C. David Sherrill
Regents' Professor
School of Chemistry and Biochemistry
School of Computational Science and Engineering
Georgia Institute of Technology

I. Earned Degrees

Ph.D. Chemistry, University of Georgia, 1996
B.S. Chemistry, Massachusetts Institute of Technology, 1992

II. Employment History

Director, Center for High Performance Computing, Georgia Institute of Technology, 2021-present
Associate Director for Research and Education, Institute for Data Engineering and Science (IDEaS), Georgia Institute of Technology, 2017-present
Regents' Professor, School of Chemistry and Biochemistry and School of Computational Science and Engineering, Georgia Institute of Technology, 2021-present
Professor, School of Chemistry and Biochemistry and School of Computational Science and Engineering, Georgia Institute of Technology, 2008-2021
Associate Professor, School of Chemistry and Biochemistry, Georgia Institute of Technology, 2005-2008
Associate Professor, College of Computing, Georgia Institute of Technology, 2006-2008
Director, Center for Computational Molecular Science & Technology, Georgia Institute of Technology, 2000-present
Blanchard Assistant Professor of Chemistry, Georgia Institute of Technology, 2002-2005
Assistant Professor, School of Chemistry and Biochemistry, Georgia Institute of Technology, 1999-2005
NSF Postdoctoral Fellow, University of California, Berkeley, with M. Head-Gordon, 1996-1999

III. Honors and Awards

Elected Member, International Academy of Quantum Molecular Science (IAQMS), 2024
Herty Medal for Outstanding Contributions from a Chemist in the Southeast, Georgia Section of the American Chemical Society, 2023
Elected Board Member, World Association of Theoretical and Computational Chemists (WATOC), 2022
College of Sciences Faculty Mentor Award, Georgia Tech, 2020
Outreach Volunteer of the Year, Georgia Section of the American Chemical Society, 2017
Fellow of the American Association for the Advancement of Science, 2014
Fellow of the American Chemical Society, 2011
Fellow of the American Physical Society, 2010
Vasser Woolley Faculty Fellow, 2008-2010
Distinguished Service Award, Georgia Section of the American Chemical Society, 2008
Class of 1940 W. Howard Ector Outstanding Teacher Award, 2006
National Science Foundation CAREER Award, 2001
Wiley-International Journal of Quantum Chemistry Young Investigator Award, 2001
Camille and Henry Dreyfus New Faculty Awardee, 1999
National Science Foundation Postdoctoral Fellow, 1996-1998
ACS/IBM Graduate Award in Computational Chemistry, 1995
National Science Foundation Graduate Fellow, 1992-1995

IV. Research, Scholarship, and Creative Activities

A2. Refereed Book Chapters

1. "**Wavefunction Theory Approaches to Noncovalent Interactions**," C. D. Sherrill in *Non-Covalent Interactions in Quantum Chemistry and Physics: Theory and Applications*, edited by A. Otero de la Roza and G. A. DiLabio (Elsevier, 2017). (ISBN: 978-0128098356)

2. "**Iterative Coupled-Cluster Methods on Graphics Processing Units**," A. E. DePrince, J. R. Hammond, and C. D. Sherrill, in *Electronic Structure Calculations on Graphics Processing Units: From Quantum Chemistry to Condensed Matter Physics*, edited by R. Walker and A. Goetz (Wiley, 2016). (ISBN: 978-1-118-66178-9)
3. "**Quantum Mechanical Methods for Quantifying and Analyzing Non-Covalent Interactions and for Force- Field Development**," C. D. Sherrill and K. M. Merz, in *Many-Body Effects and Electrostatics in Biomolecules*, edited by Q. Cui, M. Meuwly, and P. Ren (Pan Stanford, 2016) (ISBN: 978-9814613927)
4. "**PSI4Education: Computational Chemistry Labs Using Free Software**," R. C. Fortenberry, A. Ringer Mc- Donald, T. D. Shepherd, M. Kennedy, and C. D. Sherrill, in *The Promise of Chemical Education: Addressing our Students' Needs*, vol. 1193 of *ACS Symposium Series*, edited by K. Daus and R. Rigsby (American Chemical Society, Washington, D.C., 2015), pages 75-88. (doi: 10.1021/bk-2015-1193.ch007)
5. **"Wavefunction Methods for Noncovalent Interactions,"** E. G. Hohenstein and C. D. Sherrill, Wiley Interdisciplinary Reviews: Computational Molecular Science 2, 304-326 (2012) (doi: 10.1002/wcms.84).
6. "**Computations of Noncovalent π Interactions**," C. D. Sherrill, in *Reviews in Computational Chemistry*, Vol. 26, edited by K. B. Lipkowitz and T. R. Cundari (Wiley, New York, 2009), pages 1-38. (doi: 10.1002/9780470399545.ch1)
7. "**Bond Breaking in Quantum Chemistry: A Comparison of Single- and Multi-Reference Methods**," C. D. Sherrill, A. Dutta, M. L. Abrams, and J. S. Sears, in *Electron Correlation Methodology*, vol. 958 of *ACS Symposium Series*, edited by A. K. Wilson and K. A. Peterson (American Chemical Society, Washington, D.C., 2007), pages 75-88. (doi: 10.1021/bk-2007-0958.ch005)
8. "**Bond Breaking in Quantum Chemistry**," C. D. Sherrill, in *Annual Reports in Computational Chemistry*, Vol. 1, edited by D. Spellmeyer (Elsevier, Amsterdam, 2005), pages 45-54. (doi: 10.1016/S1574-1400(05)01004-2)
9. "**The Configuration Interaction Method: Advances in Highly Correlated Approaches**," C. D. Sherrill and H. F. Schaefer in *Advances in Quantum Chemistry*, Vol. 34, edited by P.-O. Löwdin (Academic Press, New York, 1999), pages 143-269. (doi: 10.1016/S0065-3276(08)60532-8)

B. Refereed Publications and Submitted Articles

Google Scholar profile:
https://scholar.google.com/citations?user=PN-rzYUAAAAJ
Over 34,000 citations and h-index of 84 as of January 2024
http://orcid.org/0000-0002-5570-7666

B1. Published and Accepted Journal Articles

1. "**Accurate and Efficient Open-Source Implementation of Domain-Based Local Pair Natural Orbital (DLPNO) Coupled-Cluster Theory Using a T1-Transformed Hamiltonian**," A. Jiang, Z. L. Glick, D. Poole, J. M. Turney, C. D. Sherrill, and H. F. Schaefer, *J. Chem. Phys*. in press.

2. "**A Physics-Aware Neural Network for Protein-Ligand Interactions with Quantum Chemical Accuracy**," Z. L. Glick, D. P. Metcalf, C. T. Sargent, S. A. Spronk, A. Koutsoukas, D. L. Cheney, and C. D. Sherrill, *Chem. Sci*. in press.

3. "**A Modular, Composite Framework for the Utilization of Reduced-Scaling Coulomb and Exchange Construction Algorithms: Design and Implementation**," D. Poole, D. B. Williams-Young, A. Jiang, Z. L. Glick, and C. D. Sherrill, *J. Chem. Phys*. **161**, 052503 (2024) (doi: 10.1063/5.0216760)

4. "**Broadening Access to Small-Molecule Parameterization with the Force Field Toolkit**," Y. Zeng, A. Pavlova, P, Nelson, Z. Glick, L. Yang, Y. T. Pang, M. Spivak, G. Licari, E. Tajkhorshid, C. D. Sherrill, and J. C. Gumbart, *J. Chem. Phys*. **160**, 242501 (2024) (doi: 10.1063/5.0196848)

5. "**Directional ΔG Neural Network (DrΔG-Net): A Modular Neural Network Approach to Binding Free Energy Prediction**," D. P. Metcalf, Z. L. Glick, A. Bortolato, A. Jiang, D. L. Cheney, and C. D. Sherrill, *J. Chem. Inf. Model*. **64**, 1907-1918 (2024) (doi: 10.1021/acs.jcim.3c02054)

6. "**A Quantum Chemical Interaction Energy Dataset for Accurately Modeling Protein-Ligand Interactions**," S. A. Spronk, Z. L. Glick, D. P. Metcalf, C. D. Sherrill, and D. L. Cheney, *Sci. Data* **10**, 619 (2023) (doi: 10.1038/s41597-023-02443-1)

7. "**Approximating Large-Basis Coupled-Cluster Theory Vibrational Frequencies using Focal-Point Approximations**," P. M. Nelson, Z. L. Glick, and C. D. Sherrill, *J. Chem. Phys.* **159**, 094104 (2023) (doi: 10.1063/5.0168608)

8. "**A Quantitative Assessment of Deformation Energy in Intermolecular Interactions: How Important is it**?" C. T. Sargent, R. Kasera, Z. L. Glick, C. D. Sherrill, and D. L. Cheney, *J. Chem. Phys.* **158**, 244106 (2023) (doi: 10.1063/5.0155895)

9. "**Benchmark Coupled-Cluster Lattice Energy of Crystalline Benzene, and Assessment of Multi-Level Approximations in the Many-Body Expansion**," C. H. Borca, Z. L. Glick, D. P. Metcalf, L. A. Burns, and C. D. Sherrill, *J. Chem. Phys*. **158**, 234102 (2023) (doi: 10.1063/5.0159410)

10. "**High-Order Quantum-Mechanical Analysis of Hydrogen Bonding in Hachimoji and Natural DNA Base Pairs**," R. L. Kumawat and C. D. Sherrill, *J. Chem. Inf. Model*. 63, 3150-3157 (2023) (doi: 10.1021/acs.jcim.3c00428)

11. "**Assessment of Three-Body Dispersion Models against Coupled-Cluster Benchmarks for Crystalline Benzene, Carbon Dioxide, and Triazine**," Y. Xie, Z. L. Glick, and C. D. Sherrill, *J. Chem. Phys.* 158, 094110 (2023) (doi: 10.1063/5.0143712)

12. "**Benchmarking Two-Body Contributions to Crystal Lattice Energies and a Range-Dependent Assessment of Approximate Methods**," C. T. Sargent, D. P. Metcalf, Z. L. Glick, C. H. Borca, and C. D. Sherrill, *J. Chem. Phys.* **158**, 054112 (2023) (doi: 10.1063/5.0141872)

13. "**Range-Dependence of Two-Body Intermolecular Interactions and their Energy Components in Molecular Crystals**," D. P. Metcalf, A. Smith, Z. L. Glick, and C. D. Sherrill, *J. Chem. Phys.* **157**, 084503 (2022) (doi: 10.1063/5.0103644)

14. "**A Nonconjugated Radical Polymer with Stable Red Luminescence in Solid State**," Z. Wang, X. Zou, Y. Xie, H. Zhang, L. Hu, C. C. S. Chan, R. Zhang, J. Guo, R. T. K. Kwok, J. W. Y. Lam, I. D. Williams, Z. Zeng, K. S. Wong, C. D. Sherrill, R. Ye, and B. Z. Tang, *Mater. Horiz.* **9**, 2564-2571 (2022) (doi: 10.1039/D2MH00808D)

15. "**Implementation of Symmetry-Adapted Perturbation Theory based on Density Functional Theory and using Hybrid Exchange-Correlation Kernels for Dispersion Terms**," Y. Xie, D. G. A. Smith, and C. D. Sherrill, *J. Chem. Phys.* **156**, 194306 (2022) (doi: 10.1063/5.0090688)

16. "**The Influence of a Solvent Environment On Direct Non-Covalent Interactions Between Two Molecules: A Symmetry-Adapted Perturbation Theory Study of Polarization Tuning**

of π-π Interactions by Water," D. A. Sirianni, X. Zhu, D. F. Sitkoff, D. L. Cheney, and C. D. Sherrill, *J. Chem. Phys*. **156**, 194306 (2022) (doi: 10.1063/5.0087302)

17. "**Quantum Chemistry Common Driver and Databases (QCDB) and Quantum Chemistry Engine (QCEngine): Automation and Interoperability Among Computational Chemistry Programs**," D. G. A. Smith, A. T. Lolinco, Z. L. Glick, J. Lee, A. Alenaizan, T. A. Barnes, C. H. Borca, R. Di Remigio, D. L. Dotson, S. Ehlert, A. G. Heide, M. F. Herbst, J. Hermann, C. B. Hicks, J. T. Horton, A. G. Hurtado, P. Kraus, H. Kruse, S. J. R. Lee, J. P. Misiewicz, L. N. Naden, F. Ramezanghorbani, M. Scheurer, J. B. Schriber, A. C. Simmonett, J. Steinmetzer, J. R. Wagner, L. Ward, M. Welborn, D. Atlarawy, J. Anwar, J. D. Chodera, A. Dreuw, H. T. Kulik, F. Liu, T. J. Martínez, D. A. Matthews, H. F. Schaefer, J. Šponer, J. T. Turney, L.-P. Wang, N. De Silva, R. A. King, J. F. Stanton, M. S. Gordon, T. L. Windus, C. D. Sherrill, and L. A. Burns, *J. Chem. Phys.* **155**, 204801 (2021). (doi: 10.1063/5.0059356)

18. "**Tuning DNA Supramolecular Polymers by Addition of Small, Functionalized Nucleobase Mimics**", C. Lachance-Brais, C. Hennecker, A. Alenaizan, X. Luo, V. Toader, M. Taing, C. D. Sherrill, A. Mittermaier, and H. Sleiman, *J. Am. Chem. Soc*. **143**, 19824-19833 (2021). (doi: 10.1021/jacs.1c08972)

19. **"Optimized Damping Parameters for Empirical Dispersion Corrections to Symmetry-Adapted Perturbation Theory**," J. B. Schriber, D. A. Sirianni, D. G. A. Smith, L. A. Burns, D. Sitkoff, D. L. Cheney, and C. D. Sherrill, *J. Chem. Phys*. **154**, 234107 (2021). (doi: 10.1063/5.0049745)

20. "**Cartesian Message Passing Neural Networks for Directional Properties: Fast and Transferable Atomic Multipoles**," Z. L. Glick, A. Koutsoukas, D. L. Cheney, and C. D. Sherrill, *J. Chem. Phys.* **154**, 224103 (2021). (doi: 10.1063/5.0050444)

21. "**CLIFF: A Component-Based, Machine-Learned, Intermolecular Force Field**," J. B. Schriber, D. R. Nascimento, A. Koutsoukas, S. A. Spronk, D. L. Cheney, and C. D. Sherrill, *J. Chem. Phys*. 154, 184110 (2021). (doi: 10.1063/5.0042989)

22. "**X-ray Fiber Diffraction and Computational Analyses of Stacked Hexads in Supramolecular Polymers: Insight into Self-Assembly in Water by Prospective Prebiotic Nucleobases**," A. Alenaizan, C. H. Borca, S. C. Karunakaran, A. K. Kendall, G. Stubbs, G. B. Schuster, C. D. Sherrill, and N. V. Hud, *J. Am. Chem. Soc*. **143**, 6079-6094 (2021). (doi: 10.1021/jacs.0c12010)

23. "**Noncovalent Helicene Structure between Nucleic Acids and Cyanuric Acid**," A. Alenaizan, K. Fauche, R. Krishnamurthy, and C. D. Sherrill, *Chem. Eur. J*. **27**, 4043-4052 (2021). (doi: 10.1002/chem.202004390)

24. "**Electron-Passing Neural Networks for Atomic Charge Prediction in Systems with Arbitrary Molecular Charge**," D. P. Metcalf, A. Jiang, S. A. Spronk, D. L. Cheney, and C. D. Sherrill, *J. Chem Inf. Model.* **61**, 115 (2021). (doi: 10.1021/acs.jcim.0c01071)

25. "**The proto-Nucleic Acid Builder: A Software Tool for Constructing Nucleic Acid Analogs**," A. Alenaizan, J. L. Barnett, N. V. Hud, C. D. Sherrill, and A. S. Petrov, *Nucleic Acids Res*. **49**, 79-89 (2021). (doi: 10.1093/nar/gkaa1159)

26. "**AP-Net: An Atomic-Pairwise Neural Network for Smooth and Transferable Interaction Potentials**," Z. L. Glick, D. P. Metcalf, A. Koutsoukas, S. A. Spronk, D. L. Cheney, and C. D. Sherrill, *J. Chem. Phys*. **153**, 044112 (2020). (doi: 10.1063/5.0011521)

27. **"Psi4 1.4: Open-Source Software for High-Throughput Quantum Chemistry,"** D. G. A. Smith, L. A. Burns, A. C. Simmonett, R. M. Parrish, M. C. Schieber, R. Galvelis, P. Kraus, H. Kruse, R. Di Remigio, A. Alenaizan, A.M. James, S. Lehtola, J. P. Misiewicz, M. Scheurer, R. A. Shaw, J. B. Schriber, Y. Xie, Z. L. Glick, D. A. Sirianni, J. Senan O'Brien, J. M. Waldrop, A. Kumar, E. G. Hohenstein, B. P. Pritchard, B. R. Brooks, H. F. Schaefer, A. Yu. Sokolov, K. Patkowski, A. E. DePrince, U. Bozkaya, R. A. King, F. A. Evangelista, J. M. Turney, T. D. Crawford, and C. D. Sherrill, *J. Chem. Phys*. **152**, 184108 (2020). (doi: 10.1063/5.0006002)

28. **"Efficient and Automated Computation of Molecular Geometries using Focal-Point Approximations to Large-Basis Coupled-Cluster Theory,"** C. E. Warden, D. G. A. Smith, L. A. Burns, U. Bozkaya, and C. D. Sherrill, *J. Chem. Phys*. **152**, 124109 (2020). (doi: 10.1063/5.0004863)

29. **"Approaches for Machine Learning Intermolecular Interaction Energies and Application to Energy Components from Symmetry Adapted Perturbation Theory,"** D. P. Metcalf, A. Koutsoukas, S. A. Spronk, B. L. Claus, D. A. Loughney, S. R. Johnson, D. L. Cheney, and C. D. Sherrill, *J. Chem. Phys*. **152**, 074103 (2020). (doi: 10.1063/1.5142636)

30. **"Techniques for High-Performance Construction of Fock Matrices,"** H. Huang, C. D. Sherrill, and E. Chow, *J. Chem. Phys*. **152**, 024122 (2020). (doi: 10.1063/1.5129452)

31. **"Python Implementation of the Restrained Electrostatic Potential (RESP) Charge Model,"** A. Alenaizan, L. A. Burns, and C. D. Sherrill, *Int. J. Quantum Chem*. **120**, e26035 (2020). (doi: 10.1002/qua.26035)

32. **"CrystaLattE: Automated Computation of Lattice Energies of Organic Crystals Exploiting the Many-Body Expansion to Achieve Dual-Level Parallelism,"** C. H. Borca, B. W. Bakr, L. A. Burns, and C. D. Sherrill, *J. Chem. Phys*. **151**, 144103 (2019). (doi: 10.1063/1.5120520)

33. **"Morphology of Organic Semiconductors Electrically Doped from Solution Using Phosphomolybdic Acid,"** T.-Y. Huang, F. Larrain, C. Borca, C. Fuentes-Hernandez, H. Yan, S. Schneider, W.-F. Chou, V. A. Rogriguez-Toro, H.-G. Steinrük, C. Cao, C. D. Sherrill, B. Kippelen, and M. Toney, *Chem. Mater*. **31**, 6677-6683 (2019). (doi: 10.1021/acs.chemmater.9b01069)

34. **"Intramolecular Noncovalent Interactions Facilitate Thermally Activated Delayed Fluorescence (TADF),"** X.-K. Chen, B. W. Bakr, M. Auffray, Y. Tsuchiya, C. D. Sherrill, C. Adachi, and J. L. Brédas, *J. Phys. Chem. Lett*. **10**, 3260-3268 (2019). (doi: 10.1021/acs.jpclett.9b01220)

35. **"Water Bridges Conduct Sequential Proton Transfer in Photosynthetic Oxygen Evolution,"** U. Brahmachari, J. F. Gonthier, C. D. Sherrill, and B. A. Barry, *J. Phys. Chem. B* **123**, 4487-4496 (2019). (doi: 10.1021/acs.jpcb.9b01523)

36. **"Tipping the Balance between S-π and O-π Interactions,"** J. Hwang, P. Li, M. D. Smith, C. E. Warden, D. A. Sirianni, E. C. Vik, J. M. Maier, C. J. Yehl, C. D. Sherrill, and K. D. Shimizu, *J. Am. Chem. Soc*. **140**, 13301-13307 (2018). (doi: 10.1021/jacs.8b07617)

37. **"Analysis of Transition State Stabilization by Non-Covalent Interactions in Organocatalysis: Application of Atomic and Functional-Group Partitioned Symmetry-Adapted Perturbation Theory to the Addition of Organoboron Reagents to Fluoroketones,"** B. W. Bakr and C. D. Sherrill, *Phys. Chem. Chem. Phys*. **20**, 18241–18251 (2018). (doi: 10.1039/c8cp02029a)

38. **"PSI4NUMPY: An Interactive Quantum Chemistry Programming Environment for Reference Implementations and Rapid Development,"** D. G. A. Smith, L. A. Burns, D. A. Sirianni, D. R. Nascimento, A. Kumar, A. M. James, J. B. Schriber, T. Zhang, B. Zhang, A. S.

