Hrant Patrick Hratchian

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Research Interests

Molecular quantum chemistry and electronic structure theory; transition metal catalysis; photoelectron spectroscopy; ab initio potential energy surface exploration; mechanistic studies in organometallic chemistry.

Appointments & Employment

2021 – Present	Chair Department of Chemistry & Biochemistry University of California, Merced
2020 – Present	Associate Professor Department of Chemistry & Biochemistry University of California, Merced
2019 – 2021	Interim Co-Director Cyberinfrastructure and Research Technologies Office of Information Technology University of California, Merced
2013 – 2020	Assistant Professor Chemistry and Chemical Biology University of California, Merced
2008 – 2013	Research Scientist Gaussian, Inc. Wallingford, CT
2005 – 2008	Ernest R. Davidson Postdoctoral Fellow Postdoctoral Mentor: Prof. Krishnan Raghavachari Department of Chemistry, Indiana University Bloomington, IN

Education

2001 – 2005	Ph.D. (Theoretical Chemistry) Wayne State University, Detroit, MI Advisor: Prof. H. Bernhard Schlegel Thesis: “Development of new theoretical tools for navigating ab initio potential energy surfaces and applications of electronic structure methods to organometallic and inorganic chemistries.”
1997 – 2001	B.S. *cum laude* (Professional Chemistry) Eastern Michigan University, Ypsilanti, MI Advisor: Prof. Maria C. Milletti Senior Thesis: “Theoretical study of the Ru−Si bond in a series of transition metal substituted base-stabilized silylene complexes.”

Selected Honors & Awards

2019	National Science Foundation CAREER Award
2017 – 2018	Hellman Faculty Fellowship
2005 – 2008	Ernest R. Davidson Postdoctoral Fellowship, Indiana University
2005	Dan Trivich Memorial Award, Wayne State University
2001 – 2005	NSF-IGERT Fellowship, Wayne State University

Teaching Experience

2013 – Present	Courses Taught at UC Merced: SPRK 001, CHEM 002H, CHEM 010H, CHEM 112, CHEM 212, CHEM 225
2012 – 2016	Lecturer, *NSCCS Gaussian Workshops*, Imperial College London.
2008 – 2019	Instructor, Gaussian User Workshops, *Introduction to Gaussian: Theory and Practice*. Locations: Sydney, Australia (2008); Ulm, Germany (2009); Columbus, OH (2010), Santiago de Compostela, Spain (2011);Chennai, India (2012), Tokyo, Japan (2012), Columbus, OH (2012), Delhi, India (2012), Wroclaw, Poland (2013); Perth, Australia (2016); Ulm, Germany (2019).
2012	Guest Lecturer, *Physical Chemistry for the Life Sciences (CHEM 381)*, Wesleyan University.
2011	Guest Lecturer, *Physical Chemistry IV: Quantum Chemistry (CHEM 340)*, Wesleyan University.
2004	Guest Lecturer, *Applications of Modeling and Simulation (SCP 7400)*, Wayne State University.
2004	Guest Lecturer, *Quantum Mechanics and Molecular Spectroscopy (CHEM 561)*, Eastern Michigan University.
2003 – 2004	Lecturer, *Fundamentals of Chemistry and Lab (CHEM 117/118)*; *General Chemistry I Lab (CHEM 122)*, Eastern Michigan University.

Selected Recent Talks & Seminars

1. Invited Presenter and Panelist, *Building an On-Ramp to the Research Pathway*, Supporting Diversity and Excellence in Research Pathways at UC Merced. A Workshop Hosted by The National Academies and the University of California Merced (October, 2021).
2. Invited Seminar, Theory and Simulation of Electronic and Optical Processes in Molecules and Materials Virtual Seminar Series (October, 2021).
3. Invited Seminar, Department of Chemistry, St. Mary's University, Halifax, NS, Canada (October, 2021).
4. Invited Seminar, Department of Chemistry and Biochemistry, Auburn University, Auburn, AL (April, 2021).
5. Invited Talk, *American Physical Society March Meeting*, (virtual) (March, 2021).
6. Invited Talk, *Advanced Light Source User's Meeting, LBNL*, (virtual) (August, 2020).
7. Invited Seminar, Department of Chemistry and Biochemistry, University of Oklahoma, Norman, OK (February, 2020).
8. Invited Seminar, Department of Chemistry, California State University, Sacramento (October, 2019).
9. Invited Seminar, Department of Chemistry, University of California, Riverside, CA (April, 2019).
10. Invited Seminar, Department of Chemistry, Wayne State University, Detroit, MI (April, 2019).

