C. David Sherrill
Professor
School of Chemistry and Biochemistry
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

Associate Director for Research and Education, Institute for Data Engineering and Science (IDEaS), Georgia Institute of Technology, 2017-
Professor, School of Chemistry and Biochemistry and School of Computational Science and Engineering, Georgia Institute of Technology, 2008-
Associate Professor, School of Chemistry and Biochemistry, Georgia Institute of Technology, 2005-2008
Associate Professor, College of Computing, Georgia Institute of Technology, 2006-2008
Co-director, Center for Computational Molecular Science & Technology, Georgia Institute of Technology, 2000-
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

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 24,000 citations and h-index of 74 as of June 2020.
http://orcid.org/0000-0002-5570-7666

B1. Published and Accepted Journal Articles

1. "**Editorial: 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)

2. "**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)

3. **"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)

4. **"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)

5. **"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)

6. **"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)

7. **"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)

8. **"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)

9. **"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)

10. **"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)

11. **"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)

12. **"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)

13. **"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)

14. **"PSI4NUMPY: An Interactive Quantum Chemistry Programming Environment for Reference Implementa- tions 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)

15. **"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)

16. **"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)

17. **"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)

18. "**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)

19. **"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)

20. "**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)

21. "**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)

22. "**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)

23. "**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)

24. "**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)

25. "**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)

26. "**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)

27. "**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)

28. "**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)

29. "**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)

30. "**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)

31. "**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)

32. "**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)

33. "**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)

34. "**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)

35. "**Co(III) Complexes of Tetradentate X_3L 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)

36. "**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)

37. "**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)

38. "**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)

39. "**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)

40. "**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)

41. "**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)

42. "**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)

43. "**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)

44. "**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)

45. "**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)

46. "**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. Mart´ınez, *J. Chem. Phys.* **140**, 181102 (2014). (doi: 10.1063/1.4876016)

47. **"Editorial: 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)

48. "**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)

49. "**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)

50. "**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)

51. "**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)

52. "**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)

53. "**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)

54. "**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)

55. "**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)

56. "**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)

57. "**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)

58. "**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)

59. "**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)

60. "**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)

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

62. "**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)

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159. "**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)

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B4. Submitted Journal Articles

1. "**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, submitted.
2. "**Noncovalent Helicene Structure between Nucleic Acids and Cyanuric Acid**," A. Alenaizan, K. Fauche, R. Krishnamurthy, and C. D. Sherrill, submitted.
3. "**The proto-Nucleic Acid Builder: A Software Tool for Constructing Nucleic Acid Analogs,"** A. Alenaizan, J. Barnett, N. V. Hud, C. D. Sherrill, and A. S. Petrov, manuscript in preparation.