Abbott, E. J. Berquist, M. H. Lechner, L. A. Cunha, A. G. Heide, J. M. Waldrop, T. Y. Takeshita, A. Alenaizan, D. Neuhauser, R. A. King, A. C. Simmonett, J. M. Turney, H. F. Schaefer, F. A. Evangelista, A. E. DePrince, T. D. Crawford, K. Patkowski, and C. D. Sherrill, *J. Chem. Theory Comput*. **14**, 3504-3511 (2018). (doi: 10.1021/acs.jctc.8b00286)

39. **"Assessment of Density Functional Methods for Geometry Optimization of Bimolecular van der Waals Complexes,"** D. A. Sirianni, A. Alenaizan, D. L. Cheney, and C. D. Sherrill, *J. Chem. Theory Comput*. **14**, 3004-3013 (2018). (doi: 10.1021/acs.jctc.8b00114)

40. **"Understanding Many-Body Basis Set Superposition Error: Beyond Boys and Bernardi,"** R. M. Richard, B. W. Bakr, and C. D. Sherrill, *J. Chem. Theory Comput*. **14**, 2386-2400 (2018). (doi: 10.1021/acs.jctc.7b01232)

41. **"Reassigning the CaH^+ $1\,^1\Sigma \rightarrow 2\,^1\Sigma$ Vibronic Transition with CaD^+,"** J. Condoluci, S. Janardan, A. T. Calvin, R. Rugango, G. Shu, C. D. Sherrill, and K. R. Brown, *J. Chem. Phys*. **147**, 214309 (2017). (doi: 10.1063/1.5016556)

42. "**Chloride Maintains a Protonated Internal Water Network in the Photosynthetic Oxygen Evolving Complex**," U. Brahmachari, J. F. Gonthier, C. D. Sherrill, and B. A. Barry, *J. Phys. Chem. B* **121,** 10327-10337 (2017). (doi: 10.1021/acs.jpcb.7b08358)

43. **"C–H···O Hydrogen Bonding. The Prototypical Methane–Formaldehyde System: A Critical Assessment,"** K. B. Moore, K. Sadeghian, C. D. Sherrill, C. Ochsenfeld, and H. F. Schaefer, *J. Chem. Theory Comput*. **13**, 5379- 5395 (2017). (doi: 10.1021/acs.jctc.7b00753)

44. "**The BioFragment Database (BFDb): An Open-Data Platform for Computational Chemistry Analysis of Noncovalent Interactions**," L. A. Burns, J. C. Faver, Z. Zheng, M. S. Marshall, D. G. A. Smith, K. Vanommeslaeghe, A. D. MacKerell, K. M. Merz, and C. D. Sherrill, *J. Chem. Phys.* **147**, 161727 (2017). (doi: 10.1063/1.5001028)

45. "**Analytic Energy Gradients for the Coupled-Cluster Singles and Doubles with Perturbative Triples Method with the Density-Fitting Approximation**," U. Bozkaya and C. D. Sherrill, *J. Chem. Phys.* **147**, 044104 (2017). (doi: 10.1063/1.4994918)

46. "**Psi4 1.1: An Open-Source Electronic Structure Program Emphasizing Automation, Advanced Libraries, and Interoperability**," R. M. Parrish, L. A. Burns, D. G. A. Smith, A. C. Simmonett, A. E. DePrince, E. G. Hohen- stein, U. Bozkaya, A. Yu. Sokolov, R. Di Remigio, R. M. Richard, J. F. Gonthier, A. M. James, H. R. McAlexander, A. Kumar, M. Saitow, X. Wang, B. P. Pritchard, P. Verma, H. F. Schaefer, K. Patkowski, R. A. King, E. F. Valeev, F. A. Enganvelista, J. M. Turney, T. D. Crawford, and C. D. Sherrill, *J. Chem. Theory Comput.* **13**, 3185-3197 (2017). (doi: 10.1021/acs.jctc.7b00174)

47. "**The Surprising Importance of Peptide Bond Contacts in Drug-Protein Interactions**," R. M. Parrish, D. F. Sitkoff, D. L. Cheney, and C. D. Sherrill, *Chem. Eur. J.* **23**, 7887-7890 (2017). (doi: 10.1002/chem.201701031)

48. "**Comparison of Explicitly Correlated Methods for Computing High-Accuracy Benchmark Energies for Non-covalent Interactions**," D. A. Sirianni, L. A. Burns, and C. D. Sherrill, *J. Chem. Theory Comput.* **13**, 86-99 (2017). (doi: 10.1021/acs.jctc.6b00797)

49. "**Density-Fitted Open-Shell Symmetry-Adapted Perturbation Theory and Application to π-Stacking in Benzene Dimer Cation and Ionized DNA Base Pair Steps**," J. F. Gonthier and C. D. Sherrill, *J. Chem. Phys.* **145**, 134106 (2016). (doi: 10.1063/1.4963385)

50. "**Revised Damping Parameters for the D3 Dispersion Correction to Density Functional Theory**," D. G. A. Smith, L. A. Burns, K. Patkowski, and C. D. Sherrill, *J. Phys. Chem. Lett.* **7**, 2197-2203 (2016). (doi: 10.1021/acs.jpclett.6b00780)

51. "**Analytic Energy Gradients for the Coupled-Cluster Singles and Doubles Methods with the Density-Fitting Approximation**," U. Bozkaya and C. D. Sherrill, *J. Chem. Phys.* **144**, 174103 (2016). (doi: 10.1063/1.4948318)

52. "**Analysis of Transition State Stabilization by Non-Covalent Interactions in the Houk-List Model of Organocatalyzed Intermolecular Aldol Additions using Functional-Group Symmetry-Adapted Perturbation Theory**," B. W. Bakr and C. D. Sherrill, *Phys. Chem. Chem. Phys.* **18**, 10297-10308 (2016). (doi: 10.1039/c5cp07281f)

53. "**Accurate Ionization Potentials and Electron Affinities of Acceptor Molecules IV: Electron–Propagator Methods**," O. Dolgounitcheva, M. D´ıaz-Tinoco, V. G. Zakrzewski, R. M. Richard, N. Marom, C. D. Sherrill, and J. V. Ortiz, *J. Chem. Theory Comput.* **12**, 627-637 (2016). (doi: 10.1021/acs.jctc.5b00872)

54. "**Accurate Ionization Potentials and Electron Affinities of Acceptor Molecules I. Reference Data at the CCSD(T) Complete Basis Set Limit**," R. M. Richard, M. S. Marshall, O. Dolgounitcheva, J. V. Ortiz, J. L. Bredás, N. Marom, and C. D. Sherrill, *J. Chem. Theory Comput.* **12**, 595-604 (2016). (doi: 10.1021/acs.jctc.5b00875)

55. "**Competition Between π-π and C–H/π Interactions: A Comparison of the Structural and Electronic Properties of Alkoxy-Substituted 1,8-bis((Propyloxyphenyl)ethynyl)naphthalenes**," B. E. Carson, T. M. Parker, E. G. Hohenstein, G. L. Brizius, W. Komorner, R. A. King, D. M. Collard, and C. D. Sherrill, *Chem. Eur. J.* **21**, 19168-19175 (2015). (doi: 10.1002/chem.201502363)

56. "**Assessment of Empirical Models versus High-Accuracy Ab Initio Methods for Nucleobase Stacking: Evaluating the Importance of Charge Penetration**," T. M. Parker and C. D. Sherrill, *J. Chem. Theory Comput.* **11**, 4197-4202 (2015). (doi: 10.1021/acs.jctc.5b00588)

57. "**Communication: Practical Intramolecular Symmetry Adapted Perturbation Theory via Hartree–Fock Embedding**," R. M. Parrish, J. F. Gonthier, C. Corminboeuf, and C. D. Sherrill, *J. Chem. Phys.* **143**, 051103 (2015). (doi: 10.1063/1.4927575)

58. "**Rubrene: The Interplay between Intramolecular and Intermolecular Interactions Determines the Planarization of its Tetracene Core in the Solid State**," C. Sutton, M. S. Marshall, C. D. Sherrill, C. Risko, and J. L. Brédas, *J. Am. Chem. Soc.* **137**, 8775-8782 (2015). (doi: 10.1021/jacs.5b04066)

59. "**Co(III) Complexes of Tetradentate X3L Type Ligands: Synthesis, Electronic Structure, and Reactivity**," Y. Feng, L. A. Burns, C. D. Sherrill, and C. W. Jones, *Inorg. Chim. Acta* **430**, 30-35 (2015). (doi: 10.1016/j.ica.2015.01.036)

60. "**Advances in Molecular Quantum Chemistry Contained in the Q-Chem 4 Program Package**," Y. Shao, et al., *Mol. Phys.* **113**, 184-215 (2105). (doi: 10.1080/00268976.2014.952696)

61. "**Counterion and Substrate Effects on Barrier Heights of the Hydrolytic Kinetic Resolution of Terminal Epoxides Catalyzed by Co(III)-salen**," M. R. Kennedy, L. A. Burns, and C. D. Sherrill, *J. Phys. Chem. A* **119**, 403-409 (2015). (doi: 10.1021/jp511261z)

62. "**Appointing Silver and Bronze Standards for Noncovalent Interactions: A Comparison of Spin-Component-Scaled (SCS), Explicitly Correlated (F12), and Specialized Wavefunction Approaches**," L. A. Burns, M. S. Marshall, and C. D. Sherrill, *J. Chem. Phys.* **141**, 234111 (2014). (doi: 10.1063/1.4903765)

63. "**Quantum Mechanical Evaluation of π-π vs. Substituent-π Interactions in π-Stacking: Direct Evidence for the Wheeler-Houk Picture**," R. M. Parrish and C. D. Sherrill, *J. Am. Chem. Soc.* **136**, 17386-17389 (2014). (doi: 10.1021/ja5101245)

64. "**Orbital-Optimized MP2.5 and its Analytic Gradients: Approaching CCSD(T) Quality for Open-Shell Non- covalent Interactions**," U. Bozkaya and C. D. Sherrill, *J. Chem. Phys.* **141**, 204105 (2014). (doi: 10.1063/1.4902226)

65. "**A Tyrosine-Rich Cell Surface Protein in the Diatom Amphora coffeaeformis Identified through Transcrip- tome Analysis and Genetic Transformation**," M. T. Buhmann, N. Poulsen, J. Klemm, M. R. Kennedy, C. D. Sherrill, and N. Kröger, *PLOS ONE* **9**, e110369 (2014). (doi: 10.1371/journal.pone.0110369)

66. "**Erratum: Accurate Prediction of Noncovalent Interaction Energies with the Effective Fragment Potential Method: Comparison of Energy Components to Symmetry-Adapted Perturbation Theory for the S22 Test set (vol 8, pg. 2835, 2012)**," J. C. Flick, D. Kosenkov, E. G. Hohenstein, C. D. Sherrill, and L. V. Slipchenko, *J. Chem. Theory Comput.* **10**, 4759-4760 (2014). (doi: 10.1021/ct500658b)

67. "**Chemical Assignment of Symmetry-Adapted Perturbation Theory Interaction Energy Components: The Functional-Group SAPT Partition**," R. M. Parrish, T. M. Parker, and C. D. Sherrill, *J. Chem. Theory Comput.* **10**, 4417-4431 (2014). (doi: 10.1021/ct500724p)

68. "**The CH-π Interactions of Methyl Ethers as a Model for Carbohydrate-N-Heteroarene Interactions**," P. Li, T. M. Parker, J. Hwang, F. Deng, M. D. Smith, P. J. Pellachia, C. D. Sherrill, and K. D. Shimizu, *Org. Lett.* **16**, 5064-5067 (2014). (doi: 10.1021/ol502418k)

69. "**Spatial Assignment of Symmetry Adapted Perturbation Theory Interaction Energy Components: The Atomic SAPT Partition**," R. M. Parrish and C. D. Sherrill, *J. Chem. Phys.* **141**, 044115 (2014). (doi: 10.1063/1.4889855)

70. "**Communication: Acceleration of Coupled Cluster Singles and Doubles via Orbital-Weighted Least-Squares Tensor Hypercontraction**" R. M. Parrish, C. D. Sherrill, E. G. Hohenstein, S. I. L. Kokkila, and T. J. Martínez, *J. Chem. Phys.* **140**, 181102 (2014). (doi: 10.1063/1.4876016)

71. "**Communication: Resolving the Three-Body Contribution to the Lattice Energy of Crystalline Benzene**," M. R. Kennedy, A. Ringer McDonald, A. E. DePrince, M. S. Marshall, R. Podeszwa, and C. D. Sherrill, *J. Chem. Phys.* **140**, 121104 (2014). (doi: 10.1063/1.4869686)

72. "**Accurate Description of Torsion Potentials in Conjugated Polymers Using Density Functionals with Re- duced Self-Interaction Error**," C. Sutton, T. Körzdörfer, M. T. Gray, M. Brunsfeld, R. M. Parrish, C. D. Sherrill, J. S. Sears, and J. L. Brédas, *J. Chem. Phys.* **140**, 054310 (2014). (doi: 10.1063/1.4863218)

73. "**Density Fitted Singles and Doubles Coupled Cluster on Graphics Processing Units**," A. E. DePrince, M. R. Kennedy, B. G. Sumpter, and C. D. Sherrill, *Mol. Phys.* **112**, 844-852 (2014). (doi: 10.1080/00268976.2013.874599)

74. "**Levels of Symmetry Adapted Perturbation Theory (SAPT). I. Efficiency and Performance for Interaction Energies**," T. M. Parker, L. A. Burns, R. M. Parrish, A. G. Ryno, and C. D. Sherrill, *J. Chem. Phys.* **140**, 094106 (2014). (doi: 10.1063/1.4867135)

75. "**Comparing Counterpoise-Corrected, Uncorrected, and Averaged Binding Energies for Benchmarking Non-covalent Interactions**," L. A. Burns, M. S. Marshall, and C. D. Sherrill, *J. Chem. Theory Comput.* **10**, 49-57 (2014). (doi: 10.1021/ct400149j)

76. "**Tractability Gains in Symmetry-Adapted Perturbation Theory Including Coupled Double Excitations: CCD+ST(CCD) Dispersion with Natural Orbital Truncations**," R. M. Parrish, E. G. Hohenstein, and C. D. Sherrill, *J. Chem. Phys.* **139**, 174102 (2013). (doi: 10.1063/1.4826520)

77. "**Mechanisms of H_2O Desorption from Amorphous Solid Water by 157-nm Irradiation: An Experimental and Theoretical Study**," A. J. DeSimone, V. D. Crowell, C. D. Sherrill, and T. M. Orlando, *J. Chem. Phys.* **139**, 164702 (2013). (doi: 10.1063/1.4825239)

78. "**Tensor Hypercontraction: A Universal Technique for the Resolution of Matrix Elements of Local, Finite- Range N -Body Potentials in Many-Body Quantum Problems**," R. M. Parrish, E. G. Hohenstein, N. F. Schunck, C. D. Sherrill, and T. J. Martınez, *Phys. Rev. Lett.*, **111**, 132505 (2013). (doi: 10.1103/PhysRevLett.111.132505)

79. "**Redox-Linked Conformational Control of Proton Coupled Electron Transfer: Y122 in the Ribonucleotide Reductase β2 Subunit**," A. R. Offenbacher, L. A. Burns, C. D. Sherrill, and B. A. Barry, *J. Phys. Chem. B* **117**, 8457-8468 (2013). (doi: 10.1021/jp404757r)

80. "**Orbital-Optimized Coupled-Electron Pair Theory and Its Analytic Gradients: Applications to Equilibrium Geometries, Harmonic Vibrational Frequencies, and Hydrogen Transfer Reactions**," U. Bozkaya and C. D. Sherrill, *J. Chem. Phys.* **139**, 054104 (2013). (doi: 10.1063/1.4816628)

81. "**Accuracy and Efficiency of Coupled-Cluster Theory Using Density Fitting / Cholesky Decomposition, Frozen Natural Orbitals, and a t_1-Transformed Hamiltonian**," A. E. DePrince and C. D. Sherrill, *J. Chem. Theory Com- put.* **9**, 2687-2696 (2013). (doi: 10.1021/ct400250u)

82. "**Discrete Variable Representation in Electronic Structure Theory: Quadrature Grids for Least-Squares Ten- sor Hypercontraction**," R. M. Parrish, E. G. Hohenstein, T. J. Mart´ınez, and C. D. Sherrill, *J. Chem. Phys.* **138**, 194107 (2013). (doi: 10.1063/1.4802773)

83. "**Analytic Energy Gradients for the Orbital-Optimized Second-Order Møller-Plesset Perturbation Theory**," U. Bozkaya and C. D. Sherrill, *J. Chem. Phys.* **138**, 184103 (2013). (doi: 10.1063/1.4803662)

84. "**Energy Component Analysis of π Interactions**," C. D. Sherrill, *Acc. Chem. Res.* **46**, 1020-1028 (2013). (doi: 10.1021/ar3001124)

85. "**Quantum Mechanical Analysis of the Energetic Contributions to π Stacking in Nucleic Acids versus Rise, Twist, and Slide**," T. M. Parker, E. G. Hohenstein, R. M. Parrish, N. V. Hud, and C. D. Sherrill, *J. Am. Chem. Soc.* **135**, 1306-1316 (2013). (doi: 10.1021/ja3063309)

86. "**Accurate Noncovalent Interaction Energies Using Truncated Basis Sets Based on Frozen Natural Orbitals**," E. DePrince and C. D. Sherrill, *J. Chem. Theory Comput.* **9**, 293-299 (2013). (doi: 10.1021/ct300780u)

87. "**Energetics of Zinc-Mediated Interactions in the Allosteric Pathways of Metal Sensor Proteins**," D. Chakravorty, T. Parker, A. Guerra, C. D. Sherrill, D. Giedroc, and K. M. Merz, *J. Am. Chem. Soc.* **135**, 30-33 (2013). (doi: 10.1021/ja309170g)

88. "**Communication: Tensor Hypercontraction. III. Least-Squares Tensor Hypercontraction for the Determination of Correlated Wavefunctions**," E. G. Hohenstein, R. M. Parrish, C. D. Sherrill, and T. J. Mart´ınez, *J. Chem. Phys.* **137**, 221101 (2012). (doi: 10.1063/1.4768241)

89. "**Tensor Hypercontraction. II. Least-Squares Renormalization**," R. M. Parrish, E. G. Hohenstein, T. J. Martinez, and C. D. Sherrill, *J. Chem. Phys.* **137**, 224106 (2012). (doi: 10.1063/1.4768233)

90. "**Buckyplates and Buckybowls: Examining the Effects of Curvature on π-π Interactions**," M. R. Kennedy, L. A. Burns, and C. D. Sherrill, *J. Phys. Chem. A* **116**, 11920-11926 (2012). (doi: 10.1021/jp305700k)

91. "**Assessment of the Performance of Tuned Range-Separated Hybrid Density Functionals in Predicting Accurate Quasiparticle Spectra**," T. Körzdörfer, R. M. Parrish, N. Marom, J. S. Sears, C. D. Sherrill, and J. L. Brédas, *Phys. Rev. B* **86**, 205110 (2012). (doi: 10.1103/PhysRevB.86.205110)

92. "**On the Relationship between Bond-Length Alternation and Many-Electron Self-Interaction Error**," T. Körzdörfer, R. M. Parrish, J. S. Sears, C. D. Sherrill, and J. L. Brédas, *J. Chem. Phys.* **137**, 124305 (2012). (doi: 10.1063/1.4752431)

93. "**Accurate Prediction of Non-Covalent Interaction Energies with the Effective Fragment Potential Method: Comparison of Energy Components to Symmetry-Adapted Perturbation Theory for the S22 Test Set**," J. C. Flick, D. Kosenkov, E. G. Hohenstein, C. D. Sherrill, and L. V. Slipchenko, *J. Chem. Theory Comput.* **8**, 2835-2843 (2012). (doi: 10.1021/ct200673a)

94. "**Do Deuteriums form Stronger CH-π Interactions?**," C. Zhao, R. M. Parrish, M. D. Smith, P.J. Pelluchia, C. D. Sherrill, and K. D. Shimizu, *J. Am. Chem. Soc.* **134**, 14306-14309 (2012). (doi: 10.1021/ja305788p)

95. "PSI4**: An Open-Source *Ab Initio* Electronic Structure Program**," J. M. Turney, A. C. Simmonett, R. M. Parrish,E. G. Hohenstein, F. Evangelista, J. F. Fermann, B. J. Mintz, L. A. Burns, J. J. Wilke, M. L. Abrams, N. J. Russ, M. L. Leininger, C. L. Janssen, E. T. Seidl, W. D. Allen, H. F. Schaefer, R. A. King, C. D. Sherrill, and T. D. Crawford, *WIREs: Comput. Mol. Sci.* **2**, 556-565 (2012). (doi: 10.1002/wcms.93).