Selected Service Activities

Outreach: Working with Prof. Ryan Baxter (UC Merced), we have developed and presented a chemistry outreach show at local elementary schools. For a video from a show in 2018, visit https://bit.ly/2HjErY0.

American Chemical Society Project SEED, Mentor to high school students Kaneen Muldrow (2019), Leonardo Canchola Colin (2018), Adrian Gomez (2017), Erika Sanchez (2016), Leonor Alcaraz-Guzman (2015), and James Willis (2014).

SELECTED SERVICE ACTIVITIES, CONTINUED

Department and School Service: Chemistry & Biochemistry Graduate Group Educational Policy Committee member (2020–Present); Faculty Co-Director, Chemistry Center (Undergraduate Tutoring Center); Chemical Sciences Faculty Assessment Organizer (2015–2020); Chemistry & Chemical Biology Graduate Group Education Policy Committee Chair & Executive Committee Member (2015–2020); Member of multiple faculty and school staff search committees.

Campus Service: Member of the Committee on Research Computing (2015–present); Member of the Campus Budget Working Group (2018–2019); Member of the Campus Academic Reorganization Working Group (2017–2018);Member of multiple staff search committees including Research Computing System Administrator and Dean of Students.

UC Merced Academic Senate: Chair of Graduate Council (2020-2021); Vice Chair of Graduate Council (2018–2020); Member of Graduate Council (2016–Present); Member of Senate Analyst search committee (2018 – 2019).

National Meeting Program Board Member, ACS COMP Division. In addition to engaging in program planning and related decisions for the COMP Division, I have co-organized the ACS National Meeting COMP Standing Symposium on Quantum Mechanics with A. E. DePrince since 2018 (occurs twice each year).

Recent Specialized Symposia Organized: *Exploring Transition Metal Chemistry & Spectroscopy with Quantum Chemistry*, Fall 2019 ACS National Meeting, San Diego, CA (with N. Mayhall); *ACS Award for Computers in Chemical & Pharmaceutical Research: Symposium in Honor of H. B. Schlegel*, Spring 2013 ACS National Meeting, New Orleans, LA. (with G. Cisneros, M. D. Halls, R. Lord, and J. L. Sonnenberg).

Guest Editor (with X. S. Li), Special Issue Honoring H. Bernhard Schlegel, *Journal of Chemical Theory and Computation*, January, 2013.

Reviewer and Panelist for the Center for Nanoscale Materials Proposal Evaluation Board (member since 2014), National Science Foundation, US Department of Energy, and Petroleum Research Fund.

Journal Reviewer for *Chemical Sciences*, *Journal of Chemical Physics*, *Journal of Physical Chemistry*, *Journal of Physical Chemistry Letters*, *Journal of Chemical Theory and Computation*, *Chemical Physics Letters*, *Journal of Computational Chemistry*, *International Journal of Quantum Chemistry*, *Molecular Physics*, *Physical Chemistry Chemical Physics*.

AFFILIATIONS

American Chemical Society; American Physical Society; American Association for the Advancement of Science

STUDENTS & POSTDOCTORALS

Summer High School and ACS SEED Students: Kaneen Muldrow (2019), Leonardo Canchola Colin (2018), Adrian Gomez (2017), Sophia Ortiz (2016), Erika Sanchez (2016), Leonor Alcaraz-Guzman (2015, 2016), and James Willis (2014)

Undergraduate Students: Jonathan Loera, Jorge Vazquez, Yogev Gluzman (B.S., 2019), Bryce Fairless (B.S., 2019), Anissa Abdullah (B.S., 2019), Preston Griffon, (B.S., 2018), Susana Calderon, (B.S., 2018), Sheyda Partovi (B.S., 2017), Nicole Giddings (B.S., 2015), Stephen Flaherty (B.S., 2015), Euna Chung (B.S., 2015), Ashlee Chan (B.S., 2015), Victor Lee (B.S., 2014), and Nicole Degregorio (B.S., 2014)

