

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**

Interim Executive Director, Institute for Data Engineering and Science (IDEaS), Georgia Institute of Technology, 2025  
Associate Director for Research and Education, Institute for Data Engineering and Science (IDEaS), Georgia Institute of Technology, 2017-2024  
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  $\pi$  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 36,000 citations and h-index of 87 as of December 2024

<http://orcid.org/0000-0002-5570-7666>

### B1. Published and Accepted Journal Articles

1. **“Evaluating Wavefunction Methods, the Counterpoise Correction, and the Frozen Core Approximation for the Optimization of van der Waals Dimers,”** C. S. Glick, R. L. Kumawat, and C. D. Sherrill, *J. Chem. Phys.* in press
2. **“PyVPT2: Interoperable Software for Anharmonic Vibrational Frequency Calculations,”** P. M. Nelson and C. D. Sherrill, *J. Chem. Phys.* **162**, 162, 032501 (2025) (doi: 10.1063/5.0251445)
3. **“Convergence of the Many-body Expansion with Respect to Distance Cutoffs in Crystals of Polar Molecules: Acetic Acid, Formamide, and Imidazole,”** P. M. Nelson and C. D. Sherrill, *J. Chem. Phys.* **161**, 214105 (2024) (doi: 10.1063/5.0234883)

4. **“QCManyBody: A Flexible Implementation of the Many-Body Expansion,”** L. A. Burns, C. D. Sherrill, and B. P. Pritchard, *J. Chem. Phys.* **161**, 152501 (2024) (doi: [10.1063/5.0231843](https://doi.org/10.1063/5.0231843))
5. **“Electrostatically Embedded Symmetry Adapted Perturbation Theory,”** C. S. Glick, A. Alenaizan, C. E. Cavender, and C. D. Sherrill, *J. Chem. Phys.* **161**, 134112 (2024) (doi: [10.1063/5.0221974](https://doi.org/10.1063/5.0221974))
6. **“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.* **161**, 114115 (2024) (doi: [10.1063/5.0219185](https://doi.org/10.1063/5.0219185))
7. **“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.* **161**, 082502 (2024) (doi: [10.1063/5.0219963](https://doi.org/10.1063/5.0219963))
8. **“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.* **15** 13313-13324 (2024) (doi: [10.1039/D4SC01029A](https://doi.org/10.1039/D4SC01029A))
9. **“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](https://doi.org/10.1063/5.0216760))
10. **“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](https://doi.org/10.1063/5.0196848))
11. **“Directional  $\Delta G$  Neural Network (Dr $\Delta G$ -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](https://doi.org/10.1021/acs.jcim.3c02054))
12. **“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](https://doi.org/10.1038/s41597-023-02443-1))
13. **“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](https://doi.org/10.1063/5.0168608))
14. **“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](https://doi.org/10.1063/5.0155895))
15. **“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](https://doi.org/10.1063/5.0159410))
16. **“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](https://doi.org/10.1021/acs.jcim.3c00428))

17. "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](https://doi.org/10.1063/5.0143712))
18. "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](https://doi.org/10.1063/5.0141872))
19. "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](https://doi.org/10.1063/5.0103644))
20. "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](https://doi.org/10.1039/D2MH00808D))
21. "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](https://doi.org/10.1063/5.0090688))
22. "The Influence of a Solvent Environment On Direct Non-Covalent Interactions Between Two Molecules: A Symmetry-Adapted Perturbation Theory Study of Polarization Tuning of  $\pi$ - $\pi$  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](https://doi.org/10.1063/5.0087302))
23. "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](https://doi.org/10.1063/5.0059356))
24. "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](https://doi.org/10.1021/jacs.1c08972))
25. "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](https://doi.org/10.1063/5.0049745))
26. "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](https://doi.org/10.1063/5.0050444))
27. "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](https://doi.org/10.1063/5.0042989))

28. **“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](https://doi.org/10.1021/jacs.0c12010))
29. **“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](https://doi.org/10.1002/chem.202004390))
30. **“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](https://doi.org/10.1021/acs.jcim.0c01071))
31. **“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](https://doi.org/10.1093/nar/gkaa1159))
32. **“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](https://doi.org/10.1063/5.0011521))
33. **“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](https://doi.org/10.1063/5.0006002))
34. **“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](https://doi.org/10.1063/5.0004863))
35. **“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](https://doi.org/10.1063/1.5142636))
36. **“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](https://doi.org/10.1063/1.5129452))
37. **“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](https://doi.org/10.1002/qua.26035))
38. **“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](https://doi.org/10.1063/1.5120520))