96. "**Isotopic Ratios in Titan's Methane: Measurements and Modeling**," C. A. Nixon, B. Temelso, S. Vinatier, N. Teanby, B. Bezard, R. K. Achterberg, K. E. Mandt, C. D. Sherrill, P. G. J. Irwin, D. E. Jennings, P. N. Romani, A. Coustenis, and F. M. Flasar, Astrophys. J. 749, 159 (2012). (doi: 10.1088/0004-637X/749/2/159).

97. "**Dispersion-weighted explicitly correlated coupled-cluster theory [DW-CCSD(T**)-F12]**," M. S. Marshall and C. D. Sherrill, *J. Chem. Theory Comput.* **7**, 3978-3982 (2011). (doi: 10.1021/ct200600p).

98. "**The Role of Long-Range Directed Lewis Acid-Base van der Waals Interactions in the Formation of Nanoparticle Clusters**," G. V. Gibbs, T. D. Crawford, A. F. Wallace, D. F. Cox, R. M. Parrish, E. G. Hohenstein, and C. D. Sherrill, *J. Phys. Chem. A* **115**, 12933-12940 (2011). (doi: 10.1021/jp204044k)

99. "**Wavefunction Methods for Noncovalent Interactions**," E. G. Hohenstein and C. D. Sherrill, *WIREs: Comput. Mol. Sci.* **2**, 304-326 (2012) (doi: 10.1002/wcms.84).

100. "**Basis Set Convergence of the Coupled-Cluster Correction: Best Practices for Benchmarking Non-Covalent Interactions and the Attendant Revision of the S22, NBC10, HBC6, and HSG Databases**," M. S. Marshall, L. A. Burns, and C. D. Sherrill, *J. Chem. Phys.* **135**, 194102 (2011). (doi: 10.1063/1.3659142) [Se- lected for the November 15, 2011 issue of the APS/AIP Virtual Journal of Biological Physics Research.]

101. "**Large-scale Symmetry-adapted Perturbation Theory Computations via Density Fitting and Laplace Trans- formation Techniques: Investigating the Fundamental Forces of DNA-Intercalator Interactions**," E. G. Hohenstein, R. M. Parrish, C. D. Sherrill, J. M. Turney, and H. F. Schaefer, *J. Chem. Phys.* **135**, 174107 (2011). (doi: 10.1063/1.3656681) [Selected for the November 15, 2011 issue of the APS/AIP Virtual Journal of Biological Physics Research.]

102. "**Quadratically-Convergent Orbital-Optimized Coupled-Cluster Doubles Method (QC-OD) and Orbital-Optimized Second-Order Møller-Plesset Perturbation Theory (QC-OMP2)**," U. Bozkaya, J. M. Turney, Y. Yamaguchi, H. F. Schaefer, and C. D. Sherrill, *J. Chem. Phys.* **135**, 104103 (2011). (doi: 10.1063/1.3631129)

103. "**Structures of Protonated Benzene Dimer and Intermolecular Interaction Analysis via Symmetry-Adapted Perturbation Theory**," H. M. Jaeger, H. F. Schaefer, E. G. Hohenstein, and C. D. Sherrill, *Comp. Theor. Chem.* **973**, 47-52 (2011). (doi: 10.1016/j.comptc.2011.06.027)

104. "**Accurate Interaction Energies for Problematic Dispersion-Bound Complexes: Homogeneous Dimers of NCCN, P_2 and PCCP**," E. G. Hohenstein, H. M. Jaeger, E. J. Carrell, G. S. Tschumper, and C. D. Sherrill, *J. Chem. Theory Comput.* **7**, 2842-2851 (2011). (doi: 10.1021/ct200374m)

105. "**Origin of the Surprising Enhancement of Electrostatic Energies by Electron-Donating Substituents in Substituted Sandwich Benzene Dimers**," E. G. Hohenstein, J. Duan, and C. D. Sherrill, *J. Am. Chem. Soc.* **133**, 13244-13247 (2011). (doi: 10.1021/ja204294q)

106. "**Challenges of Laser-Cooling Molecular Ions**," J. H. V. Nguyen, C. R. Viteri, E. G. Hohenstein, C. D. Sherrill, K. R. Brown, and B. Odom, *New J. Phys.* **13**, 063023 (2011). (doi: hrefhttp://dx.doi.org/10.1088/1367-2630/13/6/06302310.1088/1367- 630/13/6/063023)

107. "**The Energy Computation Paradox and ab initio Protein Folding**," J. C. Faver, M. L. Benson, X. He, B. P. Roberts, B. Wang, M. S. Marshall, C. D. Sherrill, and K. M. Merz, *PLOS ONE* **6**, e18868 (2011). (doi: 10.1371/jour-nal.pone.0018868)

108. "**Formal Estimation of Errors in Computed Absolute Interaction Energies for Protein-Ligand Complexes**," J. Faver, M. L. Benson, X. He, B. P. Roberts, B. Wang, M. S. Marshall, M. R. Kennedy, C. D. Sherrill, and K. M. Merz, *J. Chem. Theory Comput.* **7**, 790-797 (2011). (doi: 10.1021/ct100563b)

109. "**The Bigger, the Better: Ring-size Effects of Macrocyclic Oligomeric Co(III)-salen Catalysts**," Y. Liu, J. Rawlston, A. T. Swann, T. Takatani, C. D. Sherrill, P. J. Ludovice, and M. Weck, *Chem. Sci.* **2**, 429-438 (2011). (doi: 10.1039/c0sc00517g)

110. "**Density-Functional Approaches to Noncovalent Interactions: A Comparison of Dispersion Corrections (DFT-D), Exchange-Hole Dipole Moment (XDM) Theory, and Specialized Functionals**," L. A. Burns, Á. Vázquez-Mayagoitia, B. G. Sumpter, and C. D. Sherrill, *J. Chem. Phys.* **134**, 084107 (2011). (doi: 10.1063/1.3545971)

111. "**Assessment of the Performance of DFT and DFT-D Methods for Describing Distance Dependence of Hydrogen- Bonded Interactions**," K. S. Thanthiriwatte, E. G. Hohenstein, L. A. Burns, and C. D. Sherrill, *J. Chem. Theory Comput.* **7**, 88-96 (2011). (doi: 10.1021/ct100469b)

112. "**An Error and Efficiency Analysis of Approximations to Møller-Plesset Perturbation Theory**," M. S. Marshall, J. S. Sears, L. A. Burns, J. L. Brédas, and C. D. Sherrill, *J. Chem. Theory Comput.* **6**, 3681-3687 (2010). (doi: 10.1021/ct100468f)

113. "**Assessing the Performance of Density Functional Theory for the Electronic Structure of Metal-Salens: The M06 Suite of Functionals and the d^4-Metals**," T. Takatani, J. S. Sears, and C. D. Sherrill, *J. Phys. Chem. A* **114**, 11714-11718 (2010). (doi: 10.1021/jp1046084)

114. "**Efficient Evaluation of Triple Excitations in Symmetry-Adapted Perturbation Theory via Second-order Møller-Plesset Perturbation Theory Natural Orbitals**," E. G. Hohenstein and C. D. Sherrill, *J. Chem. Phys.* **133**, 104107 (2010). (doi: 10.1063/1.3479400)

115. "**Density Fitting of Intramonomer Correlation Effects in Symmetry-Adapted Perturbation Theory**," E. G. Hohenstein and C. D. Sherrill, *J. Chem. Phys.* **133**, 014101 (2010). (doi: 10.1063/1.3451077)

116. "**Density Fitting and Cholesky Decomposition Approximations in Symmetry-Adapted Perturbation Theory: Implementation and Application to Probe the Nature of π-π Interactions in Linear Acenes**," E. G. Hohenstein and C. D. Sherrill, *J. Chem. Phys.* **132**, 184111 (2010). (doi: 10.1063/1.3426316)

117. "**Basis Set Consistent Revision of the S22 Test Set of Noncovalent Interaction Energies**," T. Takatani, E. G. Hohenstein, M. Malagoli, M. S. Marshall, and C. D. Sherrill, *J. Chem. Phys.* **132**, 144104 (2010). (doi: 10.1063/1.3378024)

118. "**Redox-Active Ligands Facilitate Bimetallic O_2 Homolysis at Five-Coordinate Oxorhenium(V) Centers**," C. Lippert, S. A. Arnstein, C. D. Sherrill, and J. D. Soper, *J. Am. Chem. Soc.* **132**, 3879-3892 (2010). (doi: 10.1021/ja910500a)

119. "**Perspective: Frontiers in Electronic Structure Theory**," C. D. Sherrill, *J. Chem. Phys.* **132**, 110902 (2010). (doi: 10.1063/1.3369628)

120. "**Accurately Characterizing the π-π Interaction Energies of Indole-Benzene Complexes**," Y. Geng, T. Takatani, and C. D. Sherrill, *J. Phys. Chem. A* **114**, 3576-3582 (2010). (doi: 10.1021/jp9099495)

121. "**An Assessment of Density Functional Methods for Potential Energy Curves of Nonbonded Interactions: The XYG3 and B97-D Approximations**," A. Vázquez-Mayagoitia, C. D. Sherrill, E. Aprà, and B. G. Sumpter, *J. Chem. Theory Comput.* **6**, 727-734 (2010). (doi: 10.1063/1.3545971)

122. "**Potential Energy Curves for Cation-π Interactions: Off-Axis Configurations Are Also Attractive**," M. S. Marshall, R. P. Steele, K. S. Thanthiriwatte, and C. D. Sherrill, *J. Phys. Chem. A* **113**, 13628-13632 (2009). (doi: 10.1021/jp906086x)

123. "**An Assessment of Theoretical Methods for Nonbonded Interactions: Comparison to Complete Basis Set Limit Coupled-Cluster Potential Energy Curves for the Benzene Dimer, the Methane Dimer, Benzene-Methane, and Benzene-H_2S**," C. D. Sherrill, T. Takatani, and E. G. Hohenstein, Centennial Feature Article, *J. Phys. Chem. A* **113**, 10146-10159 (2009). (doi: 10.1021/jp9034375)

124. "**Assessment of Standard Force Field Models against High-Quality *ab initio* Potential Curves for Prototypes of π-π, CH/π, and SH/π Interactions**," C. D. Sherrill, B. G. Sumpter, M. O. Sinnokrot, M. S. Marshall, E. G. Hohenstein, and I. R. Gould, *J. Comput. Chem.* **30**, 2187-2193 (2009). (doi: 10.1002/jcc.21226)

125. "**Assessing the Performance of Density Functional Theory for the Electronic Structure of Metal-Salens: The d^6-Metals**," T. Takatani, J. S. Sears, and C. D. Sherrill, *J. Phys. Chem. A* **113**, 9231-9236 (2009). (doi: 10.1021/jp903865t)

126. "**Oscillations in Meta-GGA Potential Energy Surfaces for Dispersion-Bound Complexes**," E. R. Johnson, A. D. Becke, C. D. Sherrill, and G. A. DiLabio, *J. Chem. Phys.* **131**, 034111 (2009). (doi: 10.1063/1.3177061)

127. "**A Versatile Co(bisalen) Unit for Homogeneous and Heterogeneous Cooperative Catalysis in the Hydrolytic Kinetic Resolution of Epoxides**," K. Venkatasubbaiah, C. S. Gill, T. Tatakani, C. D. Sherrill, and C. W. Jones, *Chem. Eur. J.* **15**, 3951-3955 (2009). (doi: 10.1002/chem.200900030)

128. "**Substituent Effects in Sandwich Configurations of Multiply Substituted Benzene Dimers are Not Solely Governed by Electrostatic Control**," A. L. Ringer and C. D. Sherrill, *J. Am. Chem. Soc.* **131**, 4574-4575 (2009). (doi: 10.1021/ja809720r)

129. "**Desorption Electrospay Ionization Mass Spectrometry (DESI MS) of Natural Products of a Marine Alga**," L. Nyadong, E. G. Hohenstein, A. Galhena, A. L. Lane, J. Kubanek, C. D. Sherrill, and F. M Fernández, *Anal. Bioanal. Chem.* **394**, 245-254 (2009). (doi: 10.1007/s00216-009-2674-3)

130. "**Macrocyclic Cyclooctene-supported Salen(AlCl) Catalysts for Conjugated Addition Reactions: Effect of Linker and Support-structure on Catalysis**," N. Madhavan, T. Takatani, C. D. Sherrill, and M. Weck, *Chem. Eur. J.* **15**, 1186-1194 (2009). (doi: 10.1002/chem.200801611)

131. "**Effects of Heteroatoms on Aromatic π-π Interactions: Benzene-Pyridine and Pyridine Dimer**," E. G. Hohen- stein and C. D. Sherrill, *J. Phys. Chem. A* **113**, 878-886 (2009). (doi: 10.1021/jp809062x)

132. "**Assessment of the Performance of Hybrid Meta Exchange-Correlation Functionals for Noncovalent Intera- cions in Biomolecules**," E. G. Hohenstein, S. T. Chill, and C. D. Sherrill, *J. Chem. Theor. Comput.* **4**, 1996-2000 (2008). (doi: 10.1021/ct800308k)

133. "**Desorption Electrospray Ionization Reactions Between Host Crown Ethers and the Influenza Neuraminidase Inhibitor Oseltamivir for the Rapid Screening of Tamiflu**," L. Nyadong, E. G. Hohenstein, K. Johnson, C. D. Sherrill, M. D. Green, and F. M. Fernández, *Analyst* **133**, 1513-1522 (2008). (doi: 10.1039/b809471c)

134. "**Assessing the Performance of Density Functional Theory for the Electronic Structure of Metal–Salens: The d^2-Metals**," J. S. Sears and C. D. Sherrill, *J. Phys. Chem. A* **112**, 6741-6752 (2008). (doi: 10.1021/jp802249n)

135. "**Substituent Effects in Parallel-Displaced π-π Interactions**," S. A. Arnstein and C. D. Sherrill, *invited Cover Article*, *Phys. Chem. Chem. Phys.* **10**, 2646-2655 (2008). (doi: 10.1039/b718742d)

136. "**Assessing the Performance of Density Functional Theory for the Electronic Structure of Metal-Salens: The $3d^0$ Metals**," J. S. Sears and C. D. Sherrill, *J. Phys. Chem. A* **112**, 3466-3477 (2008). (doi: 10.1021/jp711595w)

137. "**Improvement of the Coupled-Cluster Singles and Doubles Method via Scaling Same- and Opposite-Spin Components of the Double Excitation Correlation Energy**," T. Takatani, E. G.Hohenstein, and C. D. Sherrill, *J. Chem. Phys.* **128**, 124111 (2008). (doi: 10.1063/1.2883974)

138. "**First Principles Computation of Lattice Energies of Organic Solids: The Benzene Crystal**," A. L. Ringer and C. D. Sherrill, *Chem. Eur. J.* **14**, 2542-2547 (2008). (doi: 10.1002/chem.200701622)

139. "**Low-lying Singlet Excited States of Isocyanogen**," A. L. Ringer, C. D. Sherrill, R. A. King, and T. D. Crawford, *Int. J. Quantum Chem.* **108**, 1137-1140 (2008). (doi: 10.1002/qua.21586)

140. "**Performance of Spin-Component-Scaled Møller-Plesset Theory (SCS-MP2) for Potential Energy Curves of Noncovalent Interactions**," T. Takatani and C. D. Sherrill, *Phys. Chem. Chem. Phys.* **9**, 6106-6114 (2007). (doi: 10.1039/b709669k)

141. "**Benchmark Full Configuration Interaction and Equation-of-Motion Coupled-Cluster Model with Single and Double Substitutions for Ionized Systems Results for Prototypical Charge Transfer Systems: Noncovalent Ionized Dimers**," P. A. Pieniazek, S. A. Arnstein, S. E. Bradforth, A. I. Krylov, and C. D. Sherrill, *J. Chem. Phys.* **127**, 164110 (2007). (doi: 10.1063/1.2795709)

142. "**Models of S/π Interactions in Protein Structures: Comparison of the H_2S-Benzene Complex with PDB Data**," A. L. Ringer, A. Senenko, and C. D. Sherrill, *Protein Science* **16**, 2216-2223 (2007). (doi: 10.1110/ps.073002307)

143. "***Ab Initio* Thermochemistry of the Hydrogenation of Hydrocarbon Radicals Using Silicon, Germanium, Tin and Lead Substituted Methane and Isobutane**," B. Temelso, C. D. Sherrill, R. C. Merkle, and R. A. Freitas, *J. Chem. Phys. A* **111**, 8677-8688 (2007). (doi: 10.1021/jp071797k)

144. "PSI 3**: An Open-Source *Ab Initio* Electronic Structure Package**," T. D. Crawford, C. D. Sherrill, E. F. Valeev, J. T. Fermann, R. A. King, M. L. Leininger, S. T. Brown, C. L. Janssen, E. T. Seidl, J. P. Kenny, and W. D. Allen, *J. Comput. Chem.* **28**, 1610-1616 (2007). (doi: 10.1002/jcc.20573)