Graduate Students: Abdul Zamani, Cristian Sarabia, Andrew Bovill, Madison Martin, Ali Abou Taka (Ph.D., 2021), Samantha Bidwell (Ph.D., 2021), Hassan Harb (Ph.D., 2021), Xianghai Sheng (Ph.D., 2019), Stephen Flaherty (Applied Math, 2016), and Lisa Gong (2015–2016)

Postdoctorals: Hector Corzo, Lee Thompson (2014–2017; Assistant Prof., Univ. of Louisville)

RECENT COLLABORATORS

Carlo Adamo (Ecole Nationale Supérieure de Chimie de Paris), Ryan D. Baxter (UC Merced), Michael J. Frisch (Gaussian, Inc.), Christine M. Isborn (UC Merced), Caroline Chick Jarrold (Indiana University), Daniel M. Neumark (UC Berkeley), Aurora Pribram-Jones (UC Merced), Christopher A. Reed (UC Riverside), Nadia Rega (Università di Napoli)

GRANTS AWARDED

National Science Foundation. "MRI Acquisition of Pinnacles – Raising Research Computing to New Heights in California's Central Valley", PI: H. P. Hratchian, co-PIs: A. M. Martini, S. Sindi. $700,000 (plus $300,000 cost-share funds from UCM, 2020–2023 (ACI-2019144).

National Science Foundation. "CAREER: Development of Efficient Spin Projection Models for Applications to Transition Metal Catalysis", PI: H. P. Hratchian. $625,000, 2019–2024 (CHE-1848580).

Department of Energy. "Improved methods for modeling functional transition metal compounds in complex environments: Ground states, excited states, and spectroscopies", PI: H. P. Hratchian, co-PIs: C. .M. Isborn, A. Pribram-Jones, L. Shi, D. .A. Strubbe. $1,580,000, 2018–2022 (DE-SC0019053).

National Science Foundation. "Building Capacity: Improving the Undergraduate Chemistry Experience at HSIs by Bridging the GAP (through Green chemistry, Active-learning, and Peer-led experiences)", PI: E. Menke, co-PIs: H. P. Hratchian, C. M. Isborn, J. M. Leslie, B. Stokes. $1,442,497, 2018–2023 (DUE-1832538).

Petroleum Research Fund (ACS). "Computational Studies of Fundamental Organic Transformations Catalyzed by Metal Oxides", PI: H. P. Hratchian. $110,000, 2016–2019 (56806-DNI6).

Hellman Family Foundation. "Exploring the Structure and Chemistry of Metal Oxide Clusters", PI: H. P. Hratchian. $10,000, 2017–2018.

UC Merced Center for Engaged Teaching and Learning. "Theoretical/Computational concept modules for General Chemistry / General Chemistry Honors", PI: H. P. Hratchian, co-PI: E. Menke. $25,000, 2017–2018.

UC Merced Center for Engaged Teaching and Learning. "Writing and Honors General Chemistry - Learning community", PI: P. Gibbons, co-PIs: E. Menke, H. P. Hratchian, A. Zanzucchi. $25,000, 2017–2018.

National Science Foundation. "MRI Acquisition: Multi-Environment Research Computer for Exploration and Discovery (MERCED) Cluster", PI: H. P. Hratchian, co-PIs: J. Q. Sun, S. Sindi. $515,842, 2014–2017 (ACI-1429783).

PUBLICATIONS

ISI *h*–index: 21 | Google Scholar *h*–index: 44; Citations $>$ 150,000

**** indicates HPH is a corresponding author.**

Publications as UC Merced Faculty

59. ** J. L. Mason, H. Harb, A. Abou Taka, C. D. Huizenga, H. Corzo, H. P. Hratchian, and C. C. Jarrold, "New Photoelectron–Valence Electron Interactions Evident in the Photoelectron Spectrum of Gd_2O^-", *J. Phys. Chem. A* **125**, 9892–9903 (2021).