39. **“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. Steinrück, C. Cao, C. D. Sherrill, B. Kippelen, and M. Toney, *Chem. Mater.* **31**, 6677-6683 (2019). (doi: [10.1021/acs.chemmater.9b01069](https://doi.org/10.1021/acs.chemmater.9b01069))
40. **“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.jpcllett.9b01220](https://doi.org/10.1021/acs.jpcllett.9b01220))
41. **“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.jpccb.9b01523](https://doi.org/10.1021/acs.jpccb.9b01523))
42. **“Tipping the Balance between S- $\pi$  and O- $\pi$  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](https://doi.org/10.1021/jacs.8b07617))
43. **“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](https://doi.org/10.1039/c8cp02029a))
44. **“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](https://doi.org/10.1021/acs.jctc.8b00286))
45. **“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](https://doi.org/10.1021/acs.jctc.8b00114))
46. **“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](https://doi.org/10.1021/acs.jctc.7b01232))
47. **“Reassigning the CaH<sup>+</sup> 1<sup>1</sup> $\Sigma$   $\rightarrow$  2<sup>1</sup> $\Sigma$  Vibronic Transition with CaD<sup>+</sup>,”** 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](https://doi.org/10.1063/1.5016556))
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## B4. Submitted Journal Articles

1. “Levels of Symmetry Adapted Perturbation Theory (SAPT). II. Convergence of Interaction Energy Components,” J. B. Schriber, A. M. Wallace, D. L. Cheney, and C. D. Sherrill, submitted.
2. “SparcleQC: Automated Input File Creation for QM/MM Studies of Protein:Ligand Complexes,” C. S. Glick, I. P. Berry, and C. D. Sherrill, submitted

## 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](https://doi.org/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](https://doi.org/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](https://doi.org/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](https://doi.org/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](https://doi.org/10.1080/00268970902909382))

### Computational Chemistry Software Contributions

1. “QCManyBody: A Flexible Implementation of the Many-Body Expansion,” L. A. Burns, C. D. Sherrill, and B. P. Pritchard, *J. Chem. Phys.* **161**, 152501 (2024) (doi: [10.1063/5.0231843](https://doi.org/10.1063/5.0231843))
2. “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. Martinez, 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](https://doi.org/10.1063/5.0059356))
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](https://doi.org/10.1063/5.0006002))
4. “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](https://doi.org/10.1093/nar/gkaa1159))
5. “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](https://doi.org/10.1002/qua.26035))

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8. **“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. Engangelista, J. M. Turney, T. D. Crawford, and C. D. Sherrill, *J. Chem. Theory Comput.* **13**, 3185-3197 (2017). (doi: [10.1021/acs.jctc.7b00174](https://doi.org/10.1021/acs.jctc.7b00174))
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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](https://doi.org/10.1039/b517914a))
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## Press

1. **“Herty Medal Goes to David Sherrill,”** Chemical & Engineering News, vol.101, issue 10, 25 March 2023
2. Quoted in **“Computational chemists welcome ‘living’ journal,”** Chemical & Engineering News, vol. 97, issue 1, 7 January 2019
3. Psi4 mentioned in Bloomberg article, **“Google Debuts Software to Open Up Quantum Computers for Chemists,”** 23 October 2017
4. Interviewed in **“Cyber Forged: Advanced Computer Technologies Speed Development of Real-World Materials,”** R. Robinson, Georgia Tech Research Horizons Issue 2, 2016. ([article link](#))
5. 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](#))
6. 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

7. "National Chemistry Week: The Chemistry of Candy," Inside The Black Box, WREK 91.1 FM Atlanta, 22 October 2014
8. Quoted in "Pi-stacking better without the aromatics?" RSC Chemistry World News, 8 July 2011
9. "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
10. "Chemistry: What is it Good For?" Inside the Black Box, WREK 91.1 FM Atlanta, 21 October 2009
11. "Supramolecular chemistry: Another piece of the  $\pi$ ," Research Highlights, Nature Chemistry, 23 January 2009 (doi: 10.1038/nchem.117)
12. "Science in Your Life," Georgia Public Radio, February 2001