145. "**Some Simple Results following from Löwdin's Partitioning Technique**," A. D. Bochevarov and C. D. Sherrill, *J. Math. Chem.* **42**, 59-64 (2007). (doi: 10.1007/s10910-006-9097-6)

146. "**High-level Ab Initio Studies of Hydrogen Abstraction from Prototype Hydrocarbon Systems**," B. Temelso, C. D. Sherrill, R. C. Merkle, and R. A. Freitas, *J. Phys. Chem. A* **100**, 11160-11173 (2006). (doi: 10.1021/jp061821e)

147. "**Aliphatic C-H/π Interactions: Methane-Benzene, Methane-Phenol, and Methane-Indole Complexes**," A. L. Ringer, M. S. Figgs, M. O. Sinnokrot, and C. D. Sherrill, *J. Phys. Chem. A* **110**, 10822-10828 (2006). (doi: 10.1021/jp0627401)

148. "**High-Accuracy Quantum Mechanical Studies of π-π Interactions in Benzene Dimers**," M. O. Sinnokrot and C. D. Sherrill, *invited Feature Article*, *J. Phys. Chem. A*, **110**, 10656-10668 (2006). (doi: 10.1021/jp0610416)

149. "**Advances in Methods and Algorithms in a Modern Quantum Chemistry Program Package**," Y. Shao, L. F. Molnar, Y. Jung, *et al*., *Phys. Chem. Chem. Phys.* **8**, 3172-3191 (2006). (doi: 10.1039/b517914a)

150. "**Hybrid Correlation Models Based on Active-Space Partitioning: Seeking Accurate** (N^5) **ab initio Methods for Bond Breaking**," A. D. Bochevarov, B. Temelso, and C. D. Sherrill, *J. Chem. Phys.* **125**, 054109 (2006). (doi: 10.1063/1.2222350)

151. "**The Effect of Multiple Substituents on Sandwich and T-Shaped π-π Intearactions**," A. L. Ringer, M. O. Sinnokrot, R. P. Lively, and C. D. Sherrill, *Chem. Eur. J.* **12**, 3821-3828 (2006). (doi: 10.1002/chem.200501316)

152. "**The Electronic Structure of oxo-Mn(salen): Single- and Multi-Reference Approaches**," J. S. Sears and C. D. Sherrill, *J. Chem. Phys.* **124**, 144314 (2006). (doi: 10.1063/1.2187974)

153. "**Orbital-Dependence of Important Configurations in Configuration Interaction and Coupled-Cluster Wave Functions**," M. L. Abrams and C. D. Sherrill, *Mol. Phys.* **103**, 3315-3320 (2005). (doi: 10.1080/00268970500302436)

154. "**Beyond the Benzene Dimer: An Investigation of the Additivity of π-π Interactions**," T. P. Tauer and C. D. Sherrill, *J. Phys. Chem. A* **109**, 10475-10478 (2005). (doi: 10.1021/jp0553479)

155. "**Important Configurations in Configuration Interaction and Coupled-Cluster Wave Functions**," M. L. Abrams and C. D. Sherrill, *Chem. Phys. Lett.* **412**, 121-124 (2005). (doi: 10.1016/j.cplett.2005.06.107)

156. "**Investigations into the Stability of Immobilized Pd^{II} Pincer Complexes During Heck Catalysis**," W. J. Sommer, K. Yu, J. S. Sears, Y. Ji, X. Zheng, R. Davis, C. D. Sherrill, C. W. Jones, and M. Weck, *Organomet.* **24**, 4351-4361 (2005). (doi: 10.1021/om048992v)

157. "**Hybrid Correlation Models Based on Active-Space Partitioning: Correcting Second-Order Møller-Plesset Perturbation Theory for Bond-Breaking Reactions**," A. D. Bochevarov and C. D. Sherrill, *J. Chem. Phys.* **122**, 234110 (2005). (doi: 10.1063/1.1935508)

158. "**General-Order Single- and Multi-Reference Configuration Interaction and Coupled-Cluster Theory: Symmetric Dissociation of Water**," M. L. Abrams and C. D. Sherrill, *Chem. Phys. Lett.* **404**, 284 (2005). (doi: 10.1016/j.cplett.2005.01.101)

159. "**On the Choice of Reference in Multi-Reference Electronic Structure Theory: Minimal References for Bond Breaking**," J. S. Sears and C. D. Sherrill, *Mol. Phys.* **103**, 803-814 (2005). (doi: 10.1080/00268970412331333023)

160. "**The $X\ ^1\Sigma^+$, $B\ ^1\Delta_g$, and $B^{\prime}\ ^1\Sigma^+$ States of C_2: A Comparison of Renormalized Coupled-Cluster and Multireference Methods with Full Configuration Interaction Benchmarks**," C. D. Sherrill and P. Piecuch, *J. Chem. Phys.* **122**, 124104 (2005). (doi: 10.1063/1.1867379)

161. "**High Accuracy *ab initio* Studies of Li^+, Li^- and Three Isomers of Li_6**," B. Temelso and C. D. Sherrill, *J. Chem Phys.* **122**, 064315 (2005). (doi: 10.1063/1.1846671)

162. "**Estimates of the Ab Initio Limit for Sulfur-Pi Interactions: The H_2S-Benzene Dimer**," T. P. Tauer, M. E. Derrick, and C. D. Sherrill, *J. Phys. Chem. A* **109**, 191-196 (2005). (doi: 10.1021/jp046778e)

163. "**Highly Accurate Coupled Cluster Potential Energy Curves for Benzene Dimer: The Sandwich, T-Shaped, and Parallel-Displaced Configurations**," M. O. Sinnokrot and C. D. Sherrill, *J. Phys. Chem. A* **108**, 10200-10207 (2004). (doi: 10.1021/jp0469517)

164. "**Full Configuration Interaction Potential Energy Curves for the X $^1\Sigma^+$, B $^1\Delta_g$, and $B^{\prime}\ ^1\Sigma^+$ States of C_2: A Challenge for Approximate Methods**," M. L. Abrams and C. D. Sherrill, *J. Chem. Phys.* **121**, 9211-9219 (2004). (doi: 10.1063/1.1804498)

165. "**Natural Orbitals as Substitutes for Optimized Orbitals in Complete Active Space Wavefunctions**," M. L. Abrams and C. D. Sherrill, *Chem. Phys. Lett.* **395**, 227-232 (2004). (doi: 10.1016/j.cplett.2004.07.081)

166. "**A General Diagrammatic Algorithm for Contraction and Subsequent Simplification of Second-Quantized Expressions**," A. D. Bochevarov and C. D. Sherrill, *J. Chem. Phys.* **121**, 3374-3383 (2004). (doi: 10.1063/1.1774977)

167. "**Substituent Effects in π-π Interactions: Sandwich and T-shaped Configurations**," M. O. Sinnokrot and C. D. Sherrill, *J. Am. Chem. Soc.* **126**, 7690-7697 (2004). (doi: 10.1021/ja049434a)

168. "**A Comparison of One-Particle Basis Set Completeness, Higher-Order Electron Correlation, Relativistic Effects, and Adiabatic Corrections for Spectroscopic Constants of BH, CH^+, and NH**," B. Temelso, E. F. Valeev, and C. D. Sherrill, *Fritz Schaefer Issue*, *J. Phys. Chem. A* **108**, 3068-3075 (2004). (doi: 10.1021/jp036933+)

169. "**The Electron and Nuclear Orbitals Model: Current Challenges and Future Prospects**," A. D. Bochevarov, E. F. Valeev, and C. D. Sherrill, *Mol. Phys.* **102**, 111-123 (2004). (doi: 10.1080/00268970410001668525)

170. "**Unexpected Substituent Effects in Face-to-Face π-Stacking Interactions**," M. O. Sinnokrot and C. D. Sherrill, *J. Phys. Chem. A* **107**, 8377-3879 (2003). (doi: 10.1021/jp030880e)

171. "**An Assessment of the Accuracy of Multireference Configuration Interaction (MRCI) and Complete-Active-Space Second-Order Perturbation Theory (CASPT2) for Breaking Bonds to Hydrogen**," M. L. Abrams and C. D. Sherrill, *J. Phys. Chem. A* **107**, 5611-5616 (2003). (doi: 10.1021/jp034669e)

172. "**X-ray Structures, Photophysical Characterization, and Computational Analysis of Geometrically Constrained Copper(I)-phenanthroline Complexes**," J. Cody, J. Dennisson, J. Gilmore, D. G. VanDerveer, M. M. Henary, A. Gabrielli, C. D. Sherrill, Y. Zhang, C.-P. Pan, C. Burda, and C. J. Fahrni, *Inorg. Chem.* **42**, 4918-4929 (2003). (doi: 10.1021/ic034529j)

173. "**A Spin-Complete Version of the Spin-Flip Approach to Bond Breaking: What is the Impact of Obtaining Spin Eigenfunctions?**," J. S. Sears, C. D. Sherrill, and A. I. Krylov, *J. Chem. Phys.* **118**, 9084-9094 (2003). (doi:10.1063/1.1568735)

174. "**On the Accuracy Limits of Orbital Expansion Methods: Explicit Effects of *k*-Functions on Atomic and Molecular Energies**," E. F. Valeev, W. D. Allen, R. Hernandez, C. D. Sherrill, and H. F. Schaefer, *J. Chem. Phys.* **118**, 8594-8610 (2003). (doi: 10.1063/1.1566744)

175. "**The Diagonal Born-Oppenheimer Correction Beyond the Hartree-Fock Approximation**," E. F. Valeev and C. D. Sherrill, *J. Chem. Phys.* **118**, 3921-3927 (2003). (doi: 10.1063/1.1540626)

176. "**Full Configuration Interaction Potential Energy Curves for Breaking Bonds to Hydrogen: An Assessment of Single-Reference Correlation Methods**," A. Dutta and C. D. Sherrill, *J. Chem. Phys.* **118**, 1610-1619 (2003). (doi: 10.1002/jcc.20573)

177. "**A Comparison of Polarized Double-Zeta Basis Sets and Natural Orbitals for Full Configuration Interaction Benchmarks**," M. L. Abrams and C. D. Sherrill, *J. Chem. Phys.* **118**, 1604-1609 (2003). (doi: 10.1063/1.1532313)

178. "**Estimates of the *Ab Initio* Limit for π-π Interactions: The Benzene Dimer**," M. O. Sinnokrot, E. F. Valeev, and C. D. Sherrill, *J. Am. Chem. Soc.* **124**, 10887-10893 (2002). (doi: 10.1021/ja025896h)

179. "**Optimization of MCSCF Excited States Using Directions of Negative Curvature**," M. R. Hoffmann, C. D. Sherrill, M. L. Leininger, and H. F. Schaefer, *Chem. Phys. Lett.* **355**, 183-192 (2002). (doi: 10.1016/S0009-2614(02)00208-7)

180. "**The Equilibrium Geometry, Harmonic Vibrational Frequencies, and Estimated *Ab Initio* Limit for the Barrier to Planarity of the Ethylene Radical Cation**," M. L. Abrams, E. F. Valeev, C. D. Sherrill, and T. D. Crawford, *J. Phys. Chem. A* **106**, 2671-2675 (2002). (doi: 10.1021/jp0134143)

181. "**Perturbative Corrections to the Equation-of-Motion Spin-Flip SCF Model: Application to Bond-Breaking and Equilibrium Properties of Diradicals**," A. I. Krylov and C. D. Sherrill, *J. Chem. Phys.* **116**, 3194-3203 (2002). (doi: 10.1063/1.1445116)

182. "**Density Functional Theory Predictions of Anharmonicity and Spectroscopic Constants for Diatomic Molecules**," M. O. Sinnokrot and C. D. Sherrill, *J. Chem. Phys.* **115**, 2439-2448 (2001). (doi: 10.1063/1.1386412)

183. "**Systematic Study of Selected Diagonalization Methods for Configuration Interaction Matrices**," M. L. Leininger, C. D. Sherrill, W. D. Allen, and H. F. Schaefer, *J. Comp. Chem.* **22**, 1574-1589 (2001). (doi: 10.1002/jcc.1111)

184. "**The Performance of Density Functional Theory for Equilibrium Molecular Properties of Symmetry Breaking Molecules**," R. D. Cohen and C. D. Sherrill, *J. Chem. Phys.* **114**, 8257-8269 (2001). (doi: 10.1063/1.1365419)

185. "**Excited States Theory for Optimized Orbitals and Valence Optimized Orbitals Coupled-Cluster Doubles Models**," A. I. Krylov, C. D. Sherrill, and M. Head-Gordon, *J. Chem. Phys.* **113**, 6509 (2000). (doi: 10.1063/1.1311292)

186. "**Complete Basis Set Extrapolations for Low-Lying Triplet Electronic States of Acetylene and Vinylidene**," C. D. Sherrill, E. F. C. Byrd, and M. Head-Gordon, *J. Chem. Phys.* **113**, 1447-1454 (2000). (doi: 10.1063/1.481956)

187. "**Is Møller-Plesset Perturbation Theory a Convergent *Ab Initio* Method?**" M. L. Leininger, W. D. Allen, H. F. Schaefer, and C. D. Sherrill, *J. Chem. Phys.* **112**, 9213-9222 (2000). (doi: 10.1063/1.481764)

188. "**The Theoretical Prediction of Molecular Radical Species: A Systematic Study of Equilibrium Geometries and Harmonic Vibrational Frequencies**," E. F. C. Byrd, C. D. Sherrill, and M. Head-Gordon, *J. Phys. Chem. A* **105**, 9736-9747 (2001). (doi: 10.1021/jp011132x)

189. "**Q-Chem 2.0: A High Performance Ab Initio Electronic Structure Program Package**," J. Kong, C. A. White, I. Krylov, C. D. Sherrill, R. D. Adamson, T. R. Furlani, M. S. Lee, A. M. Lee, S. R. Gwaltney, T. R. Adams, H. Daschel, W. Zhang, P. P. Korambath, C. Ochsenfeld, A. T. B. Gilbert, G. S. Kedziora, D. R. Maurice, N. Nair, Y. Shao, N. A. Besley, P. E. Maslen, J. P. Dombroski, J. Baker, E. F. C. Byrd, T. Van Voorhis, M. Oumi, S. Hirata, C.-P. Hsu, N. Ishikawa, J. Florian, A. Warshel, B. G. Johnson, P. M. W. Gill, M. Head-Gordon, and J. A. Pople, *J. Comp. Chem.* **21**, 1532-1548 (2000). (doi: 10.1002/1096-987X(200012)21:16<1532::AID-JCC10>3.0.CO;2-W)

190. "**Second Order Perturbation Corrections to Singles and Doubles Coupled-Cluster Methods: General Theory and Application to the Valence Optimized Doubles Model**," S. R. Gwaltney, C. D. Sherrill, M. Head-Gordon, and A. I. Krylov, *J. Chem. Phys.* **113**, 3548-3560 (2000). (doi: 10.1063/1.1286597)

191. "**On the Performance of Density Functional Theory for Symmetry Breaking Problems**," C. D. Sherrill, M. S. Lee, and M. Head-Gordon, *Chem. Phys. Lett.* **302**, 425-430 (1999). (doi: 10.1016/S0009-2614(99)00206-7)

192. "**Size-Consistent Wavefunctions for Non-Dynamical Correlation Energy: The Valence Active Space Optimized Orbital Coupled-Cluster Doubles Model**," A. I. Krylov, C. D. Sherrill, E. F. C. Byrd, and M. Head-Gordon, *J. Chem. Phys.* **109**, 10669-10678 (1998). (doi: 10.1063/1.477764)

193. "**Energies and Analytic Gradients for a Coupled-Cluster Doubles Model Using Variational Brueckner Or- bitals: Application to Symmetry Breaking in O^+**," C. D. Sherrill, A. I. Krylov, E. F. C. Byrd, and M. Head- Gordon, *J. Chem. Phys.* **109**, 4171-4181 (1998). (doi: 10.1063/1.477023)

194. "**Full Configuration Interaction Energies, Geometries, and Quartic Force Fields of the Nitrenium Ion**," T. J. Van Huis, M. L. Leininger, C. D. Sherrill, and H. F. Schaefer, *Collect. Czech. Chem. Commun.* **63**, 1107-1142 (1998). (doi: 10.1135/cccc19981107)

195. "**The $\tilde{X}\,^3B_1$, $\tilde{a}\,^1A_1$, $\tilde{b}\,^1B_1$, and $\tilde{c}\,^1\Sigma^+$ Electronic States of NH^+**," J. C. Stephens, Y. Yamaguchi, C. D. Sherrill, and H. F. Schaefer, *J. Phys. Chem. A* **102**, 3999-4006 (1998). (doi: 10.1021/jp980779n)

196. "**Benchmark Configuration Interaction Spectroscopic Constants for $\tilde{X}\,^1\Sigma^+$ C_2 and $\tilde{X}\,^1\Sigma^+$ CN^+**," M. L. Leininger, C. D. Sherrill, W. D. Allen, and H. F. Schaefer, *J. Chem. Phys.* **108**, 6717-6721 (1998). (doi: 10.1063/1.476087)

197. "**Structures and Vibrational Frequencies in the Full Configuration Interaction Limit: Predictions for Four Electronic States of Methylene Using a Triple-Zeta Plus Double Polarization (TZ2P) Basis**," C. D. Sherrill, M. L. Leininger, T. J. Van Huis, and H. F. Schaefer, *J. Chem. Phys.* **108**, 1040-1049 (1998). (doi: 10.1063/1.475465)

198. "**Comparison Between Molecular Geometry and Harmonic Vibrational Frequency Predictions from CISD[TQ] and CISDTQ Wavefunctions for Hydrogen Sulfide**," B. C. Hoffman, C. D. Sherrill, and H. F. Schaefer, *J. Chem. Phys.*, **107**, 10616-10619 (1997). (doi: 10.1063/1.474176)

199. "**The $\tilde{X}\,^1A_1$, $\tilde{a}\,^3B_1$, $\tilde{A}\,^1B_1$, and 2 $^1A_1$ Electronic States of SiH_2**," Y. Yamaguchi, T. J. Van Huis, C. D. Sherrill, and H. F. Schaefer, *Theor. Chem. Accounts* **97**, 341-349 (1997). (doi: 10.1007/s002140050270)

200. "**Molecular Geometry and Vibrational Frequency Predictions from the CISD[TQ] Wavefunction: The Water Molecule**," R. A. King, C. D. Sherrill, and H. F. Schaefer, *Spectrochimica Acta Part A*, **53**, 1163-1168 (1997). (doi: 10.1016/S1386-1425(97)00023-1)

201. "**The $\tilde{X}\,^1A_1$, $\tilde{a}\,^3B_1$, $\tilde{A}\,^1B_1$, and $\tilde{B}\,^1A_1$ Electronic States of PH^+**," T. J. Van Huis, Y. Yamaguchi, C. D. Sherrill, and H. F. Schaefer, *J. Phys. Chem. A*, **101**, 6955-6963 (1997). (doi: 10.1021/jp970980i)

202. "**Full Configuration Interaction Benchmarks for the $\tilde{X}\,^3B_1$, $\tilde{a}\,^1A_1$, $\tilde{b}\,^1B_1$, and $\tilde{c}\,^1A_1$ States of Methylene**," C. D. Sherrill, T. J. Van Huis, Y. Yamaguchi, and H. F. Schaefer, *Theochem*, **400**, 139-156 (1997).

203. "**Monomethyl Gallium: Prelude to Spectroscopy**," B. C. Hoffman, C. D. Sherrill, and H. F. Schaefer, *Theochem*, **370**, 93-95 (1996).

