fellowship, Wayne State University
- 2003 Best Student Talk, Anachem/SAS Symposium, Livonia, MI
- 2001 NSF Graduate Research Fellowship – Honorable Mention
- 2001 USAToday All American Academic Team – Honorable Mention
- 2001 B. W. Peet Award, Eastern Michigan University
- 2001 Gold Medallion Student Leader Award, Eastern Michigan University
- 1999-2001 Undergraduate Research Assistantship, Eastern Michigan University
- 2000 Outstanding Student Leader, Michigan Association of Governing Boards
- 2000 R. W. Collins Senior Research Scholarship, Eastern Michigan University
- 1998 Perry S. Brundage Endowment Scholarship, Eastern Michigan University

RESEARCH EXPERIENCE

- 2005-2008 Post-Doctoral Fellow, Indiana University
- 2001-2005 Research Assistant, Wayne State University
- 2002 Visiting Scientist, Eötvös Loránd University, Budapest, Hungary
- 2000 Undergraduate Summer Research, Wayne State University
- 1998-2001 Undergraduate Honors Research, Eastern Michigan University

TEACHING EXPERIENCE

- 2003-2004 Lecturer, CHEM 117/118 (Fundamentals of Chemistry and Lab) and CHEM 122 (General Chemistry I Lab), Eastern Michigan University
- 2004 Guest Lecturer, "Practical Aspects of Electronic Structure Calculations", SCP 7400 (Scientific Computing I: Applications of Modeling and Simulation), Wayne State University
- 2004 Guest Lecturer, "Ab Initio Molecular Dynamics", CHEM 561 (Quantum Mechanics and Molecular Spectroscopy), Eastern Michigan University
- 2000-2001 Teaching Assistant, CHEM 118 (Fundamentals of Chemistry Lab), CHEM 122 (General Chemistry Lab I), CHEM 101 (Science for Teachers Lab), Eastern Michigan University
- 1998-2000 Chemistry Department Tutor, Eastern Michigan University
- 1998-1999 Supplemental Instructor, CHEM 121 (General Chemistry I), Eastern Michigan University
- 1998-2001 Resident Advisor, Goddard and Hoyt Residence Halls, Eastern Michigan University

AFFILIATIONS AND SERVICE ACTIVITIES

- 2002-Present American Chemical Society (Student Affiliate Member, 1998-2002)
- 2003-Present American Association for the Advancement of Science
- 2003-2005 Alumni Representative, Eastern Michigan University Honors Advisory Committee
- 2000-2004 Association of Michigan Universities (Chairman, 2001-2004)

COLLABORATORS

- Bruce E. Bursten, University of Tennessee
- Ödön Farkas, Eötvös Loránd University, Budapest
- P. Jefferey Hay, Los Alamos National Laboratory
- Richard L. Martin, Los Alamos National Laboratory
- Michael J. Frisch, Gaussian, Inc.
- John Montgomery, University of Michigan
- Claudio Verani, Wayne State University

SELECTED TALKS AND INVITED SEMINARS

1. H. P. Hratchian, P. V. Parandekar, K. Raghavachari, "Developments in QM/QM electronic embedding theory", Midwest Theoretical Chemistry Conference, Bloomington, IN. 2007.
2. H. P. Hratchian, R. Fenno, U. Das, K. Raghavachari, T. Vreven, M. J. Frisch, "QM/QM electronic embedding for electronic structure studies of surface chemistry", 232nd American Chemical Society National Meeting, Division of Computers in Chemistry, San Francisco, CA. 2006.
3. H. P. Hratchian, R. Fenno, K. Raghavachari, "Efficient modeling of silicon and silicon oxide surface chemistry with electronic structure theory using pseudo-atoms", 232nd American Chemical Society National Meeting, Division of Physical Chemistry, San Francisco, CA. 2006.
4. H. P. Hratchian, "Developments in ab Initio energy surface exploration with applications to Ni(0) catalyzed addition reactions", *Invited Seminar*, Department of Chemistry, Ohio State University, Columbus, OH. 2005.
5. H. P. Hratchian, H. B. Schlegel, "Using distance weighted interpolants to improve the efficiency of nudged elastic band reaction path optimization", Midwest Theoretical Chemistry Conference, Columbia, MO. 2005.
6. H. P. Hratchian, H. B. Schlegel, "A new efficient and accurate reaction path following algorithm", 227th American Chemical Society National Meeting, Division of Physical Chemistry, Anaheim, CA. 2004.
7. H. P. Hratchian, "Navigating potential energy surfaces to understand chemical reactions", *Invited Seminar*, Department of Chemistry, Eastern Michigan University, Ypsilanti, MI. 2004.
8. H. P. Hratchian, "Navigating potential energy surfaces to understand chemical reactions", *Invited Seminar*, Department of Chemistry, Ohio State University, Columbus, OH. 2003.
9. H. P. Hratchian, "Efforts in modeling intermolecular interactions and retention in gas chromatography using polymer stationary phases", Anachem/SAS Meeting, Livonia, MI. 2003.
10. H. P. Hratchian, H. B. Schlegel, "New qualitative and quantitative reaction path following methods", Midwest Theoretical Chemistry Conference, Ames, IA. 2003.
11. H. P. Hratchian, H. B. Schlegel, "Building upon dynamics to follow reaction pathways and to locate first order saddle points", *Invited Seminar*, Department of Organic Chemistry, Eötvös Loránd University, Budapest, Hungary. 2002.