#### D. Presentations

1. Plenary Lecture, 64<sup>th</sup> Sanibel Symposium, St. Augustine, FL, 28 February 2025
2. Innovations in Computational Chemistry, Georgia Institute of Technology, Atlanta, GA, 21 March 2025
3. Data Analytics and AI for Manufacturing and Healthcare, American Chemical Society National Meeting, San Diego, CA, 25 March 2025
4. The Role of Data and Modeling in Life Processes, Southeastern Regional Meeting of the ACS (SERMACS), Atlanta, GA, 23-26 October 2024
5. Quantum-Based Modeling of Complex Environments: Methods, Software and Applications (A Symposium in Honor of Herty Medalist David Sherrill), Southeastern Regional Meeting of the ACS (SERMACS), Atlanta, GA, 24-25 October 2024
6. Department of Chemistry, Vanderbilt University, Nashville, TN, 30 September 2024
7. Elevating Biomolecular Simulations with Data-Driven Approaches, National Meeting of the American Chemical Society, Denver, CO, 18-22 August 2024
8. Plenary Talk, OpenMolcas Developers' Meeting, Toronto, Canada, 22-24 June 2024
9. Many-Body Interactions: From Quantum Mechanics to Force Fields, Telluride Science & Innovation Center, Telluride, CO, 15-19 June 2024
10. Departmental Seminar, University of Tennessee at Chattanooga, 24 May 2024
11. Keynote Lecture: Southeast Theoretical Chemistry Association (SETCA), Virginia Tech, Blacksburg, VA, 16 May 2024
12. Departmental Seminar, Department of Chemistry, Virginia Commonwealth University, 29 February 2024
13. Keynote Address, 18<sup>th</sup> Herty Medalist Undergraduate Research Symposium, Georgia Gwinnett College, 22 September 2023
14. Herty Medal Award Address, Georgia Section of the American Chemical Society, 21 September 2023
15. Free and Open Source Software: Harnessing the Power of Data, National Meeting of the American Chemical Society, San Francisco, CA, 13-17 August 2023
16. NanoFANS Forum: Trends in Machine Learning for Biology, Institute for Electronics and Nanotechnology, Georgia Tech, 22 June 2023
17. Tinker Workshop, Washington University in St. Louis, St. Louis, MO, 15-16 June 2023
18. Challenges for Physical Chemists, Harnessing the Power of Chemistry Presidential Symposium, National Meeting of the American Chemical Society, Indianapolis, IN, 26-30 March 2023
19. Physical Chemistry Seminar, Department of Chemistry, University of Florida, 25 October 2022
20. 17<sup>th</sup> Herty Medalist Undergraduate Research Symposium, Georgia Gwinnett College, 16 September 2022
21. 12<sup>th</sup> Triennial Congress of the World Association of Theoretical and Computational Chemists (WATOC), Vancouver, Canada, 3-8 July 2022
22. 10<sup>th</sup> Triennial Conference on Molecular Quantum Mechanics (MQM), Virginia Tech, Blacksburg, VA, 26 June – 1 July 2022