204. "**Cyclopropyne and Silacyclopropyne: A World of Difference**," C. D. Sherrill, C. G. Brandow, W. D. Allen, and H. F. Schaefer, *J. Amer. Chem. Soc.*, **118**, 7158-7163 (1996). (doi: 10.1021/ja960762n)

205. "**The $\tilde{A}\,^1A_u$ State and T_2 Potential Surface of Acetylene: Implications for Triplet Perturbations in the Flu-orescence Spectra of the $\tilde{A}$ State**," C. D. Sherrill, G. Vacek, Y. Yamaguchi, H. F. Schaefer, J. F. Stanton, and J. Gauss, *J. Chem. Phys.* **104** 8507-8515 (1996). (doi: 10.1063/1.471658)

206. "**The $\tilde{X}\,^3B_1$, $\tilde{a}\,^1A_1$, $\tilde{b}\,^1B_1$, and $\tilde{c}\,^1A_1$ Electronic States of CH_2**," Y. Yamaguchi, C. D. Sherrill, and H. F. Schaefer, *James L. Kinsey Issue, J. Phys. Chem.*, **100**, 7911-7918 (1996). (doi: 10.1021/jp953150i)

207. "**Compact Variational Wave Functions Incorporating Limited Triple and Quadruple Substitutions**," C. D. Sherrill and H. F. Schaefer, *Boys/Shavitt Issue, J. Phys. Chem.*, **100**, 6069-6075 (1996). (doi: 10.1021/jp9527719)

208. "**The Anomalous Behavior of the Zeeman Anticrossing Spectra of $\tilde{A}\,^1A_u$ Acetylene: Theoretical Considerations**," G. Vacek, C. D. Sherrill, Y. Yamaguchi, and H. F. Schaefer, *J. Chem. Phys.*, **104**, 1774-1778 (1996). (10.1063/1.471646)

209. "**N_8: A Structure Analogous to Pentalene, and Other High Energy Density Minima**," M. L. Leininger, C. D. Sherrill, and H. F. Schaefer, *J. Phys. Chem.* **99**, 2324-2328 (1995). (doi: 10.1021/j100008a013)

210. "**1-Silavinylidene: The First Unsaturated Silylene**," C. D. Sherrill and H. F. Schaefer, *J. Phys. Chem.* **99**, 1949- 1952 (1995). (doi: 10.1021/j100007a026)

211. "**The $\tilde{A}^1A''$ State of Isocyanogen (CNCN)**," C. D. Sherrill and H. F. Schaefer, *J. Chem. Phys.* **100**, 8920-8924 (1994). (doi: 10.1063/1.466696)

212. "**Benchmark Studies of Electron Correlation in Six-Electron Systems**," J. T. Fermann, C. D. Sherrill, T. D. Crawford, and H. F. Schaefer, *J. Chem. Phys.* **100**, 8132-8139 (1994). (doi: 10.1063/1.466807)

213. "**Acetylene: Synergy between Theory and Experiment**," J. K. Lundberg, R. W. Field, C. D. Sherrill, E. T. Seidl, Y. Xie, and H. F. Schaefer, *J. Chem. Phys.* **98**, 8384-8391 (1993). (doi: 10.1063/1.464496)

214. "**Closs's Diradical: Some Surprises on the Potential Energy Hypersurface**," C. D. Sherrill, E. T. Seidl, and H. F. Schaefer, *J. Phys. Chem.* **96**, 3712-3716 (1992). (doi: 10.1021/j100188a029)

B4. Submitted Journal Articles

1. "**QCManyBody: A Flexible Implementation of the Many-Body Expansion**," L. A. Burns, C. D. Sherrill, and B. P. Pritchard, submitted.
2. "**Electrostatically Embedded Symmetry Adapted Perturbation Theory**," C. S. Glick, A. Alenaizan, C. E. Cavender, and C. D. Sherrill, *J. Chem. Phys*., submitted.
3. "**Optimization of Damping Function Parameters for -D3 and -D4 Dispersion Models for Hartree-Fock Based Symmetry-Adapted Perturbation Theory**," A. M. Wallace and C. D. Sherrill, *J. Chem. Phys*., submitted.
4. "**Levels of Symmetry Adapted Perturbation Theory (SAPT). II. Convergence of Interaction Energy Components**," J. B. Schriber, D. L. Cheney, and C. D. Sherrill, submitted.
5. "**Comparison of Coulomb and Exchange Matrix Construction Algorithms for Chemical Systems of Increasing Size**," D. Poole, A. Jiang, Z. L. Glick, and C. D. Sherrill

C. Other Publications and Creative Products

Editorials

1. "**Chemical Physics Software**," C. D. Sherrill*, D. E. Manolopoulos, T. J. Martinez, M. Ceriotti, and A. Michaelides, *J. Chem. Phys*. **155**, 010401 (2021). (doi: 10.1063/5.0059886)
2. "**JCP Emerging Investigator Special Collection 2019**," M. D. Ediger, L. Jensen, D. E. Manolopoulos, T. J. Martinez, A. Michaelides, D. R. Reichman, C. D. Sherrill, Q. Shi, J. E. Straub, C. Vega, L.-S. Wang, E. C. Brigham, and T. Lian, *J. Chem. Phys*. **153**, 110402 (2020). (doi: 10.1063/5.0021946)
3. "**Electronic Structure Software**," C. D. Sherrill*, D. E. Manolopoulos, T. J. Martinez, and A. Michaelides, *J. Chem. Phys*. **153**, 070401 (2020). (doi: 10.1063/5.0023185)
4. **"Reflections on Fifty Years of Density Functional Theory,"** W. Kohn and C. D. Sherrill, J. Chem. Phys. 140, 18A201 (2014). (doi: 10.1063/1.4870815)
5. "**A Special Issue of Molecular Physics Honoring Prof. Henry F. Schaefer III**," T. D. Crawford and C. D. Sherrill, *Mol. Phys.* **107**, 711 (2009). (doi: 10.1080/00268970902909382)

Computational Chemistry Software Contributions

1. "**Quantum Chemistry Common Driver and Databases (QCDB) and Quantum Chemistry Engine (QCEngine): Automation and Interoperability Among Computational Chemistry Programs**," D. G. A. Smith, A. T. Lolinco, Z. L. Glick, J. Lee, A. Alenaizan, T. A. Barnes, C. H. Borca, R. Di Remigio, D. L. Dotson, S. Ehlert, A. G. Heide, M. F. Herbst, J. Hermann, C. B. Hicks, J. T. Horton, A. G. Hurtado, P. Kraus, H. Kruse, S. J. R. Lee, J. P. Misiewicz, L. N. Naden, F. Ramezanghorbani, M. Scheurer, J. B. Schriber, A. C. Simmonett, J. Steinmetzer, J. R. Wagner, L. Ward, M. Welborn, D. Atlarawy, J. Anwar, J. D. Chodera, A. Dreuw, H. T. Kulik, F. Liu, T. J. Martínez, D. A. Matthews, H. F. Schaefer, J. Šponer, J. T. Turney, L.-P. Wang, N. De Silva, R. A. King, J. F. Stanton, M. S. Gordon, T. L. Windus, C. D. Sherrill, and L. A. Burns, *J. Chem. Phys.* **155**, 204801 (2021). (doi: 10.1063/5.0059356)

2. **"Psi4 1.4: Open-Source Software for High-Throughput Quantum Chemistry,"** D. G. A. Smith, L. A. Burns, A. C. Simmonett, R. M. Parrish, M. C. Schieber, R. Galvelis, P. Kraus, H. Kruse, R. Di Remigio, A. Alenaizan, A.M. James, S. Lehtola, J. P. Misiewicz, M. Scheurer, R. A. Shaw, J. B. Schriber, Y. Xie, Z. L. Glick, D. A. Sirianni, J. Senan O'Brien, J. M. Waldrop, A. Kumar, E. G. Hohenstein, B. P. Pritchard, B. R. Brooks, H. F. Schaefer, A. Yu. Sokolov, K. Patkowski, A. E. DePrince, U. Bozkaya, R. A. King, F. A. Evangelista, J. M. Turney, T. D. Crawford, and C. D. Sherrill, *J. Chem. Phys*. **152**, 184108 (2020). (doi: 10.1063/5.0006002)

3. "**The proto-Nucleic Acid Builder: A Software Tool for Constructing Nucleic Acid Analogs**," A. Alenaizan, J. L. Barnett, N. V. Hud, C. D. Sherrill, and A. S. Petrov, *Nucleic Acids Res*. **49**, 79-89 (2021). (doi: 10.1093/nar/gkaa1159)

4. **"Python Implementation of the Restrained Electrostatic Potential (RESP) Charge Model,"** A. Alenaizan, L. A. Burns, and C. D. Sherrill, *Int. J. Quantum Chem*. **120**, e26035 (2020). (doi: 10.1002/qua.26035)

5. **"CrystaLattE: Automated Computation of Lattice Energies of Organic Crystals Exploiting the Many-Body Expansion to Achieve Dual-Level Parallelism,"** C. H. Borca, B. W. Bakr, L. A. Burns, and C. D. Sherrill, *J. Chem. Phys*. **151**, 144103 (2019). (doi: 10.1063/1.5120520)

6. **"PSI4NUMPY: An Interactive Quantum Chemistry Programming Environment for Reference Implementations and Rapid Development,"** D. G. A. Smith, L. A. Burns, D. A. Sirianni, D. R. Nascimento, A. Kumar, A. M. James, J. B. Schriber, T. Zhang, B. Zhang, A. S. Abbott, E. J. Berquist, M. H. Lechner, L. A. Cunha, A. G. Heide, J. M. Waldrop, T. Y. Takeshita, A. Alenaizan, D. Neuhauser, R. A. King, A. C. Simmonett, J. M. Turney, H. F. Schaefer, F. A. Evangelista, A. E. DePrince, T. D. Crawford, K. Patkowski, and C. D. Sherrill, *J. Chem. Theory Comput*. **14**, 3504-3511 (2018). (doi: 10.1021/acs.jctc.8b00286)

7. "PSI4 **1.1: An Open-Source Electronic Structure Program Emphasizing Automation, Advanced Libraries, and Interoperability**," R. M. Parrish, L. A. Burns, D. G. A. Smith, A. C. Simmonett, A. E. DePrince, E. G. Hohenstein, U. Bozkaya, A. Yu. Sokolov, R. Di Remigio, R. M. Richard, J. F. Gonthier, A. M. James, H. R. McAlexander, A. Kumar, M. Saitow, X. Wang, B. P. Pritchard, P. Verma, H. F. Schaefer, K. Patkowski, R. A. King, E. F. Valeev, F. A. Enganvelista, J. M. Turney, T. D. Crawford, and C. D. Sherrill, *J. Chem. Theory Comput.* **13**, 3185-3197 (2017). (doi: 10.1021/acs.jctc.7b00174)

8. "PSI4**: An Open-Source *Ab Initio* Electronic Structure Program**," J. M. Turney, A. C. Simmonett, R. M. Parrish, E. G. Hohenstein, F. Evangelista, J. F. Fermann, B. J. Mintz, L. A. Burns, J. J. Wilke, M. L. Abrams, N. J. Russ, M. L. Leininger, C. L. Janssen, E. T. Seidl, W. D. Allen, H. F. Schaefer, R. A. King, C. D. Sherrill, and T. D. Crawford, *WIREs: Comput. Mol. Sci.* **2**, 556-565 (2012). (doi: 10.1002/wcms.93)

3. "PSI **3: An Open-Source *Ab Initio* Electronic Structure Package**," T. D. Crawford, C. D. Sherrill, E. F. Valeev, J. T. Fermann, R. A. King, M. L. Leininger, S. T. Brown, C. L. Janssen, E. T. Seidl, J. P. Kenney, and W. D. Allen, *J. Comput. Chem.* **28**, 1610-1616 (2007). (doi: 10.1002/jcc.20573)

4. "**Advances in Methods and Algorithms in a Modern Quantum Chemistry Program Package**," Y. Shao, L. F. Molnar, Y. Jung, *et al.*, *Phys. Chem. Chem. Phys.* **8**, 3172-3191 (2006). (doi: 10.1039/b517914a)
5. "**Q-Chem 2.0: A High Performance Ab Initio Electronic Structure Program Package**," J. Kong, C. A. White, A. I. Krylov, C. D. Sherrill, R. D. Adamson, T. R. Furlani, M. S. Lee, A. M. Lee, S. R. Gwaltney, T. R. Adams, H. Daschel, W. Zhang, P. P. Korambath, C. Ochsenfeld, A. T. B. Gilbert, G. S. Kedziora, V. A. Rassolov, D. R. Maurice, N. Nair, Y. Shao, N. A. Besley, P. E. Maslen, J. P. Dombroski, J. Baker, E. F. C. Byrd, T. Van Voorhis, M. Oumi, S. Hirata, C.-P. Hsu, N. Ishikawa, J. Florian, A. Warshel, B. G. Hohnson, P. M. W. Gill, M. Head-Gordon, and J. A. Pople, *J. Comput. Chem.* **21**, 1532-1548 (2000). (doi: 10.1002/1096-987X(200012)21:16<1532::AID-JCC10>3.0.CO;2-W)

Press

1. Quoted in "Computational chemists welcome 'living' journal," Chemical & Engineering News, vol. 97, issue 1, 7 January 2019
2. Psi4 mentioned in Bloomberg article, "Google Debuts Software to Open Up Quantum Computers for Chemists," 23 October 2017
3. Interviewed in "Cyber Forged: Advanced Computer Technologies Speed Development of Real-World Materials," R. Robinson, Georgia Tech Research Horizons Issue 2, 2016. (article link)
4. Interviewed in Big Chemistry segment of "Data Driven: How Traditional Research is Being Rebooted," T. J. Becker, Georgia Tech Research Horizons Issue 2, 2016. (article link)
5. Interviewed by Chemical & Engineering News: "Quantum Chemistry's Modular Movement: ACS Meeting News: Software developers seek to reduce redundancy by writing reusable code," C&EN, vol. 92, issue 34, p. 26, 25 August 2014
6. "National Chemistry Week: The Chemistry of Candy," Inside The Black Box, WREK 91.1 FM Atlanta, 22 October 2014
7. Quoted in "Pi-stacking better without the aromatics?" RSC Chemistry World News, 8 July 2011
8. "The Bigger, the Better: Ring-size Effects of Macrocyclic Oligomeric Co(III)-salen Catalysts," RSC Chemistry World News, 17 December 2010, and Chemie.DE, 20 December 2010, describes work with collaborator Marcus Weck
9. "Chemistry: What is it Good For?" Inside the Black Box, WREK 91.1 FM Atlanta, 21 October 2009
10. "Supramolecular chemistry: Another piece of the π," Research Highlights, Nature Chemistry, 23 January 2009 (doi: 10.1038/nchem.117)
11. "Science in Your Life," Georgia Public Radio, February 2001

D. Presentations

1. Plenary Talk, OpenMolcas Developers' Meeting, Toronto, Canada, 22-24 June 2024
2. Many-Body Interactions: From Quantum Mechanics to Force Fields, Telluride Science & Innovation Center, Telluride, CO, 15-19 June 2024
3. Departmental Seminar, University of Tennessee at Chattanooga, 24 May 2024
4. Keynote Lecture: Southeast Theoretical Chemistry Association (SETCA), Virginia Tech, Blacksburg, VA, 16 May 2024
5. Departmental Seminar, Department of Chemistry, Virginia Commonwealth University, 29 February 2024
6. Keynote Address, 18th Herty Medalist Undergraduate Research Symposium, Georgia Gwinnett College, 22 September 2023
7. Herty Medal Award Address, Georgia Section of the American Chemical Society, 21 September 2023
8. Free and Open Source Software: Harnessing the Power of Data, National Meeting of the American Chemical Society, San Francisco, CA, 13-17 August 2023

9. NanoFANS Forum: Trends in Machine Learning for Biology, Institute for Electronics and Nanotechnology, Georgia Tech, 22 June 2023
10. Tinker Workshop, Washington University in St. Louis, St. Louis, MO, 15-16 June 2023
11. Challenges for Physical Chemists, Harnessing the Power of Chemistry Presidential Symposium, National Meeting of the American Chemical Society, Indianapolis, IN, 26-30 March 2023
12. Physical Chemistry Seminar, Department of Chemistry, University of Florida, 25 October 2022
13. 17th Herty Medalist Undergraduate Research Symposium, Georgia Gwinnett College, 16 September 2022
14. 12th Triennial Congress of the World Association of Theoretical and Computational Chemists (WATOC), Vancouver, Canada, 3-8 July 2022
15. 10th Triennial Conference on Molecular Quantum Mechanics (MQM), Virginia Tech, Blacksburg, VA, 26 June – 1 July 2022
16. Many-Body Interactions: From Quantum Mechanics to Force-Fields, Telluride Science Research Center, Telluride, CO, 6-10 June 2022
17. Machine Learning in Chemical and Materials Sciences, Los Alamos National Laboratory Center for Nonlinear Studies, 23-26 May 2022 (virtual presentation)
18. Institute of Computational and Theoretical Chemistry (ICTCUB), University of Barcelona, Spain, 28 April 2022 (virtual presentation)
19. 30th Annual Suddath Symposium, Applications of Physical Chemistry to Probing and Understanding Biology, in honor of Bridgette Barry, Georgia Tech, Atlanta, GA, 13-14 January 2022 (virtual presentation)
20. Computational Quantum Chemistry: Synergism Between Theory and Experiment, International Chemical Congress of Pacific Basin Societies (Pacifichem), Honolulu, Hawaii, 16-21 December 2021 (virtual presentation)
21. High-Performance Computing Applications in Chemistry, Southeastern Regional Meeting of the American Chemical Society (SERMACS), 10-13 November 2021
22. Computational Chemistry and Machine Learning, Southeastern Regional Meeting of the American Chemical Society (SERMACS), 10-13 November 2021
23. Advanced Force Fields, National Meeting of the American Chemical Society, Atlanta, GA, 22-26 August 2021 (virtual presentation)
24. Theoretical Chemistry Seminar, Cambridge University, Cambridge, England, 12 May 2021 (virtual presentation)
25. Department of Chemistry, King Fahd University of Petroleum and Minerals, Saudi Arabia, 27 October 2020 (virtual presentation)
26. Laboratory for Computational Biology, National Institutes of Health, Bethesda MD (virtual presentation), 10 September 2020
27. Many-Body Interactions: From Quantum Mechanics to Force Fields, Telluride, CO, 8-12 June 2020
28. Telluride Science Summer Lecture Series, Telluride, CO (virtual presentation), 1 June 2020
29. Monthly Meeting of the Georgia Section of the American Chemical Society (virtual presentation), 12 March 2020
30. Computational Chemistry Applied to Interesting Problems, Southeastern Regional Meeting of the American Chemical Society (SERMACS), 20-23 October 2019
31. Student-Invited Seminar, Department of Chemistry, University of Minnesota, 3 October 2019
32. Electron-Molecule and Molecule-Molecule Interactions, National Meeting of the American Chemical Society, Orlando, FL, 31 March - 4 April 2019
33. Telluride Workshop on Intermolecular Interactions, Telluride, CO, 18-22 March 2019
34. Department of Chemistry, University of North Texas, 26 October 2018
35. Department of Chemistry, University of Tennessee, 27 September 2018
36. Many-Body Interactions: From Quantum Mechanics to Force Fields, Telluride, CO, 9-13 July 2018
37. 2018 Meeting of the Southeast Theoretical Chemistry Association (SETCA), Louisiana State University, Baton Rouge, LA, 18-19 May 2018
38. Dipole and Charge in Drug Design, National Meeting of the American Chemical Society, New Orleans, LA, 18-22 March 2018
39. Quantum Chemical Program Development in a Modern Computer and Programming Environment, National Meeting of the American Chemical Society, New Orleans, LA, 18-22 March 2018