SELECTED POSTER PRESENTATIONS

1. H. P. Hratchian, R. Fenno, U. Das, K. Raghavachari, T. Vreven, M. J. Frisch, "QM/QM electronic embedding for electronic structure studies of surface chemistry", 232nd American Chemical Society National Meeting, Division of Computers in Chemistry, San Francisco, CA. 2006.
1. H. P. Hratchian, R. Fenno, K. Raghavachari, "Efficient modeling of silicon and silicon oxide surface chemistry with electronic structure theory using pseudo-atoms", 6th Canadian Computational Chemistry Conference, Vancouver, BC. 2006.
2. J. L. Sonnenberg, H. P. Hratchian, P. J. Hay, R. L. Martin, H. B. Schlegel, B. E. Bursten, "Towards an understanding of uranyl tetrahydroxide isomerization processes in aqueous environments via electronic structure methods", 229th American Chemical Society Meeting, Division of Inorganic Chemistry, San Diego, CA. 2005.

3. H. P. Hratchian, H. B. Schlegel, “Using walkers to find transition states from reactant and product minima”, 228th American Chemical Society National Meeting, Division of Computers in Chemistry, Philadelphia, PA. 2004.
4. H. P. Hratchian, H. B. Schlegel, “Reaction path following using a Hessian based predictor-corrector integrator: An accurate and efficient method for quantitative and qualitative paths”, Midwest Theoretical Chemistry Conference, East Lansing, MI. 2004.
5. J. L. Sonnenberg, H. P. Hratchian, P. J. Hay, R. L. Martin, H. B. Schlegel, B. E. Bursten, “Uranyl dihydroxides: A bent uranyl model”, 227th American Chemical Society National Meeting, Division of Inorganic Chemistry, Anaheim, CA. 2004.
6. H. P. Hratchian, S. Chowdhury, K. K. D. Amarasinghe, H. B. Schlegel, J. Montgomery, “Investigation of Ni-catalyzed three-component coupling reactions: A density-functional study”, 225th American Chemical Society National Meeting, Division of Computers in Chemistry *(also invited and presented in Sci-Mix Symposium)*, New Orleans, LA. 2003.
7. H. P. Hratchian, H. B. Schlegel, “Finding transition states using trajectories: burning the wick from both ends”, 223rd American Chemical Society National Meeting, Division of Computers in Chemistry, Orlando, FL. 2002.
8. H. P. Hratchian, H. B. Schlegel, “Following reaction pathways using a damped – classical trajectory algorithm”, 221st American Chemical Society National Meeting, Division of Computers in Chemistry *(also invited and presented in Sci-Mix Symposium)*, San Diego, CA. 2001.
9. H. P. Hratchian, M. C. Milletti, “Theoretical determination of ^{99}Ru magnetic properties for a series of transition metal-substituted base-stabilized silylene complexes”, 221st American Chemical Society National Meeting, Division of Inorganic Chemistry, San Diego, CA. 2001.
10. H. P. Hratchian, M. C. Milletti, “Comparison of theoretical methods for calculating ^{99}Ru chemical shifts”, 219th American Chemical Society National Meeting, Division of Chemical Education, San Francisco, CA. 2000.