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

2022 – Present	Vice Provost for Graduate Education and Dean of the Graduate Division University of California, Merced
2023 – Present	Professor Department of Chemistry & Biochemistry University of California, Merced
2021 – 2022	Chair Department of Chemistry & Biochemistry University of California, Merced
2020 – 2023	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

2022	Alumni Achievement Award, Eastern Michigan University
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

Grants Awarded

National Science Foundation. "Venture for Innovation in Self-assembly and integration of Optoelectronic Nanostructures (VISION)", PI: M. Scheibner, co-PIs: H. Cai, S. Ghosh, L. Neshyba, D. Ginger. H. P. Hratchian is Senior Personnel on this award. $1,000,000, 2024–2027 (DMR-2425230).

Mellon Foundation. "Our Interwoven Futures: The Public Humanities Design Studio as a Community-Engaged Hub for Dialogue on Social Justice", PI: C. Lux, co-PIs: I. López-Calvo, R. DeLugan, H. P. Hratchian . $750,000, 2024–2027. (My participation in this project is through my role as UC Merced's Graduate Dean.)

National Science Foundation. "CC*Regional Computing: CENVAL-ARC: Central Valley Accessible Research and Computational Hub", PI: S. Chadalapaka, co-PIs: E. J. McTavish, A. Klimaszewski-Patterson, S. Sindi. H. P. Hratchian is Senior Personnel on this award. $1,000,000, 2024–2026 (OAC-2346744).

Department of Energy. "Localized electrons, ionization potentials, and non-thermal states in warm dense matter from the thermal projection-based initial maximum overlap method", PI: A. Pribram-Jones, co-PI: H. P. Hratchian. $637,400, 2023–2026 (DE-SC0024476).

Department of Energy. "Exploring photon-initiated electron-neutral interactions in strongly correlated lanthanide complexes", PI: C. C. Jarrold, co-PIs: H. P. Hratchian and L. M. Thompson. $1,356,131 ($443,709 to UCM), 2023–2026 (DE-SC0024282).

National Science Foundation. "Planning: PREC Track 2: The UC Merced/MolSSI Chemical Computation and Theory Pathway Program", PI: H. P. Hratchian, co-PIs: C. .M. Isborn, A. Pribram-Jones, L. Shi, D. .A. Strubbe. $183,978, 2023–2025 (CHE-2335166).

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.

GRANTS AWARDED, CONTINUED

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).

SELECTED SERVICE ACTIVITIES

American Chemical Society Councilor and COMP Division Executive Committee Member. The ACS Council is the Society's governance organization. ACS Councilors are elected by local sections and technical division. I serve as an elected Councilor for the Division of Computers in Chemistry (COMP). This elected position also serves as a member of the COMP Executive Committee.

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 Christina Chan (2022), Joanne Guan (2022), Kaneen Muldrow (2019), Leonardo Canchola Colin (2018), Adrian Gomez (2017), Erika Sanchez (2016), Leonor Alcaraz-Guzman (2015), and James Willis (2014).

Guest Editorships. Special Issue Honoring Krishnan Raghavachari, *Journal of Physical Chemistry A*, April, 2024 (Guest Editors: H. P. Hratchian, A. Karton, and N. J. Mayhall). Special Issue Honoring H. Bernhard Schlegel, *Journal of Chemical Theory and Computation*, January, 2013 (Guest Editors: H. .P. Hratchian and X. S. Li).

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.

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).

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*, *Nature Communications*, *WIRES: Computational Molecular Sciences*, *Physical Chemistry Chemical Physics*.

Department and School Service: Chemistry & Biochemistry Graduate Group Educational Policy Committee member (2020–2021); Faculty Co-Director, Chemistry Center, an undergraduate learning and tutoring center (2018–2021); 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.

UC Merced Academic Senate: Chair of Graduate Council (2020-2021); Merced Division representative on UC Systemwide Coordinating Committee on Graduate Affairs (2020-2021); Vice Chair of Graduate Council (2018–2020); Member of Graduate Council (2016–Present); Member of Senate Analyst search committee (2018 – 2019).

SELECTED SERVICE ACTIVITIES, CONTINUED

Campus Service: Member of the Committee on Research Computing (2015–present); Member of the Honors Program Work Group (2021–2022); Valuing Black Lives task force focused on student success (2020–2021); Member of the DFA Procurement Task Force (2021); Member of Campus Instructional Budget Guideline Review Committee (2019–2020); 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, Dean of Students, and Chief Information Officer.

PROFESSIONAL AFFILIATIONS

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

RECENT COLLABORATORS

Rebeca Arevalo (UC Merced), Ryan D. Baxter (UC Merced), Marco Caricato (Kansas University), Michael Findlater (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), Liang Shi (UC Merced), Lee M. Thompson (University of Louisville)

STUDENTS & POSTDOCTORALS

Summer High School and ACS SEED Students: Christina Chan (2022), Joanne Guan (2022), 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: Emma Brass (B.S., 2022), Jonathan Loera (B.S., 2022), Jorge Vazquez (B.S., 2022), 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: Cristian Sarabia, Andrew Bovill, Abigail Gyamfi, Brianna Aguilar-Solis, Christian Dywer, Li Ji, Abdul Zamani (Ph.D., 2023), Madison Martin (M.S., 2022), 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 (2019-2021; Staff Scientist, Oakridge National Laboratory), Lee Thompson (2014–2017; Associate Prof., Univ. of Louisville)