40. Dipole and Charge in Drug Design, National Meeting of the American Chemical Society, New Orleans, LA, 18-22 March 2018
41. Department of Chemistry, The University of the South, Sewanee, TN, 22 September 2017
42. 11th Triennial Congress of the World Association of Theoretical and Computational Chemists (WATOC), Munich, Germany, 27 August - 1 September 2017
43. Noncovalent Interactions in Quantum Chemistry and Physics: Theory and Applications, 100th Canadian Chemistry Conference, Toronto, Canada, 28 May – 1 June, 2017
44. Molecular Sciences Software Institute Workshop on Software Interoperability, Virginia Tech, 5-7 June 2017
45. Florida Meeting and Exposition of the American Chemical Society, Tampa, FL, 4-6 May 2017
46. Dow Core Research, Midland, MI, 22 March 2017
47. Molecules to Functional Supramolecular Materials, Southeast Regional Meeting of the American Chemical Society (SERMACS), Columbia, SC, 23-26 October, 2016
48. Electronic Structure: Concepts and Applications, Southeast Regional Meeting of the American Chemical Society (SERMACS), Columbia, SC, 23-26 October, 2016
49. International Conference on Theoretical and High Performance Computational Chemistry 2016 (ICT-HPCC16), Chongqing, China, October 14-17, 2016
50. Department of Chemistry, Washington University in St. Louis, 29 September 2016
51. Bristol-Myers Squibb, Princeton, NJ, 19 July 2016
52. Density- and Response Density-Based Models for Intermolecular Interactions in Molecular Assemblies and in Solids, CECAM workshop, Nancy, France, 20-23 June 2016
53. Keynote talk, 2016 Meeting of the Southeast Theoretical Chemistry Association (SETCA), Florida State University, Tallahassee, FL, 12-14 May 2016
54. Department of Chemistry, University of Kansas, April 2016
55. Open-Eye Software CUP XVI Conference, Santa Fe, NM, 7-9 March 2016
56. Practical Strategies for Modeling Non-Covalent Interactions, International Chemical Congress of Pacific Basin Societies (Pacifichem), Honolulu, Hawaii, 15-20 December 2015
57. Keynote intived talk, Control of London Dispersion Interactions in Molecular Chemistry, German DFG SPP 1807, 2015
58. Workshop, Göttingen, Germany, 19-20 October 2015
59. Intermolecular Interactions: New Challenges for ab initio Theory, Telluride, CO, 6-11 July 2015
60. Keynote talk, 2015 Meeting of the Southeast Theoretical Chemistry Association (SETCA), University of Central Florida, Orlando, FL, 15-16 May 2015
61. Southeastern Regional Meeting of the American Chemical Society, Nashville, TN, 16-19 October 2014
62. World Association of Theoretical and Computational Chemists (WATOC), Santiago, Chile, 5-10 October 2014
63. Addressing Challenges for First-Principles Based Modeling of Molecular Materials, CECAM Workshop, Lausanne, Switzerland, 25-29 August 2014
64. "Sustainable Software for Quantum Chemistry," in the symposium The Future of Computational Chemistry, National Meeting of the American Chemical Society, San Francisco, CA, 10-14 August 2014 [talk featured in the August 25, 2014 issue of *Chemical and Engineering News*]
65. Telluride Workshop on Quantum Mechanics Derived Force Fields, Telluride, CO, 15-19 June 2014
66. Department of Chemistry, Tulane University, 8 May 2014
67. NSF/LASiGMA Seminar, University of New Orleans, New Orleans, LA, 7 May 2014
68. Chemical Theory for Complex Systems, Joint International Symposium hosted by the Emerson Center (Emory University) and the Catalysis Reseach Center (Hokkaido U, Japan), Atlanta, GA, 9-10 January 2014
69. Department of Chemistry, University of Chicago, 25 November 2013
70. University Seminar, University of Tennessee, Knoxville, TN, 1 November 2013
71. Structure-Property Relationships of Molecular Precursors to Organic Electronics, CECAM Workshop, Lausanne, Switzerland, 22-25 October 2013
72. Intermolecular Interactions: New Challenges for ab initio Theory, Telluride, Colorado, 15-19 July, 2013

73. Molecular Quantum Mechanics: Electron Correlation, the Many Body Problem at the Heart of Chemistry, an International Conference in Honor of Prof. Rodney J. Bartlett, Lugano, Switzerland, 2-7 June 2013
74. 2013 Meeting of the Southeast Theoretical Chemistry Association (SETCA), Auburn University, 10-11 May 2013
75. Accurate Characterization of Non-Covalent Interactions: From Small Molecules to Supramolecular Chemistry, National Meeting of the American Chemical Society, New Orleans, LA, 7-11 April 2013
76. Potential Function Uncertainty and Validation, National Meeting of the American Chemical Society, New Orleans, LA, 7-11 April 2013
77. Department of Chemistry, University of Tennessee at Chattanooga, 1 March 2013
78. Symposium on the Occasion of Professor Joel Bowman's 65th Birthday, Emory University, Atlanta, GA, 8-9 February 2013
79. The Robert J. Silbey Memorial Symposium on Theory for Experimentalists, Georgia Tech, Atlanta, GA, 6-7 December 2012
80. Towards First-Principles Description of van der Waals Interactions in Complex Materials, CECAM Workshop, Lausanne, Switzerland, 15-19 October, 2012
81. Bridging the Gap Between Ab Initio and Classical Simulations, National Meeting of the American Chemical Society, Philadelphia, PA, 19-23 August 2012
82. Many-Body Interactions: From Quantum Mechanics to Force Fields, Telluride, Colorado, 2-6 July 2012
83. Electronic Structure Theory for Strongly Correlated Systems, An International Conference in Celebration of Per-Åke Malmqvist's 60th Birthday, Palermo, Italy, 30 May – 1 June 2012
84. 2012 Meeting of the Southeast Theoretical Chemistry Association (SETCA), University of Georgia, 17-19 May 2012
85. "Energy Component Analysis of Molecular Recognition in Biochemistry," Astrobiology Science Conference (AbSciCon) 2012, Atlanta, GA, 16-20 April 2012
86. Department of Chemistry, Ohio State University, 20 February 2012
87. Department of Chemistry, University of Wisconsin-Madison, 31 January 2012
88. "Understanding the Fundamental Nature of Non-Covalent Interactions: From the Benzene Dimer to DNA-Intercalator Interactions," Robert S. Mulliken Lecture, University of Georgia, 16 September 2011
89. 7th Congress of the International Society for Theoretical Chemical Physics (ISTCP-VII), Tokyo, Japan, 2-8 Septem ber 2011
90. 10th Annual MERCURY Conference on Undergraduate Computational Chemistry, Bucknell University, 28-30 July 2011
91. World Association of Theoretical and Computational Chemists (WATOC), 17-22 July 2011
92. Fragment and Local Orbital Methods in Electronic Structure Theory, National Meeting of the American Chemical Society, Anaheim, CA, 27-31 March 2011
93. ACS Award for Computers in Chemical and Pharmaceutical Research Award: Symposium in Honor of Thom Dunning, National Meeting of the American Chemical Society, Anaheim, CA, 27-31 March 2011
94. Student Invited Seminar, Florida International University, Miami, FL, 28 January 2011
95. Mesilla Workshop on Aromatic Interactions in Chemistry and Biology, Mesilla, New Mexico, 6-9 February 2011
96. Department of Chemistry, Auburn University, 28 October 2010
97. Department of Chemistry, Johns Hopkins University, 19 October 2010
98. Next Generation Force Fields for Nanoscience, Center for Nanophase Materials Sciences (CNMS), Oak Ridge National Laboratory, 15-16 September 2010
99. Silverton Workshop on Intermolecular Interactions: New Challenges for ab initio Theory, 9-13 August 2010, Silverton, Colorado.
100. 50th Sanibel Symposium, St. Simons Island, GA, 24 February - 2 March 2010
101. Department of Chemistry, University of Georgia, 25 September 2009
102. 238th National Meeting of the American Chemical Society, Washington, DC, 16-20 August 2009
103. School of Chemistry and Biochemistry, Georgia Institute of Technology, 4 April 2009

104. Department of Chemistry, St. Louis University, 27 February 2009
105. Department of Chemistry, University of Massachusetts, Amherst, 19 February 2009
106. Gordon Research Conference on Molecular Energy Transfer, Ventura, CA, 18-23 January 2009
107. Department of Chemistry, University of Michigan, 17 November 2008
108. Department of Chemistry, Bethel University, 1 October, 2008
109. Theory and Applications of Computational Chemistry (TACC), Shanghai, China, 23-27 September, 2008
110. World Association of Theoretical and Computational Chemists, Sydney, Australia, 14-19 September, 2008
111. 6th Congress of the International Society for Theoretical Chemical Physics (ISTCP-VI), Vancouver, Canada, 29-24 July, 2008.
112. Development of Force Fields using *Ab Initio* Electronic Structure Calculations, Telluride, Colorado, 6-11 July, 2008
113. Molecular Quantum Mechanics - Analytic Gradients and Beyond, an international conference in honor of Prof. Peter Pulay, Budapest, Hungary, 29 May - 3 June 2007
114. Department of Chemistry, University of Tennessee, Chattanooga, TN, November 2, 2007
115. Department of Chemistry, Middle Tennessee State University, Murfreesboro, TN, November 1, 2007
116. Biology and Chemistry Lecture Series, Trevecca University, Nashville, TN, October 31, 2007
117. 59th Southeastern Regional Meeting of the American Chemical Society, Greenville, SC, 25 October 2007
118. Solvay-COPE Symposium on Organic Electronics, Georgia Tech, 8 May 2007
119. Department of Chemistry, Michigan State University, 22 February 2007
120. XIth European Workshop on Quantum Systems in Chemistry and Physics (QSCP-XI), St. Petersburg, Russia, 20-25 August 2006
121. 35th Meeting of the Southeast Theoretical Chemistry Association, Emory University, 19-20 May 2000
122. Quantitative Quantum Chemistry, a conference in honor of Dr. Thom Dunning, Santa Fe, New Mexico, 17-20 March, 2006
123. Department of Chemistry, University of South Carolina, 30 January 2006
124. International Chemical Congress of Pacific Basin Societies (Pacifichem), Honolulu, Hawaii, 15-20 December 2005
125. 14th Conference on Current Trends in Computational Chemistry, Jackson, MS, 4-5 November 2005
126. Quantum Theory Project, University of Florida, 5 October 2005
127. Department of Chemistry, University of Florida, 4 October 2005
128. Highlands in Chemistry Seminar, Virginia Tech, 4 March 2005
129. 7th Congress of the World Association of Theoretically Oriented Chemists, Cape Town, South Africa, 16-21 January 2005
130. Department of Chemistry, University of North Dakota, 12 November 2004
131. Department of Chemistry, University of Southern California, 25 October 2004
132. Department of Chemistry, Rice University, 9 September 2004
133. Department of Chemistry, Imperial College, London, 23 July 2004
134. 228th National Meeting of the American Chemical Society, Philadelphia, 22-26 August 2004
135. Oak Ridge National Laboratory, 16 June 2004
136. 33rd Meeting of the Southeast Theoretical Chemistry Association, University of Mississippi, 21-22 May 2004
137. Department of Chemistry, Wake Forest University, 3 March 2004
138. Southeastern Regional Meeting of the ACS (SERMACS), Atlanta, 17 November 2003
139. 226th National Meeting of the American Chemical Society, New York, 8 September 2003
140. Symposium on Frontiers in Computational Chemistry, Emory University, 12 April 2003
141. 225th National Meeting of the American Chemical Society, New Orleans, 24 March 2003
142. Department of Chemistry, Hampton University, 30 January 2003
143. Department of Chemistry, Old Dominion University, 6 December 2002
144. Eastern Texas Section of the ACS, 24 October 2002
145. Department of Chemistry, Kilgore College, 24 October 2002
146. Department of Chemistry, Iowa State University, 20 September 2002

147. Gordon Research Conference on Computational Chemistry, Colby-Sawyer College, New London, NH, 1 July 2002
148. Atlanta Area Chemical Physics Seminar, 6 May 2002
149. University of Georgia Chemistry Graduate Student Organization, Athens, 26 April 2002
150. 223rd National Meeting of the American Chemical Society, Orlando, 9 April 2002
151. Department of Chemistry, University of Tennessee at Chattanooga, 15 February 2002
152. Quantum Theory Project, University of Florida, 17 October 2001
153. Department of Chemistry, University of Florida, 16 October 2001
154. 4th Harold Nations Symposium, Georgia Institute of Technology, 5 October 2001
155. Southeastern Regional Meeting of the ACS (SERMACS), Savannah, 24 September 2001
156. Department of Chemistry, University of Alabama, Birmingham, 6 September 2001
157. Molecular Quantum Mechanics: The Right Answer for the Right Reason, an international conference in honor of Prof. Ernest R. Davidson, Seattle, Washington, July 21-26, 2001
158. 30th Meeting of the Southeast Theoretical Chemistry Association, Auburn University, 17-19 May 2001
159. 41st Sanibel Symposium, 24 February - 2 March 2001
160. APS Centennial Meeting, Atlanta, GA, 25 March 1999
161. NASA Ames, December 1998
162. Department of Chemistry, Yale University, 14 December 1998
163. School of Chemistry and Biochemistry, Georgia Institute of Technology, 23 November 1998
164. Department of Chemistry, University of Southern California, 9 November 1998
165. 18th Annual West Coast Theoretical Chemistry Conference, Berkeley, CA, 11 April 1997
166. Department of Chemistry, Massachusetts Institute of Technology, 12 January 1997
167. 25th Meeting of the Southeast Theoretical Chemistry Association, Florida State University, 25 May 1996
168. IX Strasbourg Seminar on Computational Chemistry, Girona, Spain, 14 July 1993

Upcoming Presentations:
1. Elevating Biomolecular Simulations with Data-Driven Approaches, National Meeting of the American Chemical Society, Denver, CO, 18-22 August 2024
2. Vanderbilt University, Nashville, TN
3. The Role of Data and Modeling in Life Processes, Southeastern Regional Meeting of the ACS (SERMACS), 23-26 October 2024

E. Grants and Contracts

E1. As Principal Investigator

Title of Project: CDS&E: Theoretical Models for Potential Energy Landscapes of Challenging Chemical Systems
Agency/Company: NSF CHE
Project Period: 9/1/20-8/31/24
Total Dollar Amount: $449,879
Role: Principal Investigator

Title of Project: Computational Methods for Protein-Ligand Interactions
Agency/Company: Bristol Myers Squibb
Project Period: 7/1/20-6/20/22
Total Dollar Amount: $180,000
Role: Principal Investigator

Title of Project: Computational Methods for Protein-Ligand Interactions

Agency/Company: Bristol Myers Squibb
Project Period: 8/30/18-7/31/20
Total Dollar Amount: $240,000
Role: Principal Investigator

Title of Project: CDS&E: Theoretical Models for Potential Energy Landscapes of Challenging Chemical Systems
Agency/Company: NSF CHE
Project Period: 9/1/16-8/31/20
Total Dollar Amount: $450,000
Role: Principal Investigator

Title of Project: Computational Methods for Protein-Ligand Interactions
Agency/Company: Bristol Myers Squibb
Project Period: 12/1/15-11/30/17
Total Dollar Amount: $140,000
Role: Principal Investigator

Title of Project: CDS&E: Theoretical Models for Potential Energy Landscapes of Challenging Chemical Systems
Agency: NSF
Project Period: 9/1/13-8/31/16
Total Dollar Amount: $449,999
Role: Principal Investigator

Title of Project: Collaborative Research: SI2-SSI: Sustainable Development of Next-Generation Software in Quantum Chemistry
Agency: NSF
Project Period: 6/1/12-5/31/16
Total Dollar Amount: $450,000
Role: Principal Investigator (with E. Chow and D. Crawford)
$150k to Sherrill

Title of Project: Theoretical Models for Potential Energy Landscapes of Challenging Chemical Systems
Agency: NSF
Project Period: 9/1/10-12/31/13
Total Dollar Amount: $450,000
Role: Principal Investigator

Title of Project: CRIF:MU: Acquisition of a Cyber-Enabled Green Computer Cluster for Green Energy Research
Agency: NSF
Project Period: 1/1/2010 - 12/31/2012
Total Dollar Amount: $350,000
Role: Principal Investigator (with C. L. Liotta, J. L. Bredas, A. Bongiorno, and R. Hernandez)
Shared equipment

Title of Project: Theoretical Models for Potential Energy Landscapes of Challenging Chemical Systems
Agency: NSF
Project Period: 7/15/07-7/14/10
Total Dollar Amount: $373,749
Role: Principal Investigator

Title of Project: Theoretical Investigations of the Nature of π-π Interactions PRF
Agency: ACS Petroleum Research Fund
Project Period: 5/1/06-8/31/10
Total Dollar Amount: $80,000
Role: Principal Investigator

Title of Project: Center for Computational Molecular Science & Technology (CCMST)
Agency: NSF CRIF
Project Period: 7/1/05 – 6/30/08
Total Dollar Amount: $350,000
Role: Principal Investigator
Shared computing equipment

Title of Project: Theoretical Studies of Bond-Breaking, Diradicals, and Nondynamical Correlation
Agency: NSF CAREER
Project Period: 5/1/01 - 4/30/07
Total Dollar Amount: $450,000
Role: Principal Investigator

Title of Project: Parallelization of Linear R12 Theories
Agency: Sandia National Labs
Project Period: 10/1/01 - 9/30/04
Total Dollar Amount: $203,000
Role: Principal Investigator

Title of Project: Center for Computational Molecular Science & Technology (CCMST)
Agency: IBM SUR
Project Period: 8/24/00 - 8/24/03
Total Dollar Amount: $1,750,000
Role: Principal Investigator (with R. Hernandez)
Equipment grant

Title of Project: Theoretical Studies of the Photophysics of Mononuclear Copper(I) Complexes
Agency: NSF
Project Period: 8/1/00 - 7/31/01
Total Dollar Amount: $40,000
Role: Principal Investigator

Title of Project: Theoretical Studies of Fundamental Reactions in Organic and Interstellar
Agency: Chemistry Dreyfus Foundation
Project Period: 8/1/99 - 7/31/04
Total Dollar Amount: $40,000
Role: Principal Investigator

E2. As Co-Principal Investigator

Title of Project: MRI: Acquisition of an HPC System for Data-Driven Discovery in Computational Astrophysics, Biology, Chemistry, and Materials Science
Agency/Company: NSF MRI

Project Period: 9/1/18-8/20/22
Total Dollar Amount: $3,699,317 [equipment grant, shared by GT Researchers]
Role: Co-PI (PI: S. Aluru; Co-PI with R. Vuduc, D. Shoemaker, and S. Kalidindi)

Title of Project: Development of Exascale Software for Heterogeneous and Interfacial Catalysis
Agency/Company: DOE CCS
Project Period: 10/1/18-9/30/23
Amount to Sherrill: $266,000
Role: Co-PI (with M. Gordon et al.)

Title of Project: TRIPODS+X:EDU: Collaborative Education: Data-Driven Discovery and Alliance
Agency/Company: NSF
Project Period: 10/1/18-9/30/22
Amount to Sherrill: $99,976
Role: Co-PI (PI: P. Tetali; Co-PI with W. Liao, C. Peng, and J. Weitz)

Title of Project: Enabling GAMESS for Exascale Computing in Chemistry & Materials
Agency/Company: DOE ECP
Project Period: 10/1/18-9/30/23
Amount to Sherrill: $689,517
Role: Co-PI (with M. Gordon et al.)