C. Other Publications and Creative Products

Ab Initio Program Packages Made Available to the Community

1. "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)
2. "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. Virtual lecture, Laboratory for Computational Biology, National Institutes of Health, Bethesda MD, 10 September 2020
2. Many-Body Interactions: From Quantum Mechanics to Force Fields, Telluride, CO, 8-12 June 2020
3. Telluride Science Summer Lecture Series, Telluride, CO, 1 June 2020
4. Monthly Meeting of the Georgia Section of the American Chemical Society, 12 March 2020
5. Computational Chemistry Applied to Interesting Problems, Southeastern Regional Meeting of the American Chemical Society (SERMACS), 20-23 October 2019
6. Student-Invited Seminar, Department of Chemistry, University of Minnesota, 3 October 2019
7. Electron-Molecule and Molecule-Molecule Interactions, National Meeting of the American Chemical Society, Orlando, FL, 31 March - 4 April 2019
8. Telluride Workshop on Intermolecular Interactions, Telluride, CO, 18-22 March 2019
9. Department of Chemistry, University of North Texas, 26 October 2018
10. Department of Chemistry, University of Tennessee, 27 September 2018
11. Many-Body Interactions: From Quantum Mechanics to Force Fields, Telluride, CO, 9-13 July 2018
12. 2018 Meeting of the Southeast Theoretical Chemistry Association (SETCA), Louisiana State University, Baton Rouge, LA, 18-19 May 2018
13. Dipole and Charge in Drug Design, National Meeting of the American Chemical Society, New Orleans, LA, 18-22 March 2018
14. 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
15. Dipole and Charge in Drug Design, National Meeting of the American Chemical Society, New Orleans, LA, 18-22 March 2018
16. Department of Chemistry, The University of the South, Sewanee, TN, 22 September 2017
17. 11th Triennial Congress of the World Association of Theoretical and Computational Chemists (WATOC), Munich, Germany, 27 August - 1 September 2017
18. Noncovalent Interactions in Quantum Chemistry and Physics: Theory and Applications, 100th Canadian Chemistry Conference, Toronto, Canada, 28 May – 1 June, 2017
19. Molecular Sciences Software Institute Workshop on Software Interoperability, Virginia Tech, 5-7 June 2017
20. Florida Meeting and Exposition of the American Chemical Society, Tampa, FL, 4-6 May 2017
21. Dow Core Research, Midland, MI, 22 March 2017
22. Molecules to Functional Supramolecular Materials, Southeast Regional Meeting of the American Chemical Society (SERMACS), Columbia, SC, 23-26 October, 2016
23. Electronic Structure: Concepts and Applications, Southeast Regional Meeting of the American Chemical Society (SERMACS), Columbia, SC, 23-26 October, 2016
24. International Conference on Theoretical and High Performance Computational Chemistry 2016 (ICT-HPCC16), Chongqing, China, October 14-17, 2016
25. Department of Chemistry, Washington University in St. Louis, 29 September 2016
26. Bristol-Myers Squibb, Princeton, NJ, 19 July 2016

27. Density- and Response Density-Based Models for Intermolecular Interactions in Molecular Assemblies and in Solids, CECAM workshop, Nancy, France, 20-23 June 2016
28. Keynote talk, 2016 Meeting of the Southeast Theoretical Chemistry Association (SETCA), Florida State University, Tallahassee, FL, 12-14 May 2016
29. Department of Chemistry, University of Kansas, April 2016
30. Open-Eye Software CUP XVI Conference, Santa Fe, NM, 7-9 March 2016
31. Practical Strategies for Modeling Non-Covalent Interactions, International Chemical Congress of Pacific Basin Societies (Pacifichem), Honolulu, Hawaii, 15-20 December 2015
32. Keynote intived talk, Control of London Dispersion Interactions in Molecular Chemistry, German DFG SPP 1807
33. Workshop, Göttingen, Germany, 19-20 October 2015
34. Intermolecular Interactions: New Challenges for ab initio Theory, Telluride, CO, 6-11 July 2015
35. Keynote talk, 2015 Meeting of the Southeast Theoretical Chemistry Association (SETCA), University of Central Florida, Orlando, FL, 15-16 May 2015
36. Southeastern Regional Meeting of the American Chemical Society, Nashville, TN, 16-19 October 2014
37. World Association of Theoretical and Computational Chemists (WATOC), Santiago, Chile, 5-10 October 2014
38. Addressing Challenges for First-Principles Based Modeling of Molecular Materials, CECAM Workshop, Lausanne, Switzerland, 25-29 August 2014
39. "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*]
40. Telluride Workshop on Quantum Mechanics Derived Force Fields, Telluride, CO, 15-19 June 2014
41. Department of Chemistry, Tulane University, 8 May 2014
42. NSF/LASiGMA Seminar, University of New Orleans, New Orleans, LA, 7 May 2014
43. 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
44. Department of Chemistry, University of Chicago, 25 November 2013
45. University Seminar, University of Tennessee, Knoxville, TN, 1 November 2013
46. Structure-Property Relationships of Molecular Precursors to Organic Electronics, CECAM Workshop, Lausanne, Switzerland, 22-25 October 2013
47. Intermolecular Interactions: New Challenges for ab initio Thoery, Telluride, Colorado, 15-19 July, 2013
48. 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
49. 2013 Meeting of the Southeast Theoretical Chemistry Association (SETCA), Auburn University, 10-11 May 2013
50. 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
51. Potential Function Uncertainty and Validation, National Meeting of the American Chemical Society, New Orleans, LA, 7-11 April 2013
52. Department of Chemistry, University of Tennessee at Chattanooga, 1 March 2013
53. Symposium on the Occasion of Professor Joel Bowman's 65th Birthday, Emory University, Atlanta, GA, 8-9 February 2013
54. The Robert J. Silbey Memorial Symposium on Theory for Experimentalists, Georgia Tech, Atlanta, GA, 6-7 December 2012
55. Towards First-Principles Description of van der Waals Interactions in Complex Materials, CECAM Workshop, Lausanne, Switzerland, 15-19 October, 2012
56. Bridging the Gap Between Ab Initio and Classical Simulations, National Meeting of the American Chemical Society, Philadelphia, PA, 19-23 August 2012
57. Many-Body Interactions: From Quantum Mechanics to Force Fields, Telluride, Colorado, 2-6 July 2012