RECENT TALKS & SEMINARS

1. Invited Talk, *National ACS Meeting, COMP Division*, New Orleans, LA (March, 2024).
2. Invited Discussion Leader, *Gordon Research Conference: Molecular and Ionic Clusters*, Ventura, CA (February, 2024).
3. Invited Keynote Speaker, *Amazon Web Services Symposium at UC Merced*, Merced, CA (September, 2023).
4. Invited Talk, *West Coast Theoretical Chemistry Conference*, Davis, CA (March, 2023).
5. Invited Talk, *Austin Symposium on Molecular Structure and Dynamics*, Dallas, TX (March, 2023).
6. Invited Talk, *National ACS Meeting, COMP Division*, Chicago, IL (August, 2022).
7. Invited Talk, *Advanced Light Source User's Meeting, LBNL*, (virtual) (August, 2022).
8. Invited Talk, *WATOC*, Vancouver, BC, Canada (July, 2022).
9. Invited Seminar, New York Section of the American Chemical Society, Computers in Chemistry Topical Group Webinar (April, 2022).

TEACHING EXPERIENCE

2013 – Present	Chemistry Courses Taught at UC Merced: CHEM 002H, CHEM 010H, CHEM 112, CHEM 212, CHEM 225
2020, 2021	First Year Seminar Course Taught at UC Merced: SPARK 1, "What is a research university?"
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.

PUBLICATIONS

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

Publications as UC Merced Faculty

72. A. King, A. Rezaei, A. Bovill, H. P. Hratchian, A. Gorden, M. Findlater, "Recyclable homogeneous zinc and cobalt complexes in catalytic hydrosilylation of ketones and amides", *Organometallics*, submitted.
71. A. M. Kinyua, H. P. Hratchian, C. C. Jarrold, and L. M. Thompson, "Photoelectron–remnant interaction effect on remnant wavefunction in low-kinetic energy electron detachment events", *J. Chem. Phys.* **162**, 064304 (2025).
70. ** A. Y. Zamani and H. P. Hratchian, "Estimating vertical core-excitation energies from Møller-Plesset theory with spin projection", *Mol. Phys.*, e2398142 (2024). Sanibel Conference special issue.
69. S. Vaish, A. O. Gyamfi, C. D. Huizenga, H. P. Hratchian, and C. C. Jarrold, "Electronic structures of small stoichiometric Zn_xO_x clusters", *J. Phys. Chem. A* **128**, 6450–6461 (2024).
68. ** H. P. Hratchian, A. Karton, and N. J. Mayhall, "Tribute to Krishnan Raghavachari", *J. Phys. Chem. A* **129**, 2523–2525 (2024). *Invited Guest Editorial*.
67. ** A. Y. Zamani and H. P. Hratchian, "Δ-based composite models for calculating x-ray absorption and emission energies", *J. Chem. Phys.* **159**, 224109 (2023).
66. ** A. Abou Taka, H. H. Corzo, A. Pribram-Jones, and H. P. Hratchian, "Good Vibrations: Calculating excited state frequencies using ground state self-consistent field models", *J. Chem. Theory Comput.* **8**, 7286–7297 (2022).

PUBLICATIONS, CONTINUED

65. J. M. Herbert, M. Head-Gordon, H. P. Hratchian, T. Head-Gordon, R. Amaro, A. Aspuru-Guzik, R. Hoffmann, C. Parish, C. M. Payne, and T. Van Voorhis, "Words Matter: On the Debate over Free Speech, Inclusivity, and Academic Excellence", *J. Phys. Chem. Lett.* **13**, 7100–7104 (2022). Guest Commentary

64. ** A. Y. Zamani and H. P. Hratchian, "Assessing the performance of ΔSCF and the diagonal second-order self-energy approximation for calculating vertical core excitation energies", *J. Chem. Phys.* **157**, 084115 (2022).

63. S. I. Baker, M. Yaghoubi, S. Bidwell, S. L. Pierce, H. P. Hratchian, and R. .D. Baxter, "Enhanced Reactivity for Aromatic Bromination via Halogen-Bonding with Lactic Acid Derivatives", *J. Org. Chem.* **87**, 8492–8502 (2022).

62. ** A. Abou Taka, S. Lu, D. Gowland, T. J. Zuehlsdorff, H. H. Corzo, A. Pribram-Jones, L. Shi, H. P. Hratchian, and C. M. Isborn, "Comparison of Linear Response Theory, Projected Initial Maximum Overlap Method, and Molecular Dynamics Based Vibronic Spectra: The Case of Methylene Blue", *J. Chem. Theory Comput.* **18**, 3039–3051 (2022).

61. ** H. Harb and H. P. Hratchian, "A Density Functional Theory Investigation of the Reaction of Water with Ce_2O^-", *Comput. Theor. Chem.* **1209**, 113603 (2022).

60. ** H. H. Corzo, A. Abou Taka, A. Pribram-Jones, and H. P. Hratchian, "Using Projection Operators With Maximum Overlap Methods to Simplify Challenging Self-Consistent Field Optimization", *J. Comp. Chem.* **43**, 382–390 (2022).

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).

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).

PUBLICATIONS, CONTINUED

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).
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).

PUBLICATIONS, CONTINUED

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).
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).

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