58. C. D. Huizenga, H. P. Hratchian, and C. C. Jarrold, "Lanthanide Oxides: From Diatomics to High-Spin, Strongly Correlated Homo- and Heterometallic Clusters", *J. Phys. Chem. A* **125**, 6315–6331 (2021). Feature Article.

57. J. D. Galloway, C. Sarabia, J. C. Fettinger, H. P. Hratchian, and R. .D. Baxter, "Versatile New Reagent for Nitrosation under Mild Conditions", *Org. Lett.* **23**, 3253–3258 (2021).

56. ** H. Harb and H. P. Hratchian, "ΔSCF Dyson Orbitals and Pole Strengths From Natural Ionization Orbitals", *J. Chem. Phys.* **154**, 084104 (2021).

55. ** J. L. Mason, H. Harb, A. Abou Taka, A. J. McMahon, C. D. Huizenga, H. Corzo, H. P. Hratchian, and C. C. Jarrold, "Photoelectron Spectra of $Gd_2O_2^-$ and Nonmonotonic Photon-Energy-Dependent Variations in Populations of Close-Lying Neutral States", *J. Phys. Chem. A* **125**, 857–866 (2021).

PUBLICATIONS, CONTINUED

54. ** A. Abou Taka, M. C. Babin, X. Sheng, J. A. DeVine, D. M. Neumark, and H. P. Hratchian, "Unveiling the Coexistence of Cis and Trans Isomers in the Hydrolysis of ZrO_2: A Coupled DFT and High-Resolution Photoelectron Spectroscopy Study", *J. Chem. Phys.* **153**, 244308 (2020).

53. ** X. Sheng, L. M. Thompson, and H. P. Hratchian, "Assessing the Calculation of Exchange Coupling Constants and Spin Crossover Gaps Using the Approximate Projection Model To Improve Density Functional Calculations", *J. Chem. Theory Comput.* **16**, 154–163 (2020).

52. ** J. L. Mason, H. Harb, J. E. Topolski, H. P. Hratchian, and C. C. Jarrold, "Exceptionally Complex Electronic Structures of Lanthanide Oxides and Small Molecules", *Acc. Chem. Res.* **52**, 3265–3273 (2019).

51. ** H. Harb, L. M. Thompson, and H. P. Hratchian, "On the Linear Geometry of Lanthanide Hydroxides (Ln−OH, Ln=La-Lu)", *Phys. Chem. Chem. Phys.* **21**, 21890–21897 (2019).

50. ** L. C. Reimer, J. M. Leslie, S. .L. Bidwell, C. M. Isborn, D. Lair, E. Menke, B. J. Stokes, and H. P. Hratchian, "Aiming Toward an Effective Hispanic Serving Chemistry Curriculum", In *ACS Symposium Series. Growing Diverse STEM Communities: Methodology, Impact, and Evidence*, edited by L. L. Winfield, G. Thomas, L. M. Watkins, and Z. S. Wilson-Kennedy (American Chemical Society, Washington, D.C.), 29–66 (2019).

49. ** L. M. Thompson, H. P. Hratchian, "On approximate projection models", *Mol. Phys.* **117**, 1421–1429 (2019). (Dieter Cremer Memorial Issue)

48. ** A. M. Hua, S. L. Bidwell, S. I. Baker, H. P. Hratchian, and R. .D. Baxter, "Experimental and Theoretical Evidence for Nitrogen-Fluorine Halogen Bonding in Silver-Initiated Radical Flourinations", *ACS Catal.* **9**, 3322–3326 (2019).

47. ** J. L. Mason, H. Harb, C. D. Huizenga, J. C. Ewigleben, J. E. Topolski, H. P. Hratchian, and C. C. Jarrold, "Electronic and Molecular Structures of the CeB_6 Monomer", *J. Phys. Chem. A* **123**, 2040–2048 (2019). (Hanna Reisler Festschrift)

46. X. Cai, A. Tohti, C. Ramirez, H. Harb, J. C. Fettinger, H. P. Hratchian, and B. J. Stokes, "Dispersion-Controlled Regioselective Acid-Catalyzed Intramolecular Hydroindolation of cis-Methindolylstyrenes to Access Tetrahydrobenzo[cd]indoles", *Org. Lett.* **21**, 1574–1577 (2019).