58. 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
59. 2012 Meeting of the Southeast Theoretical Chemistry Association (SETCA), University of Georgia, 17-19 May 2012
60. "Energy Component Analysis of Molecular Recognition in Biochemistry," Astrobiology Science Conference (AbSciCon) 2012, Atlanta, GA, 16-20 April 2012
61. Department of Chemistry, Ohio State University, 20 February 2012
62. Department of Chemistry, University of Wisconsin-Madison, 31 January 2012
63. "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
64. 7th Congress of the International Society for Theoretical Chemical Physics (ISTCP-VII), Tokyo, Japan, 2-8 Septem ber 2011
65. 10th Annual MERCURY Conference on Undergraduate Computational Chemistry, Bucknell University, 28-30 July 2011
66. World Association of Theoretical and Computational Chemists (WATOC), 17-22 July 2011
67. Fragment and Local Orbital Methods in Electronic Structure Theory, National Meeting of the American Chemical Society, Anaheim, CA, 27-31 March 2011
68. 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
69. Student Invited Seminar, Florida International University, Miami, FL, 28 January 2011
70. Mesilla Workshop on Aromatic Interactions in Chemistry and Biology, Mesilla, New Mexico, 6-9 February 2011
71. Department of Chemistry, Auburn University, 28 October 2010
72. Department of Chemistry, Johns Hopkins University, 19 October 2010
73. Next Generation Force Fields for Nanoscience, Center for Nanophase Materials Sciences (CNMS), Oak Ridge National Laboratory, 15-16 September 2010
74. Silverton Workshop on Intermolecular Interactions: New Challenges for ab initio Theory, 9-13 August 2010, Silverton, Colorado.
75. 50th Sanibel Symposium, St. Simons Island, GA, 24 February - 2 March 2010
76. Department of Chemistry, University of Georgia, 25 September 2009
77. 238th National Meeting of the American Chemical Society, Washington, DC, 16-20 August 2009
78. School of Chemistry and Biochemistry, Georgia Institute of Technology, 4 April 2009
79. Department of Chemistry, St. Louis University, 27 February 2009
80. Department of Chemistry, University of Massachusetts, Amherst, 19 February 2009
81. Gordon Research Conference on Molecular Energy Transfer, Ventura, CA, 18-23 January 2009
82. Department of Chemistry, University of Michigan, 17 November 2008
83. Department of Chemistry, Bethel University, 1 October, 2008
84. Theory and Applications of Computational Chemistry (TACC), Shanghai, China, 23-27 September, 2008
85. World Association of Theoretical and Computational Chemists, Sydney, Australia, 14-19 September, 2008
86. 6th Congress of the International Society for Theoretical Chemical Physics (ISTCP-VI), Vancouver, Canada, 29-24 July, 2008.
87. Development of Force Fields using *Ab Initio* Electronic Structure Calculations, Telluride, Colorado, 6-11 July, 2008
88. Molecular Quantum Mechanics - Analytic Gradients and Beyond, an international conference in honor of Prof. Peter Pulay, Budapest, Hungary, 29 May - 3 June 2007
89. Department of Chemistry, University of Tennessee, Chattanooga, TN, November 2, 2007
90. Department of Chemistry, Middle Tennessee State University, Murfreesboro, TN, November 1, 2007
91. Biology and Chemistry Lecture Series, Trevecca University, Nashville, TN, October 31, 2007
92. 59th Southeastern Regional Meeting of the American Chemical Society, Greenville, SC, 25 October 2007
93. Solvay-COPE Symposium on Organic Electronics, Georgia Tech, 8 May 2007