23. Many-Body Interactions: From Quantum Mechanics to Force-Fields, Telluride Science Research Center, Telluride, CO, 6-10 June 2022
24. Machine Learning in Chemical and Materials Sciences, Los Alamos National Laboratory Center for Nonlinear Studies, 23-26 May 2022 (virtual presentation)
25. Institute of Computational and Theoretical Chemistry (ICTCUB), University of Barcelona, Spain, 28 April 2022 (virtual presentation)
26. 30<sup>th</sup> 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)
27. Computational Quantum Chemistry: Synergism Between Theory and Experiment, International Chemical Congress of Pacific Basin Societies (Pacifichem), Honolulu, Hawaii, 16-21 December 2021 (virtual presentation)
28. High-Performance Computing Applications in Chemistry, Southeastern Regional Meeting of the American Chemical Society (SERMACS), 10-13 November 2021
29. Computational Chemistry and Machine Learning, Southeastern Regional Meeting of the American Chemical Society (SERMACS), 10-13 November 2021
30. Advanced Force Fields, National Meeting of the American Chemical Society, Atlanta, GA, 22-26 August 2021 (virtual presentation)
31. Theoretical Chemistry Seminar, Cambridge University, Cambridge, England, 12 May 2021 (virtual presentation)
32. Department of Chemistry, King Fahd University of Petroleum and Minerals, Saudi Arabia, 27 October 2020 (virtual presentation)
33. Laboratory for Computational Biology, National Institutes of Health, Bethesda MD (virtual presentation), 10 September 2020
34. Many-Body Interactions: From Quantum Mechanics to Force Fields, Telluride, CO, 8-12 June 2020
35. Telluride Science Summer Lecture Series, Telluride, CO (virtual presentation), 1 June 2020
36. Monthly Meeting of the Georgia Section of the American Chemical Society (virtual presentation), 12 March 2020
37. Computational Chemistry Applied to Interesting Problems, Southeastern Regional Meeting of the American Chemical Society (SERMACS), 20-23 October 2019
38. Student-Invited Seminar, Department of Chemistry, University of Minnesota, 3 October 2019
39. Electron-Molecule and Molecule-Molecule Interactions, National Meeting of the American Chemical Society, Orlando, FL, 31 March - 4 April 2019
40. Telluride Workshop on Intermolecular Interactions, Telluride, CO, 18-22 March 2019
41. Department of Chemistry, University of North Texas, 26 October 2018
42. Department of Chemistry, University of Tennessee, 27 September 2018
43. Many-Body Interactions: From Quantum Mechanics to Force Fields, Telluride, CO, 9-13 July 2018
44. 2018 Meeting of the Southeast Theoretical Chemistry Association (SETCA), Louisiana State University, Baton Rouge, LA, 18-19 May 2018
45. Dipole and Charge in Drug Design, National Meeting of the American Chemical Society, New Orleans, LA, 18-22 March 2018
46. 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
47. Dipole and Charge in Drug Design, National Meeting of the American Chemical Society, New Orleans, LA, 18-22 March 2018
48. Department of Chemistry, The University of the South, Sewanee, TN, 22 September 2017
49. 11th Triennial Congress of the World Association of Theoretical and Computational Chemists (WATOC), Munich, Germany, 27 August - 1 September 2017
50. Noncovalent Interactions in Quantum Chemistry and Physics: Theory and Applications, 100th Canadian Chemistry Conference, Toronto, Canada, 28 May – 1 June, 2017
51. Molecular Sciences Software Institute Workshop on Software Interoperability, Virginia Tech, 5-7 June 2017
52. Florida Meeting and Exposition of the American Chemical Society, Tampa, FL, 4-6 May 2017
53. Dow Core Research, Midland, MI, 22 March 2017

54. Molecules to Functional Supramolecular Materials, Southeast Regional Meeting of the American Chemical Society (SERMACS), Columbia, SC, 23-26 October, 2016
55. Electronic Structure: Concepts and Applications, Southeast Regional Meeting of the American Chemical Society (SERMACS), Columbia, SC, 23-26 October, 2016
56. International Conference on Theoretical and High Performance Computational Chemistry 2016 (ICT-HPCC16), Chongqing, China, October 14-17, 2016
57. Department of Chemistry, Washington University in St. Louis, 29 September 2016
58. Bristol-Myers Squibb, Princeton, NJ, 19 July 2016
59. Density- and Response Density-Based Models for Intermolecular Interactions in Molecular Assemblies and in Solids, CECAM workshop, Nancy, France, 20-23 June 2016
60. Keynote talk, 2016 Meeting of the Southeast Theoretical Chemistry Association (SETCA), Florida State University, Tallahassee, FL, 12-14 May 2016
61. Department of Chemistry, University of Kansas, April 2016
62. Open-Eye Software CUP XVI Conference, Santa Fe, NM, 7-9 March 2016
63. Practical Strategies for Modeling Non-Covalent Interactions, International Chemical Congress of Pacific Basin Societies (Pacifichem), Honolulu, Hawaii, 15-20 December 2015
64. Keynote invited talk, Control of London Dispersion Interactions in Molecular Chemistry, German DFG SPP 1807, 2015
65. Workshop, Göttingen, Germany, 19-20 October 2015
66. Intermolecular Interactions: New Challenges for ab initio Theory, Telluride, CO, 6-11 July 2015
67. Keynote talk, 2015 Meeting of the Southeast Theoretical Chemistry Association (SETCA), University of Central Florida, Orlando, FL, 15-16 May 2015
68. Southeastern Regional Meeting of the American Chemical Society, Nashville, TN, 16-19 October 2014
69. World Association of Theoretical and Computational Chemists (WATOC), Santiago, Chile, 5-10 October 2014
70. Addressing Challenges for First-Principles Based Modeling of Molecular Materials, CECAM Workshop, Lausanne, Switzerland, 25-29 August 2014
71. "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*]
72. Telluride Workshop on Quantum Mechanics Derived Force Fields, Telluride, CO, 15-19 June 2014
73. Department of Chemistry, Tulane University, 8 May 2014
74. NSF/LASiGMA Seminar, University of New Orleans, New Orleans, LA, 7 May 2014
75. Chemical Theory for Complex Systems, Joint International Symposium hosted by the Emerson Center (Emory University) and the Catalysis Research Center (Hokkaido U, Japan), Atlanta, GA, 9-10 January 2014
76. Department of Chemistry, University of Chicago, 25 November 2013
77. University Seminar, University of Tennessee, Knoxville, TN, 1 November 2013
78. Structure-Property Relationships of Molecular Precursors to Organic Electronics, CECAM Workshop, Lausanne, Switzerland, 22-25 October 2013
79. Intermolecular Interactions: New Challenges for ab initio Theory, Telluride, Colorado, 15-19 July, 2013
80. 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
81. 2013 Meeting of the Southeast Theoretical Chemistry Association (SETCA), Auburn University, 10-11 May 2013
82. 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
83. Potential Function Uncertainty and Validation, National Meeting of the American Chemical Society, New Orleans, LA, 7-11 April 2013
84. Department of Chemistry, University of Tennessee at Chattanooga, 1 March 2013