45. J. L. Mason, H. Harb, J. E. Topolski, H. P. Hratchian, and C. C. Jarrold, "A tale of two stabilities: How one boron atom affects a switch in bonding motifs in $CeO_2B_x^-$ (x = 2, 3) complexes", *J. Phys. Chem. A* **122**, 9879–9885 (2018).

44. J. E. Topolski, J. O. Kafader,V. Marrero-Colon, S. S. Iyengar, H. P. Hratchian, and C. C. Jarrold, "Exotic electronic structures of $Sm_xCe_{3-x}O_y$ (x = 0-3; y = 2-4) clusters, and the effect of high neutral density of low-lying states on photodetachment transition intensities", *J. Chem. Phys.* **149**, 054305 (2018).

43. ** J. A. DeVine, A. Abou Taka, M. C. Babin, M. L. Weichman, H. P. Hratchian, and D. M. Neumark, "High-resolution photoelectron spectroscopy of $TiO_3H_2^-$: Probing the TiO_2^- + H_2O dissociative adduct", *J. Chem. Phys.* **148**, 222810 (2018).

42. ** L. M. Thompson, C. C. Jarrold, and H. P. Hratchian, "Simulation of low energy photoelectron transitions in $MoVO_4^-$", *J. Chem. Phys.* **146**, 104301 (2017).

41. M. J. Frisch, *et al.*, "GAUSSIAN 16", Gaussian, Inc., Wallingford, CT (2016).

40. A. Petrone, P. Cimino, G. Donati, H. P. Hratchian, M. J. Frisch, and N. Rega, "On the Driving Force of the Excited-State Proton Shuttle in the Green Fluorescent Protein: A Time-Dependent Density Functional Theory (TD-DFT) Study of the Intrinsic Reaction Path", *J. Chem. Theory Comput.* **12**, 4925–4933 (2016).

PUBLICATIONS, CONTINUED

39. ** L. M. Thompson, H. Harb, and H. P. Hratchian, "Natural Ionization Orbitals for interpreting electron detachment processes", *J. Chem. Phys.* **144**, 204117 (2016).
38. D. Presti, F. Labat, A. Pedone, M. J. Frisch, H. P. Hratchian, I. Ciofini, M. C. Menziani, and C. Adamo, "Modeling emission features of salicylidene aniline molecular crystals: A QM/QM' approach", *J. Comp. Chem.* **37**, 861–870 (2016).
37. S. Cummings, H. P. Hratchian, C. A. Reed, "The strongest acid: Protonation of carbon dioxide", *Angew. Chem. Int. Ed.* **128**, 1404–1408 (2016).
36. ** L. M. Thompson, H. P. Hratchian, "Modeling the photoelectron spectra of $MoNbO_2^-$ accounting for spin contamination in Density Functional Theory", *J. Phys. Chem. A* **119**, 8744–8751 (2015).
35. ** L. M. Thompson, H. P. Hratchian, "Second derivatives for approximate spin projection methods", *J. Chem. Phys.* **142**, 054106 (2015).
34. D. Presti, F. Labat, A. Pedone, M. J. Frisch, H. P. Hratchian, M. C. Menziani, I. Ciofini, and C. Adamo, "A computational protocol for modeling thermochromic molecular crystals: salicylidene aniline as a case study", *J. Chem. Theory Comput.* **10**, 5577–5585 (2014).
33. ** L. M. Thompson, H. P. Hratchian, "Spin projection with double hybrid density functional theory", *J. Chem. Phys.* **141**, 034108 (2014).
32. B. C. Gamoke, U. Das, H. P. Hratchian, and K. Raghavachari, "Divalent pseudoatoms in cluster modeling of Si(100) surfaces", *J. Chem. Phys.* **139**, 164708 (2013).

Publications as Research Scientist at Gaussian, Inc.