94. Department of Chemistry, Michigan State University, 22 February 2007
95. XIth European Workshop on Quantum Systems in Chemistry and Physics (QSCP-XI), St. Petersburg, Russia, 20-25 August 2006
96. 35th Meeting of the Southeast Theoretical Chemistry Association, Emory University, 19-20 May 2000
97. Quantitative Quantum Chemistry, a conference in honor of Dr. Thom Dunning, Santa Fe, New Mexico, 17-20 March, 2006
98. Department of Chemistry, University of South Carolina, 30 January 2006
99. International Chemical Congress of Pacific Basin Societies (Pacifichem), Honolulu, Hawaii, 15-20 December 2005
100. 14th Conference on Current Trends in Computational Chemistry, Jackson, MS, 4-5 November 2005
101. Quantum Theory Project, University of Florida, 5 October 2005
102. Department of Chemistry, University of Florida, 4 October 2005
103. Highlands in Chemistry Seminar, Virginia Tech, 4 March 2005
104. 7th Congress of the World Association of Theoretically Oriented Chemists, Cape Town, South Africa, 16-21 January 2005
105. Department of Chemistry, University of North Dakota, 12 November 2004
106. Department of Chemistry, University of Southern California, 25 October 2004
107. Department of Chemistry, Rice University, 9 September 2004
108. Department of Chemistry, Imperial College, London, 23 July 2004
109. 228th National Meeting of the American Chemical Society, Philadelphia, 22-26 August 2004
110. Oak Ridge National Laboratory, 16 June 2004
111. 33rd Meeting of the Southeast Theoretical Chemistry Association, University of Mississippi, 21-22 May 2004
112. Department of Chemistry, Wake Forest University, 3 March 2004
113. Southeastern Regional Meeting of the ACS (SERMACS), Atlanta, 17 November 2003
114. 226th National Meeting of the American Chemical Society, New York, 8 September 2003
115. Symposium on Frontiers in Computational Chemistry, Emory University, 12 April 2003
116. 225th National Meeting of the American Chemical Society, New Orleans, 24 March 2003
117. Department of Chemistry, Hampton University, 30 January 2003
118. Department of Chemistry, Old Dominion University, 6 December 2002
119. Eastern Texas Section of the ACS, 24 October 2002
120. Department of Chemistry, Kilgore College, 24 October 2002
121. Department of Chemistry, Iowa State University, 20 September 2002
122. Gordon Research Conference on Computational Chemistry, Colby-Sawyer College, New London, NH, 1 July 2002
123. Atlanta Area Chemical Physics Seminar, 6 May 2002
124. University of Georgia Chemistry Graduate Student Organization, Athens, 26 April 2002
125. 223rd National Meeting of the American Chemical Society, Orlando, 9 April 2002
126. Department of Chemistry, University of Tennesee at Chattanooga, 15 February 2002
127. Quantum Theory Project, University of Florida, 17 October 2001
128. Department of Chemistry, University of Florida, 16 October 2001
129. 4th Harold Nations Symposium, Georgia Institute of Technology, 5 October 2001
130. Southeastern Regional Meeting of the ACS (SERMACS), Savannah, 24 September 2001
131. Department of Chemistry, University of Alabama, Birmingham, 6 September 2001
132. 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
133. 30th Meeting of the Southeast Theoretical Chemistry Association, Auburn University, 17-19 May 2001
134. 41st Sanibel Symposium, 24 February - 2 March 2001
135. APS Centennial Meeting, Atlanta, GA, 25 March 1999
136. NASA Ames, December 1998
137. Department of Chemistry, Yale University, 14 December 1998
138. School of Chemistry and Biochemistry, Georgia Institute of Technology, 23 November 1998
139. Department of Chemistry, University of Southern California, 9 November 1998
140. 18th Annual West Coast Theoretical Chemistry Conference, Berkeley, CA, 11 April 1997
141. Department of Chemistry, Massachusetts Institute of Technology, 12 January 1997

142. 25th Meeting of the Southeast Theoretical Chemistry Association, Florida State University, 25 May 1996
143. IX Strasbourg Seminar on Computational Chemistry, Girona, Spain, 14 July 1993