Title of Project: CDS&E: Exploiting Multiple Levels of Parallelism in Quantum Chemistry Software
Agency/Company: NSF ACI
Project Period: 8/1/16-7/31/21
Total Dollar Amount: $690,711
Role: Co-PI (with E. Chow)
~40% to Sherrill

Title of Project: Collaborative Research: SI2-SSI: Removing Bottlenecks in High Performance Computational Science
Agency/Company: NSF
Project Period: 8/1/15-7/31/19
Total Dollar Amount: $3,600,000
Role: Co-PI (with M. Gordon, T. Windus, D. Crawford, T. Martinez, and L. Slipchenko)
$600k to Sherrill

Title of Project: Enabling Exascale Calculations for Electronic Structure Theory
Agency/Company: DOD HASI
Project Period: 7/1/15-6/30/17
Total Dollar Amount: $2,000,000
Role: Co-PI (with M. Gordon, T. Windus, D. Crawford, and M. Sosonkina)
25% to Sherrill

Title of Project: Basic Principles that Govern the Interaction of Organometallic Catalysts
Agency: DOE BES
Project Period: 9/15/12-9/14/16
Total Dollar Amount: $2,226,906
Role: Principal Investigator (with C. Jones, M. Weck, and S. J. Jang)
~20% to Sherrill

Title of Project: Basic Principles that Govern the Interaction of Organometallic Catalysts
Agency: DOE BES
Project Period: 9/15/09-9/14/12

Total Dollar Amount: $2,103,400
Role: Co-PI (with C. Jones, P. Ludovice, M. Weck, and R. Davis)
~15% to Sherrill

Title of Project: An Integrated Approach to the Rational Design of Chemical Catalysts, Innovative and Novel Computational Impact on Theory and Experiment (INCITE)
Agency: Department of Energy
Project Period: 2010
Total Dollar Amount: 75 million CPU hours
Role: Co-PI (with R. J. Harrison, et al.)
Shared computer time allocation

Title of Project: The Computational Chemistry End Station (ChemES)
Agency: DOE ASCR
Project Period: 1/1/08-12/31/09
Total Dollar Amount: $1,890,000
Role: Co-PI (with R. J. Harrison et al.)

Title of Project: Basic Principles that Govern the Interaction of Organometallic Catalysts
Agency: DOE BES
Project Period: 9/15/06-9/14/09
Total Dollar Amount: $2,103,401
Role: Co-PI (with C. Jones, P. Ludovice, M. Weck, and R. Davis)
~15% to Sherrill

Title of Project: Basic Principles that Govern the Interaction of Organometallic Catalysts with Supports - The Science of Immobilized Molecular Catalysts
Agency: DOE
Project Period: 9/15/03-9/14/06
Total Dollar Amount: $1,873,000
Role: Principal Investigator (with C. Jones, M. Weck, P. Ludovice, R. Davis)
~15% to Sherrill

E3. As Senior Personnel or Contributor

E4. Pending Proposals

Title of Project: EAGER: CI PAOS: A Quantum Leap in Research Data Management for Quantum Chemistry
Agency/Company: NSF OAC
Project Period: 10/1/24 – 9/30/26
Total Dollar Amount: $300,000 ($150k to CDS)
Role: lead PI

Title of Project: Collaborative Research: Frameworks: Software Infrastructure for Next-Generation Quantum Chemistry
Agency/Company: NSF OAC (Software Institutes)
Project Period: 7/1/24-6/30/29
Total Dollar Amount: $4,850,107 ($2,277,120 to GT; $884,168 to CDS)
Role: lead PI (Collaborative proposal involving E. Chow, J. Kretchmer, T. D. Crawford, J. Turney, D. Nascimento)

E5. Proposals Submitted but Not Funded (Last Two Years)

Title of Project: CDS&E: Theoretical Models for Potential Energy Landscapes of Challenging Chemical Systems
Agency/Company: NSF CHE
Project Period: 9/1/24-8/31/27
Total Dollar Amount: $540,205
Role: Principal Investigator

Title of Project: Supplement to Altering Hepatitis B Virus assembly through pharmacological intervention
Agency/Company: NIH
Project Period: 1/24-12/24
Total Dollar Amount: $236,700
Role: Co-Principal Investigator on Software Supplement to J.C. Gumbart's NIH grant (50% to Sherrill)

Title of Project: Application of Next-Generation Quantum-Based Models to Protein-Ligand Interactions
Agency/Company: Eli Lilly LRAP
Project Period: 7/1/24-6/30/25
Total Dollar Amount: $132,500
Role: Principal Investigator

Title of Project: CDS&E: Theoretical Models for Potential Energy Landscapes of Challenging Chemical Systems
Agency/Company: NSF CHE
Project Period: 9/1/23-8/31/26
Total Dollar Amount: $480,288
Role: Principal Investigator

Title of Project: Collaborative Research: Frameworks: Combining Databases, Deep Learning, and Computational Chemical Science
Agency/Company: NSF OAC (Software Institutes)
Project Period: 7/1/23-6/30/28
Total Dollar Amount: $1,000,000 to CDS
Role: PI (Collaborative proposal involving M. Gordon, T. L. Windus, A. Tiwari, L. Carrington, S. Leang, T. D. Crawford, M. Sosonkina)

Title of Project: Machine Learning for Energetically Ranking Polymorphs of Molecular Crystals
Agency/Company: Camille and Henry Dreyfus Foundation
Project Period: 8/22-7/24
Total Dollar Amount: $150,000
Role: PI

Title of Project: NRT-FW-HTF: Graduate Training in Organic and Organic/Inorganic Hybrid Electronics & Photonics for Global Sustainability – TorHES
Agency/Company: NSF DGE – NSF Research Traineeship (NRT)
Project Period: 3/1/22-2/28/27
Total Dollar Amount: $3,000,000
Role: Senior Personnel (PI: N. Stingelin; Co-PI's: T. Harris, A. Osterholm, M. Realff, C. Silva)

Title of Project: Collaborative Research: Frameworks: Combining Databases, Deep Learning, and Computational Chemical Science
Agency/Company: NSF OAC (Software Institutes)
Project Period: 7/1/22-6/30/27
Total Dollar Amount: $1,000,000 to CDS
Role: PI (Collaborative proposal involving M. Gordon, T. L. Windus, A. Tiwari, L. Carrington, S. Leang, T. D. Crawford, M. Sosonkina)

Title of Project: Development of Exascale Software for Catalysis and Interfacial Phenomena
Agency/Company: DOE Computational Chemical Sciences
Project Period: 10/22-9/25
Total Dollar Amount: $450,000 to CDS
Role: PI (Collaborative proposal involving M. Gordon, T. L. Windus, A. Tiwari, L. Carrington, S. Leang, T. D. Crawford, M. Sosonkina). Funded at $66,500 for one year.

Title of Project: Collaborative Research: DMREF: Design of Functionalized Mesoporous Materials optimized for Transport and Catalysis
Agency/Company: NSF
Project Period: 10/1/21 – 9/31/25
Total Dollar Amount: $1,400,000
Role: Co-PI (with M. Gordon, J. Evans, and I. Slowing)
$360k to Sherrill

Title of Project: Combining Data Bases, Deep Learning, and Computational Chemistry to Enhance Chemical Catalysis
Agency/Company DOE
Project Period: 10/1/2021 – 9/30/2024
Total Dollar Amount: $546,000 (GT part of collaborative proposal)
Role: Co-PI

Title of Project: AI Institute: Center for Artificial Intelligence in Polymer Chemistry (AIPoly)
Agency/Company NSF ACI
Project Period: 9/1/2020 – 8/31/2024
Total Dollar Amount: $2,426,470 (GT Portion of MIT-led project)
Role: PI of GT portion of MIT-led consortium (with GT colleagues W. Gutekunst, R. Ramprasad, L. Song)
25% to Sherrill

V. Teaching

A. Courses Taught

Term	Course	Description
F ’99, S ’02, ’05, F ’06-07, ’12-’18 F ’22	CHEM 6491	Quantum Mechanics (graduate)
F ’02	CHEM 6472	Quantum Chemistry & Molecular Spectroscopy (graduate)
F ’00, ’03, ’04 ’07; S ’06, ’10, ’12, ’16	CHEM 3412	Physical Chemistry II (undergraduate)
F ’05, S ’01, ’04, ’09, ’11, ’13, ’15, ’17-‘24	CHEM 6485/ CHEM 4485	Computational Chemistry (graduate & undergraduate)
F ’01, ’06, ’19-’21,’23	CHEM 1310	General Chemistry (undergraduate)

F '09-'11	CHEM 1310HP	General Chemistry, Honors (undergraduate)

B. Individual Student Guidance

B1-B2. Graduate Students

1. Isabel Berry (8/23 – present)
   B.S. Chemistry; CS, Applied Math, Physics Minors, Eckerd College, St. Petersburg FL, 2023
   Presidential Fellowship, Georgia Tech
   DOE Computational Science Graduate Fellowship, 2024-2027
2. Austin Wallace (8/22 – present)
   B. S. Chemistry, University of Mississippi, 2022
   Presidential Fellowship, Georgia Tech
   NSF Graduate Fellowship, 2022-2025
3. Luke Kurfman (8/22 – present)
   B.S. Chemistry, Furman University, 2022
   Presidential Fellowship, Georgia Tech
   NSF Graduate Fellowship, 2024-2027
4. Caroline Sargent (8/21 – present)
   B.S. Chemistry, Wofford College, 2021
   Presidential Fellowship, Georgia Tech
   NSF Graduate Fellowship, 2023-2026
5. Philip Nelson (8/20 – present)
   B.S. Chemistry, Colorado School of Mines, 2020
6. Joseph O'Brien (8/18 – 12/20)
   M.S. Computational Science and Engineering, Georgia Tech, 2020
   B.S. Chemistry and Mathematics, Wayne State University, 2018
   PTC Therapeutics
7. Derek Metcalf (6/18 – 10/22)
   B.S. Chemical Engineering, Michigan State University, 2018; Ph.D. Georgia Tech, 2022
   Ph.D. Thesis: Building Blocks of Neural Network Intermolecular Interaction Potentials
   NSF Graduate Fellowship, 2020-2023
   Southeast Theoretical Chemistry Association (SETCA) Poster Award, 2019
   Co-founder, Lavo Life Sciences
8. Zach Glick (8/18 – 10/22)
   B.S. Chemistry and Computer Science, Washington University in St. Louis, 2018
   Ph.D. Georgia Tech, 2022
   Ph.D. Thesis: Affordable Quantum Chemistry via Data-Driven and Local Approximations to Non-Covalent Interactions
   Presidential Fellowship, Georgia Tech
   Co-founder, Lavo Life Sciences
9. Yi Xie (7/17 – 06/22)
   B.S. Chemical Biology, Tsinghua University, Beijing, China, 2016; Ph.D. Georgia Tech, 2022
   Ph.D. Thesis: Implementation and Application of Density Functional Theory Based Symmetry-Adapted Perturbation Theory for Dimers, Trimers, and Molecular Crystals
10. Constance Warden (7/16 – 5/18)
    M.S. Chemistry, East Tennessee State University, 2016
    B.S. Chemistry, Appalachian State University, 2014
    Presidential Fellowship, Georgia Tech
11. Asim Alenaizan (8/16 – 5/21)
    M.S. Chemistry, Georgia Tech, 2018

B.S. Physics and Chemistry, King Fahd University of Petroleum and Minerals, Saudi Arabia, 2016
Ph.D. Georgia Tech, 2021
Ph.D. Thesis: Computational Analysis of the Structure and Noncovalent Interactions of Nucleic Acids and their Analogs
Professor, King Fahd University of Petroleum and Minerals

12. Matthew Schieber (5/16 – 5/18)
    M. S. Computational Science and Engineering, Georgia Tech, 2018
    B.S. Applied Mathematics, Physics, and Chemistry, Rockhurst University, 2016
    M. S. Thesis: Optimizing Computational Kernels in Quantum Chemistry
    Presidential Fellowship, Georgia Tech
    Smartleaf, Inc.
13. Marvin Lechner (8/16 - 12/16)
    M.S. exchange student from Technical University of Munich
14. Dominic Sirianni (7/15 – 3/20)
    B.S. Chemistry and Mathematics, Edinboro University of Pennsylvania; Ph.D. Georgia Tech, 2020
    Ph.D. Thesis: Electronic Structure Methods for Studying Non-Covalent Interactions in Complex Chemical Environments
    Best Student Talk, Southeast Theoretical Chemistry Association (SETCA), 2017
    Presidential Fellowship, Georgia Tech
    Assistant Professor, Daemen College, Amherst NY
15. Brandon Bakr (8/13 – 5/18)
    B.S. Chemistry with minor in Mathematics, Auburn University; Ph.D. Georgia Tech, 2018
    Ph.D. Thesis: Symmetry-Adapted Perturbation Theory for Organocatalysis
    Presidential Fellowship, Georgia Tech
    Amazon
16. Trent Parker (6/11 - 7/16)
    B.S. Chemistry, St. Louis University
    Presidential Fellowship, Georgia Tech
    Google Inc.
17. Robert Parrish (5/10 - 5/15)
    B.S. Mechanical Engineering, Georgia Tech; Ph.D. Georgia Tech, 2015
    Ph.D. Thesis: Rank Reduction Methods in Electronic Structure Theory
    Georgia Tech Chih Award, 2015
    Forbes 30 Under 30 in Science, 2015
    ACS Graduate Award in Computational Physical Chemistry, 2013
    1st Place, Graduate Student Awards Symposium, Georgia Tech, 2013
    2nd Place Poster Prize, Molecular Quantum Mechanics (Lugano, Switzerland), 2013
    DOE Computational Sciences Graduate Fellowship
    NSF Graduate Fellowship (declined)
    Travel Award, Georgia Tech Research and Innovation Conference, 2013
    2nd Place, Southeast Theoretical Chemistry Association (SETCA) Poster Award, 2011
    Fellowship to attend the 62nd Lindau Meeting of Nobel Laureates and Students, Lindau Germany, June 2012 Presidential Fellowship, Georgia Tech
    Head of Chemistry Simulations, QCWare Inc.
18. Matthew Kennedy (6/09 - 12/14)
    B.S. Chemistry and Computer Science, University of Tennessee; Ph.D. Georgia Tech 2014 Ph.D. Thesis: Non-Covalent Interactions and their Role in Biological and Catalytic Chemistry
    Outstanding Teaching Assistant Award, Georgia Tech, 2010
19. Michael S. Marshall (8/07 - 8/12)
    B.S. Physics, University of Alabama, Birmingham; Ph.D. Georgia Tech, 2012
    Ph.D. Thesis: The Construction and Role of Non-Covalent Benchmarks in Computational Chemistry
    Presidential Fellowship, Georgia Tech
    3rd Place, Graduate Student Awards Symposium, Georgia Tech, 2011

20. Edward Hohenstein (8/07 - 8/11)
    B.S. Chemistry and Mathematics, Washington College; Ph.D. Georgia Tech, 2011
    Ph.D. Thesis: Implementation and Applications of Density-Fitted Symmetry-Adapted Perturbation Theory Assistant Professor, City College of New York
    1st Place, Southeast Theoretical Chemistry Association (SETCA) Poster Award, 2011
    1st Place, Graduate Student Awards Symposium, Georgia Tech, 2010
    Student poster award, 2008 Annual Meeting of the Southeast Theoretical Chemistry Association (SETCA)
    Institute Fellowship, Georgia Tech
    Research Scientist, SLAC National Accelerator Laboratory
21. Tait Takatani (8/06 - 6/10)
    B.S., Marist College; Ph.D. Georgia Tech, 2010
    Ph.D. Thesis: Truth and Tractability: Compromising Between Accuracy and Computational Cost in Quantum Computational Chemistry Methods for Noncovalent Intearctions and Metal-Salen Catalysis Research Faculty, SUNY, 2010-present
    Finalist, Graduate Student Awards Symposium, Georgia Tech, 2009
    Cherry Emerson Fellowship, Georgia Tech
22. Steven Arnstein (8/05 - 12/08)
    B.S., Duquesne University; M.S., Georgia Tech, 2009
    M.S. Thesis: Pi-Pi to Full CI: Cation Dimers and Substitutent Effects in Noncovalent Interactions
    Molecular Biophysics Training Grant, Georgia Tech, 2007-2008
    Center for Organic Photonics and Electronics (COPE) Fellowship, Georgia Tech, 2007
    Presidential Fellowship, Georgia Tech
23. Ashley Ringer (8/04 - 5/09)
    B.S., Mississippi College; Ph.D., Georgia Tech, 2009
    Ph.D. Thesis: From Small to Big: Understanding Noncovalent Interactions in Chemical Systems from Quantum Mechanical Models
    Finalist, GT Chemistry Graduate Student Awards Symposium, 2008 AAUW Dissertation Fellowship, 2008
    Anna Louise Hoffman Award for Outstanding Graduate Research, Iota Sigma Pi, 2008
    2nd Place Poster Award, 2007 Annual Meeting of the Southeast Theoretical Chemistry Association (SETCA)
    National P.E.O. Fellowship, 2007
    Molecular Biophysics Training Grant, Georgia Tech, 2006-2007
    3rd Place Poster Award, 2006 Annual Meeting of the Southeast Theoretical Chemistry Association (SETCA)
    Fellowship to attend the 56th Lindau Meeting of Nobel Laureates and Students, Lindau, Germany, June 2006
    NSF Graduate Fellowship, 2005-2008
    DOE Computational Sciences Graduate Fellowship (declined), 2005
    Best student poster, 14th Conference on Current Trends in Computational Chemistry, Jackson, MS, 2005
    Student poster award, 2005 Annual Meeting of the Southeast Theoretical Chemistry Association (SETCA)
    Presidential Fellowship, Georgia Tech
    Associate Professor, Cal Poly San Luis Obispo
24. John Sears (5/02 - 12/07)
    B.S., University of the South (Sewanee); Ph.D., Georgia Tech, 2007
    Ph.D. Thesis: Minimalist Descriptions of Nondynamical Electron Correlation: From Bond-Breaking to Transition-Metal Catalysis
    Best student poster, 2003 Annual Meeting of the Southeast Theoretical Chemistry Association (SETCA)
    Presidential Fellowship, Georgia Tech
    Scientific Advisor, Pabst Patent Group LLP, 2012-present