31. ** H. P. Hratchian, "An efficient analytic gradient theory for approximate spin projection methods", *J. Chem. Phys.* **138**, 101101 (2013).
30. ** H. P. Hratchian and E. Kraka, "Improved predictor-corrector integrators for evaluating reaction path curvature", *J. Chem. Theory Comput.* **9**, 1481-–1488 (2013).
29. ** H. P. Hratchian and X. S. Li, "Thirty years of geometry optimization in quantum chemistry and beyond: A tribute to Berny Schlegel", *J. Chem. Theory Comput.* **8**, 4853–4855 (2012). *Invited Guest Editorial*.
28. ** H. P. Hratchian, "Using efficient predictor-corrector reaction path integrators for studies involving projected frequencies", *J. Chem. Theory Comput.* **8**, 5013–5019 (2012).
27. ** H. P. Hratchian and M. J. Frisch, "Integrating steepest-descent reaction pathways for large molecules", *J. Chem. Phys.* **134**, 204103 (2011).
26. H. P. Hratchian, A. V. Krukau, P. V. Parandekar, K. Raghavachari, M. J. Frisch, and T. Vreven, "QM:QM embedding using electronic densities within and ONIOM framework. Energies and analytic gradients", *J. Chem. Phys.* **135**, 014105 (2011).
25. F. Labat, I. Coifini, H. P. Hratchian, K. Raghavachari, M. J. Frisch, and C. Adamo, "Insights into working principles of N_3/TiO_2 dye-sensitized solar cells from first principles modeling", *J. Phys. Chem. C* **115**, 4297–4306 (2011).
24. ** H. P. Hratchian, M. J. Frisch, and H. B. Schlegel, "Steepest descent reaction path integration using a first-order predictor-corrector method", *J. Chem. Phys.* **133**, 224101 (2010).
23. N. J. Mayhall, K. Raghavachari, and H. P. Hratchian, "ONIOM-based QM:QM electronic embedding method using Löwdin atomic charges: Energies and analytic gradients", *J. Chem. Phys.* **132**, 114107 (2010).

PUBLICATIONS, CONTINUED

22. J. L. Sonnenberg, H. P. Hratchian, and H. B. Schlegel, "Spin contamination in inorganic chemistry calculations", In *Computational Inorganic and Bioinorganic Chemistry*, edited by E. I. Solomon, R. B. King, and R. A. Scott (Wiley, Chichester, U.K.), 173–186 (2009).
21. F. Labat, I. Ciofini, H. P. Hratchian, M. J. Frisch, K. Raghavachari, and C. Adamo, "First principles modeling of eosin-loaded ZnO films: A step toward the understanding of a dye-sensitized solar cell performances", *J. Am. Chem. Soc.* **131**, 14290–14298 (2009).
20. M. J. Frisch, *et al.*, "GAUSSIAN 09", Gaussian, Inc., Wallingford, CT (2009).