E. Grants and Contracts

E1. As Principal Investigator

Title of Project: Theoretical Models for Potential Energy Landscapes of Challenging Chemical Systems
Agency/Company: NSF CHE
Project Period: 9/1/20-8/31/23
Total Dollar Amount: $449,879
Role: Principal Investigator

Title of Project: 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: Center for Computational Molecular Science & Technology (CCMST)
equipment grant
Project Period: 5/1/06-8/31/10
Total Dollar Amount: $80,000
Role: Principal Investigator

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: CDS&E: Exploiting Multiple Levels of Parallelism in Quantum Chemistry Software
Agency/Company: NSF ACI
Project Period: 8/1/16-7/31/19
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

E4. Pending Proposals

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-’16	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	CHEM 6485	Computational Chemistry (graduate & undergraduate)
F ’01, ’06, ’19, ‘20	CHEM 1310	General Chemistry (undergraduate)
F ’09-’11	CHEM 1310HP	General Chemistry, Honors (undergraduate)

B. Individual Student Guidance

B1-B2. Graduate Students

1. Joseph O’Brien (8/18 - present)
   B.S. Chemistry and Mathematics, Wayne State University, 2018

2. Derek Metcalf (6/18 - present)
   B.S. Chemical Engineering, Michigan State University, 2018
   NSF Graduate Fellowship, 2020-2023
   Southeast Theoretical Chemistry Association (SETCA) Poster Award, 2019

3. Zach Glick (8/18 - present)
   B.S. Chemistry and Computer Science, Washington University in St. Louis, 2018
   Presidential Fellowship, Georgia Tech

4. Yi Xie (7/17 - present)
   B.S. Chemical Biology, Tsinghua University, Beijing, China, 2016
5. 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
6. Asim Alenaizan (8/16 - present)
   M.S. Chemistry, Georgia Tech, 2018
   B.S. Physics and Chemistry, King Fahd University of Petroleum and Minerals, Saudi Arabia, 2016
7. 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
   Smartleaf, Inc.
   Presidential Fellowship, Georgia Tech
8. Marvin Lechner (8/16 - 12/16)
   M.S. exchange student from Technical University of Munich
9. Dominic Sirianni (7/15 – 3/20)
   B.S. Chemistry and Mathematics, Edinboro University of Pennsylvania; Ph.D. Georgia Tech, 2020
   Best Student Talk, Southeast Theoretical Chemistry Association (SETCA), 2017
   Presidential Fellowship, Georgia Tech
10. 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
    Epic Systems, Inc.
    Presidential Fellowship, Georgia Tech
11. Trent Parker (6/11 - 7/16)
    B.S. Chemistry, St. Louis University
    Presidential Fellowship, Georgia Tech
12. 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
13. 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*
14. 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

15. 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
16. 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
17. 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
18. 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
    Assistant Professor, Cal Poly San Luis Obispo, 2011-present
    Postdoc, MacKerell Group, University of Maryland, 2009-
    2011 *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
19. 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
    Scientific Advisor, Pabst Patent Group LLP, 2012-
    present Research Scientist, Georgia Tech, 2010-
    2012
    Postdoc, Georgia Tech, 2008-2010

Best student poster, 2003 Annual Meeting of the Southeast Theoretical Chemistry Association (SETCA) Presidential Fellowship, Georgia Tech

20. 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 Postdoc, Shields Group, Armstrong Atlantic
    University, 2009-present *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
21. 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
    Research Scientist, Schrödinger, Inc., 2010-present
    Postdoc, Friesner group, Columbia University, 2006-
    2009
    Finalist, House-Flaschka-Ashby Student Awards Symposium, Georgia Tech, 2005
22. Fuchang Yin (8/04 - 8/05)
    B.S., Lanzhou University, China; M.S., Mississippi State University
23. 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
24. 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 Technical Director, MHM Innovations, Inc., 2011-present
    Decisive Analytics Corporation, 2008-2010
    Assistant Professor, University of Central Arkansas, 2006-2009
    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
25. 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 Recognition Assistant Professor, The Petroleum Institute, 2012-present
    Assistant Professor, University of Jordan, 2004-2012
    1st Place, House-Flaschka-Ashby Student Awards Symposium, Georgia Tech, 2003 Molecular Design Institute Fellowship, Georgia Tech