Research Scientist, Georgia Tech, 2010-2012
Postdoc, Georgia Tech, 2008-2010

25. Berhane Temelso (5/02 - 2/07)
    B.A., Berea College; Ph.D., Georgia Tech, 2007
    Ph.D. Thesis: Computation of Molecular Properties at the Ab Initio Limit
    Foresight Institute Distinguished Student Award in Nanotechnology, 2006
    Third Place, House-Flaschka-Ashby Student Awards Symposium, Georgia Tech, 2006
    Sanibel Graduate Student Poster Award, 2005
    Cherry Emerson Fellowship, Georgia Tech
    Postdoc, Shields Group, Furman University, 2009-2017
    Research Scientist, University of Charleston, 2017-present
26. Arteum Bochevarov (1/02 - 7/06)
    M.S., Kharkiv National University, Ukraine; Ph.D., Georgia Tech, 2006
    Ph.D. Thesis: Hybrid Correlation Models for Bond Breaking Based on Active Space Partitioning
    Product Manager for the Jaguar program, Schrödinger, Inc., 2012-present
    Finalist, House-Flaschka-Ashby Student Awards Symposium, Georgia Tech, 2005
    Research Scientist, Schro¨dinger, Inc., 2010-present
    Postdoc, Friesner group, Columbia University, 2006-2009
27. Fuchang Yin (8/04 - 8/05)
    B.S., Lanzhou University, China; M.S., Mississippi State University
28. Tony Tauer (8/03 - 7/05)
    B.A., Hendrix College; M.S., Georgia Tech, 2005
    M.S. Thesis: Theoretical Investigations of π-π and Sulfur-π Interactions and their Roles in Biomolecular Systems
    Presidential Fellowship, Georgia Tech
29. Micah Abrams (5/01 - 2/05)
    B.S., University of Central Arkansas; Ph.D., Georgia Tech, 2005
    Ph.D. Thesis: General-Order Single-Reference and Multi-Reference Methods in Quantum Chemistry
    Best student lecture, 2004 Annual Meeting of the Southeast Theoretical Chemistry Association (SETCA)
    1st Place, House-Flaschka-Ashby Student Awards Symposium, Georgia Tech, 2004
    Presidential Fellowship, Georgia Tech
    Technical Director, MHM Innovations, Inc., 2011-present
    Decisive Analytics Corporation, 2008-2010
    Assistant Professor, University of Central Arkansas, 2006-2009
30. Mutasem Sinnokrot (8/00 - 7/04)
    B.S., University of Jordan; M.S., Georgia Tech; Ph.D., Georgia Tech, 2004
    Ph.D. Thesis: Theoretical Investigations of π-π Interactions and Their Role in Molecular
    1st Place, House-Flaschka-Ashby Student Awards Symposium, Georgia Tech, 200
    Molecular Design Institute Fellowship, Georgia Tech
    Chemistry Professor, American University of Iraq-Baghdad, 2022-present
    Senior Lecturer, Khalifa University, 2011-2021
    Assistant Professor, University of Jordan, 2004-2011

B3. Undergraduate Researchers

Melody Lee	1/24 –5/24	Testing coupled-cluster code
Jaden Yon	5/23 – 9/23	NSF REU student: high-accuracy for vdW dimers
Matthew Shammami	5/21 – 9/21	NSF REU student: solute-solvent interactions
Andrew Smith	5/21 – 7/21	NSF REU student: organic crystal polymorphs
Andy Jiang	1/20 - 5/23	Protein-ligand interactions
Tom Regan	5/19 – 7/19	NSF REU student: focal-point frequencies
Donna Odhiambo	5/18 – 7/18	NSF REU student: Noncovalent interactions
Mike Zott	8/15 - 8/17	Clusters and QM/MM interface

Nick Petosa	8/16 - 5/17	Database backend
Seth Polansky	5/16 - 7/16	Ab initio force fields
Leonardo dos Anjos Cunha	8/15 - 7/16	(exchange student) Open-shell SAPT
Omar Hayek	8/15 -12/15	SMP parallelization
Addison Schile	5/15 - 7/15	NSF REU student: Natural orbital coupled-cluster
Christopher Cook	2/12 - 5/15	DFT benchmarking; SETCA Undergrad poster prize, 2015
Georgia Murray	9/12 - 5/14	(High-school student) force-field models
Nihit Pokhrel	8/12 - 12/12	(visitor from Wesleyan College) noncovalent model systems
Christian Loftus	10/11 - 5/12	Range-separated DFT
Jiana Duan	8/10 - 5/11	Charge penetration effects
Rob Parrish	2/09 - 8/10	Density fitting and DFT implementation
Yue Geng	8/08 - 8/09	Indole-benzene
Alvin Yates	5/06 - 7/06	Group databases
Anastasia Senenko	5/06 - 7/06	Perl scripts for PDB searches
Mohini Jain	8/05 - 12/05	Noncovalent interactions
Ryan West	1/05 - 5/06	Protein structure data-mining
Ryan Lively	1/04 - 8/04	GT PURA student: π-π interactions
Michelle Figgs	5/04 - 7/04	NSF REU student: Noncovalent interactions
Pamela Mashburn	8/03 - 12/03	Symmetry breaking
Hugh Heldenbrand	5/03 - 7/03	NSF REU student: Noncovalent interactions
Michelle Szeto	9/02 - 4/03	Cation-π interactions
Ryan Steele	5/02 - 7/02	NSF REU student: Cation-π interactions
Anne Margaret Huss	5/01 - 8/01	Pfizer Summer Undergraduate: Excited states of 1-naphthol
Amanda Jacob	8/01 - 5/01	Cu(I) complexes
Brendan Sullivan	1/01 - 5/01	Electronic structure visualization
Ryan Cohen	5/00 - 8/00	NSF REU student: DFT for symmetry breaking
Daniel Baker	1/00 - 5/00	Twisting induced charge transfer effect
Alfred Park	12/99 - 8/02	Scientific computing
Michael McGinley	9/99 - 5/00	Computer benchmarking
Jennifer Ayers	9/99 - 12/99	Computer benchmarking

B5. Postdoctoral Fellows and Visiting Scholars

1. Dr. Rameshwar Kumawat (11/21 – 5/23)
   Ph.D., Indian Institute of Technology Indore (IIT Indore)
2. Dr. David Poole, Postdoc (9/21 – Present)
   Ph.D., Iowa State University
3. Dr. Jeff Schriber, Postdoc (5/19 – 7/22)
   Ph.D., Emory University
   Assistant Professor, Iona College, New York
4. Dr. Carlos Borca, Postdoc (9/17 - 3/20)
   Ph.D., Purdue University
   Postdoc, Princeton University
5. Dr. Daniel Nascimento, Postdoc (2/18 - 3/19)
   Ph.D., Florida State University
   Assistant Professor, University of Memphis
6. Dr. Daniel Smith, Postdoc (1/16 - 4/17)
   Ph.D., Auburn University
   Staff Scientist, Entos Inc.
7. Dr. Jerome Gonthier, Postdoc (3/14 - 7/16)
   Ph.D., École Polytechnique fédérale de Lausanne (EPFL), Switzerland
   Zapata Inc.

8. Dr. Ryan Richard, Postdoc (1/14 - 3/17)
   Ph.D., Ohio State University
   Research Scientist, Ames National Laboratory
9. Dr. Lori Burns, Research Scientist (6/09 - present)
   Ph.D., Yale University
10. Dr. Eugene DePrince, Research Scientist (9/11 - 7/13)
    Ph.D., University of Chicago
    Assistant Professor, Florida State University, 2013-present
11. Prof. Ugur Bozkaya, Attaturk University, Turkey (7/12 - 5/13)
    Ph.D., Middle East Technical University
12. Dr. Sahan Thanthiriwatte, Postdoc (1/09 - 12/10)
    Ph.D., Mississippi State University
    High-Performance Computing Manager, Federal Reserve Bank of Atlanta
13. Dr. Massimo Malagoli, CCMST Research Scientist (1/09 - 7/12)
14. Dr. Gerry Hyde, Postdoc (10/01 - 03/02)
    Ph.D., Cambridge University
15. Dr. Antara Dutta, Visiting Scientist (5/02 - 2/03)
    Ph.D., Jadavpur University, India
16. Dr. Edward Valeev, CCMST Research Scientist (2/01 - 8/06)
    Ph.D., University of Georgia
    Professor, Virginia Tech

Visiting Faculty

1. Prof. Mary Van Vleet, Visiting Professor (9/22 – present)
   Spelman University
2. Prof. Ugur Bozkaya (7/12 - 5/13)
   Attaturk University, Turkey (Psi4 Project)
3. Dr. Justin Fermann (9/10 - 10/10)
   University of Massachusetts, Amherst (PSI4 Project)
4. Prof. Elizabeth Derrick (1/03 - 12/03)
   Valdosta State University (NSF Faculty Development Program)
5. Prof. Alan Gabrielli (Summers 2000 and 2001)
   Southern Polytechnic State Univ. (NSF Faculty Development Program)

C. Other Teaching Activities

Course Development

1. In 2013, created the "Psi4Education" team of faculty throughout the U.S. to develop an open-source lab manual for computational chemistry using open-source and freely-available software for the computational labs; manual is available at (http://www.psicode.org/labs.php). These labs have been used in CHEM 3412 and CHEM 6491.
2. Instituted and developed computational chemistry exercises for freshman chemistry, which have been used by hundreds of students every year since 2011.
3. Instituted and developed new Computational Chemistry course (CHEM 6481) for graduate students and advanced undergraduates. This is a popular course; it has drawn more than 20 registered students and frequently has several additional students sitting in.

4. Instituted and developed new computational chemistry laboratory module for the senior laboratory course, CHEM 4681 (1999). Taught this module for three semesters.

Additional Teaching Service

1. Instructor, STACC Virtual Workshop in Introductory Computational Chemistry (a two-week workshop for undergraduates, with typically a dozen participants from around the U.S., organized by Prof. Josh Kretchmer), 2022-present
2. Organizer, Data Science Bootcamp, NSF TRIPODS+X and GT Institute for Data Engineering and Science (IDEaS), one-week intensive bootcamp with morning lectures and afternoon hands-on activities, with more than 80 participating undergraduate and graduate students from Georgia Tech, Morehouse, Spelman, Agnes Scott, and Kennesaw State, August 2019
3. Organizer, GT IDEaS Summer Skills Workshop in Data Science and Scientific Computing, a 5-week program with one lecture and one hands-on session per week with 60+ attendees, Summers 2017-8
4. Python Programming Workshop for Chemistry graduate students, Spring, 2010 (http://vergil.chemistry.gatech.edu/courses/python/index.html)
5. Developed Honors section of General Chemistry and taught it 2009-2011
6. Instituted and co-taught (with Prof. Rigoberto Hernandez) a Summer Lecture Series in Theoretical Chemistry for NSF REU theory students, taught in various forms nearly continually from 2000-present.
7. PERL Programming Workshop for Chemistry graduate students, Spring, 2006 (http://vergil.chemistry.gatech.edu/courses/perl/index.html).

Teaching Beyond Georgia Tech

1. Created a public video lecture series on YouTube on introductory topics in Computational Chemistry (https://www.youtube.com/c/DavidSherrill1)
2. Organizer and instructor for a half-day workshop on using the Psi4 Quantum Chemistry program for educational lab modules, 4 May 2017, Florida Meeting and Exposition of the American Chemical Society
3. Developed an extensive set of on-line lecture notes in quantum chemistry, from undergraduate-level to graduate- level (http://vergil.chemistry.gatech.edu/notes/index.html). These notes are used extensively at other institutions, including UC Berkeley, University of Delhi, University of Madrid. See *Chemical & Engineering News*, 11 October 1999.
4. Developed and co-taught (with Prof. Rigoberto Hernandez) the NSF Workshop in Theoretical and Computational Chemistry, summers of 2002-2005, 2009, 2011, 2013-4. Over 100 faculty from 2- and 4-year colleges have participated in this program.
5. Appeared on radio programs, "Inside the Black Box" (October 2009) and "Science in Your Life" (February 2001) and advised the Food Network on an episode of their television program, "Good Eats."

VI. Service

A. Professional Contributions

Symposia Organized

1. Co-organizer, Southeast Theoretical Chemistry Association (SETCA) Annual Meeting, Atlanta, GA, 19-21 May 2022
2. Co-organizer, Computational Quantum Chemistry: Synergism Between Theory and Experiment, International Chemical Congress of Pacific Basin Societies (Pacifichem), Honolulu, Hawaii, December 16-21, 2021

3. Co-organizer, Advanced Research Computing (ARC) Symposium, Georgia Institute of Technology, Atlanta, GA, November 17, 2021
4. Program Chair, Division of Physical Chemistry, American Chemical Society National Meeting, Atlanta, GA, 22-26 August 2021
5. Program Chair, Division of Physical Chemistry, American Chemical Society National Meeting, Virtual Meeting, 5-16 April 2021
6. Organizer, Hive Supercomputer Symposium, Georgia Institute of Technology, Atlanta, GA, March 24, 2021
7. Organizer, PsiCon20, virtual conference for developers and users of Psi4, 3-5 December 2020
8. Co-organizer, Computational Quantum Chemistry- From Promise to Prominence: Symposium in Honor of Henry F. Schaefer III, National Meeting of the American Chemical Society, San Diego, CA, August 25-29, 2019
9. Co-organizer, Machine Learning in Science and Engineering, Georgia Tech, June 10-12, 2019
10. Co-organizer, Machine Learning in Science and Engineering, Carnegie Mellon University, June 6-8, 2018
11. Program Chair, Southeastern Regional Meeting of the American Chemical Society (SERMACS), Atlanta, GA, November 12-16, 2013. Largest ACS regional meeting in 2013, with over 1100 abstracts and 1700 attendees. Winner, ChemLuminary Award for Best 2013 Regional Meeting.
12. Vice-Chair, Gordon Research Conference on Molecular Energy Transfer, Ventura, CA, Jan. 13-18, 2013
13. Co-organizer, "Molecular Quantum Mechanics: From Methylene to DNA and Beyond," an international conference in honor of Professor Henry F. Schaefer III, Berkeley, CA, May 24-29, 2010
14. Co-organizer, "New Frontiers in Electronic Structure Theory," National APS Meeting, Portland, Oregon, Mar. 15- 19, 2010
15. Co-organizer, "Advances in Electronic Structure Theory and First Principles Dynamics," National ACS Meeting, Salt Lake City, Utah, Mar. 22-26, 2009
16. Co-organizer, "Computational Exploration of Energy Landscapes: Challenges and Solutions," National ACS Meeting, Washington, DC, Aug. 28 - Sept. 1, 2005
17. Co-organizer, 31st Southeast Theoretical Chemistry Association (SETCA) conference, Atlanta, GA, May 24-25, 2002
18. Co-organizer, "Frontiers in Biomolecular Simulations," 4th Annual Nations Symposium, Atlanta, GA, Oct. 5, 2001
19. Co-organizer, "Open-shell Molecules and Symmetry Breaking Problems: A Challenge for Quantum Chemistry" joint Southeast/Southwest ACS Meeting, New Orleans, LA, Dec. 6-8, 2000
20. Co-organizer, Twelfth Annual Workshop on Recent Developments in Electronic Structure Methods, Atlanta, GA, May 19-22, 2000

Review Activities

Frequent reviewer for *J. Phys. Chem. A*, *J. Chem. Phys.*, *J. Am. Chem. Soc.*, and *Int. J. Quantum Chem.*, and occasional reviewer for *Phys. Chem. Chem. Phys.*, *J. Comput. Chem.*, *Chem. Phys. Lett.*, *THEOCHEM*, *J. Chem. Theor. Comput.*, *Mol. Phys.*, Academic Press, and Cambridge University Press.

Editorial Activities

Associate Editor, *Journal of Chemical Physics*, 2009-present
Guest Editor, Fritz Schaefer Issue of *Molecular Physics*, 2008-2009 Editorial Board, *Advances in Physical Chemistry*, 2008-2017
Editorial Board, *International Journal of Quantum Chemistry*, 2007-2016

B. Public and Community Service

1. Chair, fundraising committee, ACS Award in Theoretical Chemistry, 2022
2. Science and Software Advisory Board, Molecular Sciences Software Institute (MolSSI), 2019-2022; Chair, 2021-2
3. Past-Chair, Division of Physical Chemistry, American Chemical Society (ACS/PHYS), 8/2022-present

4. Chair, Division of Physical Chemistry, American Chemical Society (ACS/PHYS), 8/2021-8/2022
5. Chair-elect, Division of Physical Chemistry, American Chemical Society (ACS/PHYS), 8/2020-8/2021
6. Vice-chair, Division of Physical Chemistry, American Chemical Society (ACS/PHYS), 8/2019-8/2020
7. Vice-chair-elect, Physical Chemistry Division of the American Chemical Society (ACS/PHYS), 8/2018-8/2019
8. Scientific Advisory Committee, Center for Scalable Predictive Methods for Excitations and Correlated Phenomena (SPEC), Department of Energy Computational Chemical Sciences Program, 2018-2021
9. External Review Committee, Department of Chemistry, University of Nevada, Reno, 2014
10. American Chemical Society Petroleum Research Fund Advisory Board, 2008-2011
11. Chair, Theoretical Chemistry Subdivision of the American Chemical Society, 8/2010-8/2011
12. Chair-elect, Theoretical Chemistry Subdivision of the American Chemical Society, 8/2009-8/2010
13. Vice-chair, Theoretical Chemistry Subdivision of the American Chemical Society, 8/2008-8/2009
14. Executive Committee, Physical Chemistry Division of the American Chemical Society (ACS/PHYS), 8/2007-2010
15. Councilor, Georgia Section of the American Chemical Society, 2008-present
16. National Chemistry Week Chair, Georgia Section of the American Chemical Society, 2009-2022 (GA section a National ChemLuminary Award winner, 2011, 2019)
17. Chair, Georgia Section of the American Chemical Society, 7/2005-2006 (GA section a winner of **four** and finalist for **seven** National ChemLuminary Awards for 2006)
18. Chair-Elect, Georgia Section of the American Chemical Society, 2005

C. Institute Contributions

1. Chair Search Committee, School of Chemistry and Biochemistry (10/23 – 3/24)
2. Undergraduate and Graduate Academic Programs Committee (1/23 – present)
3. Advisory Board, Georgia Tech Open Source Program Office (10/23 – present)
4. Research Next Task Force, Phase II, (1/21 – 5/21)
5. Diversity, Equity, and Inclusion Committee, School of Chemistry and Biochemistry (1/21 – 7/23)
6. Virtual Faculty Professional Development Advisory Committee (8/20 – 7/21)
7. Chair, Strategic Planning Committee, School of Chemistry and Biochemistry (3/20 – 5/20)
8. Chair, Faculty Search Committee, School of Chemistry and Biochemistry (8/18 - 7/19)
9. Seminar Committee, School of Chemistry and Biochemistry (8/18 - 7/19)
10. Strategic Planning Committee, School of Chemistry and Biochemistry (8/17 – 7/18)
11. Search Committee, School of Chemistry and Biochemistry (8/16 - 7/17)
12. Reappointment, Promotion, and Tenure Committee, College of Sciences (10/15 – 5/18)
13. Reappointment, Promotion, and Tenure Committee, School of Chemistry and Biochemistry (8/14 - 7/16, 1/23-present; chair, 4/24-present)
14. Graduate Curriculum Committee, School of Chemistry and Biochemistry (8/15 – 7/18)
15. Georgia Tech Academic Senate (8/12 - 7/15)
16. Chair Search Committee, School of Chemistry and Biochemistry (7/12 - 5/13)
17. Institute for Data and HPC (IDH) Advisory Committee (4/10 - 8/13)
18. Institute Task Force for High Performance Computing (2/06 - 5/06, 5/09 - 5/10)
19. Computational Science and Engineering PhD Program Committee (8/08 - present)
20. Advisory Search Committee for the College of Computing Dean (1/09 - 4/10)
21. Provost's Task Force on Interdisciplinary Activities (8/07 - 5/08)
22. Internal Review Committee, Georgia Tech Bioinformatics Degree Program (8/07 - 12/07)

23. Freshman Chemistry Committee (1/06 - 7/14)
24. Internal Advisory Board, Division of Computational Science and Engineering, College of Computing (8/05 - 8/08)
25. Awards Committee, School of Chemistry and Biochemistry (8/03 - 8/13; chair, 8/06 - 8/09; 8/20 - present)
26. Services Committee, School of Chemistry and Biochemistry (8/99 - 7/07, 8/13 - 7/16)
27. Executive Committee, School of Chemistry and Biochemistry (8/03 - 8/05; 8/08 - 8/12; 1/18 – 12/21)
28. Graduate Committee, School of Chemistry and Biochemistry (8/99 - 7/03)
29. Seminar Committee, School of Chemistry and Biochemistry (8/99 - 7/00)