Publications as Student/Postdoc Prior to Independent Career

19. P. V. Parandekar, H. P. Hratchian, and K. Raghavachari, "Applications and assessment of QM:QM electronic embedding using generalized asymmetric Mulliken atomic charges", *J. Chem. Phys.* **129**, 145101 (2008).
18. H. P. Hratchian, P. V. Parandekar, K. Raghavachari, M. J. Frisch, and T. Vreven, "QM:QM electronic embedding using Mulliken atomic charges. Energies and analytic gradients in an ONIOM framework", *J. Chem. Phys.* **128**, 034107 (2008).
17. R. Shakya, S. S. Hindo, L. Wu, M. Allard, M. J. Heeg, H. P. Hratchian, B. R. McGarvey, S. R. P. da Rocha, and C. N. Verani, "Archetypical modeling and amphiphilic behavior of cobalt(II)-containing soft-materials with asymmetric tridentate ligands", *Inorg. Chem.* **46**, 9808–9818 (2007).
16. ** R. Shakya, S. S. Hindo, L. Wu, S. Ni, M. Allard, M. J. Heeg, S. R. P. da Rocha, G. T. Yee, H. P. Hratchian, and C. N. Verani, "Amphiphilic and magnetic properties of a new class of cluster-bearing $[L_2Cu_4(\mu_4-O)(\mu_2-\text{carboxylato})_4]$ soft materials", *Chem. Eur. J.* **13**, 9948–9956 (2007).
15. H. E. Herbert, M. D. Halls, H. P. Hratchian, and K. Raghavachari, "Hydrogen-bonding interactions in peptide nucleic acid: A comparative study", *J. Phys. Chem. B* **110**, 3336–3343 (2006).
14. R. Shakya, C. Imbert, H. P. Hratchian, M. Lanznaster, M. J. Heeg, H. B. Schlegel, B. R. McGarvey, and C. N. Verani, "Structural, spectroscopic, and electrochemical behavior of trans-phenolato cobalt(III) complexes of asymmetric NN'O ligands as archetypes for metallomesogens", *Dalton Trans.* **2006**, 2517–2525 (2006). Selected as the issue's "Hot Article".
13. J. E. Knox, M. D. Halls, H. P. Hratchian, H. B. Schlegel, "Chemical failure modes of AlQ3-based OLEDs: AlQ3 hydrolysis", *Phys. Chem. Chem. Phys.* **8**, 1371–1377 (2006).
12. M. Lanznaster, H. P. Hratchian, M. J. Heeg, L. M. Hryhorczuk, B. R. McGarvey, H. B. Schlegel, and C. N. Verani, "Structural and electronic behavior of unprecedented five-coordinate iron(III) and gallium(III) complexes with a new phenol-rich electroactive ligand", *Inorg. Chem.* **45**, 955–957 (2006).
11. ** H. P. Hratchian, J. L. Sonnenberg, P. J. Hay, R. L. Martin, B. E. Bursten, and H. B. Schlegel, "Theoretical investigation of uranyldihydroxide: Oxo ligand exchange, water catalysis, and vibrational spectra", *J. Phys. Chem. A* **109**, 8579–8586 (2005).
10. C. Imbert, H. P. Hratchian, M. Lanznaster, M. J. Heeg, L. M. Hryhorczuk, B. R. McGarvey, H. B. Schlegel, and C. N. Verani, "Influence of ligand rigidity and ring substitution on the structural and electronic behavior of trivalent iron and gallium complexes with asymmetric tridentate ligands", *Inorg. Chem.* **44**, 7414–7422 (2005).

PUBLICATIONS, CONTINUED

9. H. P. Hratchian and H. B. Schlegel, "Finding minima, transition states, and following reaction pathways on ab initio potential energy surfaces", In *Theory and Applications of Computational Chemistry: The First 40 Years*, edited by C. E. Dykstra, G. Frenking, K. S. Kim, and G. E. Scuseria (Elsevier, Amsterdam), 195–249 (2005).
8. H. P. Hratchian and H. B. Schlegel, "Using Hessian updating to increase the efficiency of a Hessian based predictor-corrector reaction path following method", *J. Chem. Theory Comput.* **1**, 61–69 (2005).
7. H. P. Hratchian and M. C. Milletti, "First principles determination of ^{99}Ru chemical shifts using moderately sized basis sets", *J. Mol. Struc.* **724**, 45–52 (2005).
6. H. P. Hratchian, S. K. Chowdury, V. M. Gutiérrez-García, H. B. Schlegel, and J. Montgomery, "Combined experimental and computational investigation of the mechanism of nickel-catalyzed three-component addition processes", *Organometallics* **23**, 4636–4646 (2004). [Addition/Correction: 23, 5652 (2005)]
5. H. P. Hratchian and H. B. Schlegel, "Reaction path following using a Hessian based predictor-corrector algorithm", *J. Chem. Phys.* **120**, 9918–9924 (2004).
4. J. E. Knox, H. P. Hratchian, N. Trease, J. Struble, H. B. Schlegel, and H. Holmes, "Using stationary points on potential energy surfaces to model intermolecular interactions and retention in gas chromatography", *Chromatographia* **59**, 329–334 (2004).
3. M. J. Frisch, *et al.*, "GAUSSIAN 03", Gaussian, Inc., Wallingford, CT (2004).
2. H. P. Hratchian and H. B. Schlegel, "Following reaction pathways using a damped classical trajectory algorithm", *J. Phys. Chem. A* **106**, 165–169 (2002).
1. H. P. Hratchian, T. Prendergast, and M. C. Milletti, "Theoretical investigation of substituent effects on the silicon-metal bond for a series of transition metal-substituted base-stabilized silylene complexes", *Polyhedron* **20**, 209–213 (2001).