B3. Undergraduate Researchers

Andy Jiang	1/20 -	Protein-ligand interactions
Sarim Khan	11/17 - 1/18	Molecular torsion balances (visitor from IIT Roorkee)
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. Jeff Schriber, Postdoc (5/19 - Present)
   Ph.D., Emory University
2. Dr. Carlos Borca, Postdoc (9/17 - 3/20)
   Ph.D., Purdue University
   Postdoc, Princeton University
3. Dr. Daniel Nascimento, Postdoc (2/18 - 3/19)
   Ph.D., Florida State University
   Postdoc, Pacific Northwest National Laboratory
4. Dr. Daniel Smith, Postdoc (1/16 - 4/17)
   Ph.D., Auburn University
   Staff Scientist, Molecular Sciences Software Institute
5. Dr. Ryan Richard, Postdoc (1/14 - 3/17)
   Ph.D., Ohio State University
   Research Scientist, Ames National Laboratory
6. Dr. Jerome Gonthier, Postdoc (3/14 - 7/16)
   Ph.D., École Polytechnique fédérale de Lausanne (EPFL), Switzerland
   Zapata Inc.
7. Dr. Ryan Richard, Postdoc (1/14 - 3/17)
   Ph.D., Ohio State University

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

Visiting Faculty

1. Prof. Ugur Bozkaya (7/12 - 5/13)
   Attaturk University, Turkey (PSI4 Project)
2. Dr. Justin Fermann (9/10 - 10/10)
   University of Massachusetts, Amherst (PSI4 Project)
3. Prof. Elizabeth Derrick (1/03 - 12/03)
   Valdosta State University (NSF Faculty Development Program)
4. 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. 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 partici- pating undergraduate and graduate students from Georgia Tech, Morehouse, Spelman, Agnes Scott, and Kennesaw State

2. 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
3. Python Programming Workshop for Chemistry graduate students, Spring, 2010 (http://vergil.chemistry.gatech.edu/courses/python/index.html)
4. Developed Honors section of General Chemistry and taught it 2009-2011
5. 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.
6. PERL Programming Workshop for Chemistry graduate students, Spring, 2006 (http://vergil.chemistry.gatech.edu/courses/perl/index.html).

Teaching Beyond Georgia Tech

1. 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
2. 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.
3. 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 partic- ipated in this program.
4. Appeared on radio programs, "Inside the Black Box" (October 2009) and "Science in Your Life" (February 2001) and advised the Food Network television program, "Good Eats."

VI. Service

A. Professional Contributions

Symposia Organized

1. Co-organizer, Computational Quantum Chemistry: Synergism Between Theory and Experiment, International Chemical Congress of Pacific Basin Societies (Pacifichem), Honolulu, Hawaii, December 15-20, 2020
2. Co-organizer, Computational Quantum Chemistry- From Promise to Prominence: Symposium in Honor of Henry
3. F. Schaefer III, National Meeting of the American Chemical Society, San Diego, CA, August 25-29, 2019
4. Co-organizer, Machine Learning in Science and Engineering, Georgia Tech, June 10-12, 2019
5. Co-organizer, Machine Learning in Science and Engineering, Carnegie Mellon University, June 6-8, 2018
6. 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.
7. Vice-Chair, Gordon Research Conference on Molecular Energy Transfer, Ventura, CA, Jan. 13-18, 2013
8. 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
9. Co-organizer, "New Frontiers in Electronic Structure Theory," National APS Meeting, Portland, Oregon, Mar. 15- 19, 2010

10. Co-organizer, “Advances in Electronic Structure Theory and First Principles Dynamics,” National ACS Meeting, Salt Lake City, Utah, Mar. 22-26, 2009
11. Co-organizer, “Computational Exploration of Energy Landscapes: Challenges and Solutions,” National ACS Meeting, Washington, DC, Aug. 28 - Sept. 1, 2005
12. Co-organizer, 31st Southeast Theoretical Chemistry Association (SETCA) conference, Atlanta, GA, May 24-25, 2002
13. Co-organizer, “Frontiers in Biomolecular Simulations,” 4th Annual Nations Symposium, Atlanta, GA, Oct. 5, 2001
14. 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
15. Co-organizer, Twelfth Annual Workshop on Recent Developments in Electronic Structure Methods, Atlanta, GA, May 19-22, 2000

B. Public and Community Service

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

Other Service Activities

1. Science and Software Advisory Board, Molecular Sciences Software Institute (MolSSI), 2019-present
2. Chair-elect, Physical Chemistry Division of the American Chemical Society (ACS/PHYS), 8/2020-8/2021
3. Vice-chair, Physical Chemistry Division of the American Chemical Society (ACS/PHYS), 8/2019-8/2020
4. Vice-chair-elect, Physical Chemistry Division of the American Chemical Society (ACS/PHYS), 8/2018-8/2019
5. Scientific Advisory Committee, Center for Scalable Predictive Methods for Excitations and Correlated Phenomena (SPEC), Department of Energy Computational Chemical Sciences Program, 2018-present
6. External Review Committee, Deparment of Chemistry, University of Nevada, Reno, 2014
7. American Chemical Society Petroleum Research Fund Advisory Board, 2008-2011
8. Chair, Theoretical Chemistry Subdivision of the American Chemical Society, 8/2010-8/2011
9. Chair-elect, Theoretical Chemistry Subdivision of the American Chemical Society, 8/2009-8/2010
10. Vice-chair, Theoretical Chemistry Subdivision of the American Chemical Society, 8/2008-8/2009
11. Executive Committee, Physical Chemistry Division of the American Chemical Society (ACS/PHYS), 8/2007-2010
12. Councilor, Georgia Section of the American Chemical Society, 2008-2019
13. National Chemistry Week Chair, Georgia Section of the Americal Chemical Society, 2009-present (National ChemLuminary Award winner, 2011)
14. 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)
15. Chair-Elect, Georgia Section of the American Chemical Society, 2005

C. Institute Contributions

1. Virtual Faculty Professional Development Advisory Committee (8/20 – 7/21)
2. Chair, Strategic Planning Committee, School of Chemistry and Biochemistry (3/20 – 5/20)
3. Chair, Faculty Search Committee, School of Chemistry and Biochemistry (8/18 - 7/19)
4. Seminar Committee, School of Chemistry and Biochemistry (8/18 - 7/19)
5. Strategic Planning Committee, School of Chemistry and Biochemistry (8/17 – 7/18)
6. Search Committee, School of Chemistry and Biochemistry (8/16 - 7/17)
7. Reappointment, Promotion, and Tenure Committee, College of Science (10/15 – 5/18)
8. Reappointment, Promotion, and Tenure Committee, School of Chemistry and Biochemistry (7/14 - 7/16)
9. Graduate Curriculum Committee, School of Chemistry and Biochemistry (7/15 - present)
10. Georgia Tech Academic Senate (8/12 - 7/15)
11. Chair Search Committee, School of Chemistry and Biochemistry (7/12 - 5/13)
12. Institute for Data and HPC (IDH) Advisory Committee (4/10 - 8/13)
13. Institute Task Force for High Performance Computing (2/06 - 5/06, 5/09 - 5/10)
14. Computational Science and Engineering PhD Program Committee (8/08 - present)
15. Advisory Search Committee for the College of Computing Dean (1/09 - 4/10)
16. Provost's Task Force on Interdisciplinary Activities (8/07 - 5/08)
17. Internal Review Committee, Georgia Tech Bioinformatics Degree Program (8/07 - 12/07)
18. Freshman Chemistry Committee (1/06 - 7/14)
19. Internal Advisory Board, Division of Computational Science and Engineering, College of Computing (8/05 - 8/08)
20. Awards Committee, School of Chemistry and Biochemistry (8/03 - 8/13; chair, 8/06 - 8/09)
21. Services Committee, School of Chemistry and Biochemistry (8/99 - 7/07, 8/13 - 7/16)
22. Executive Committee, School of Chemistry and Biochemistry (8/03 - 8/05; 8/08 - 8/12)
23. Graduate Committee, School of Chemistry and Biochemistry (8/99 - 7/03)
24. Seminar Committee, School of Chemistry and Biochemistry (8/99 - 7/00)