85. Symposium on the Occasion of Professor Joel Bowman's 65th Birthday, Emory University, Atlanta, GA, 8-9 February 2013
86. The Robert J. Silbey Memorial Symposium on Theory for Experimentalists, Georgia Tech, Atlanta, GA, 6-7 December 2012
87. Towards First-Principles Description of van der Waals Interactions in Complex Materials, CECAM Workshop, Lausanne, Switzerland, 15-19 October, 2012
88. Bridging the Gap Between Ab Initio and Classical Simulations, National Meeting of the American Chemical Society, Philadelphia, PA, 19-23 August 2012
89. Many-Body Interactions: From Quantum Mechanics to Force Fields, Telluride, Colorado, 2-6 July 2012
90. 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
91. 2012 Meeting of the Southeast Theoretical Chemistry Association (SETCA), University of Georgia, 17-19 May 2012
92. "Energy Component Analysis of Molecular Recognition in Biochemistry," Astrobiology Science Conference (AbSciCon) 2012, Atlanta, GA, 16-20 April 2012
93. Department of Chemistry, Ohio State University, 20 February 2012
94. Department of Chemistry, University of Wisconsin-Madison, 31 January 2012
95. "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
96. 7th Congress of the International Society for Theoretical Chemical Physics (ISTCP-VII), Tokyo, Japan, 2-8 September 2011
97. 10th Annual MERCURY Conference on Undergraduate Computational Chemistry, Bucknell University, 28-30 July 2011
98. World Association of Theoretical and Computational Chemists (WATOC), 17-22 July 2011
99. Fragment and Local Orbital Methods in Electronic Structure Theory, National Meeting of the American Chemical Society, Anaheim, CA, 27-31 March 2011
100. 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
101. Student Invited Seminar, Florida International University, Miami, FL, 28 January 2011
102. Mesilla Workshop on Aromatic Interactions in Chemistry and Biology, Mesilla, New Mexico, 6-9 February 2011
103. Department of Chemistry, Auburn University, 28 October 2010
104. Department of Chemistry, Johns Hopkins University, 19 October 2010
105. Next Generation Force Fields for Nanoscience, Center for Nanophase Materials Sciences (CNMS), Oak Ridge National Laboratory, 15-16 September 2010
106. Silverton Workshop on Intermolecular Interactions: New Challenges for ab initio Theory, 9-13 August 2010, Silverton, Colorado.
107. 50th Sanibel Symposium, St. Simons Island, GA, 24 February - 2 March 2010
108. Department of Chemistry, University of Georgia, 25 September 2009
109. 238th National Meeting of the American Chemical Society, Washington, DC, 16-20 August 2009
110. School of Chemistry and Biochemistry, Georgia Institute of Technology, 4 April 2009
111. Department of Chemistry, St. Louis University, 27 February 2009
112. Department of Chemistry, University of Massachusetts, Amherst, 19 February 2009
113. Gordon Research Conference on Molecular Energy Transfer, Ventura, CA, 18-23 January 2009
114. Department of Chemistry, University of Michigan, 17 November 2008
115. Department of Chemistry, Bethel University, 1 October, 2008
116. Theory and Applications of Computational Chemistry (TACC), Shanghai, China, 23-27 September, 2008
117. World Association of Theoretical and Computational Chemists, Sydney, Australia, 14-19 September, 2008
118. 6th Congress of the International Society for Theoretical Chemical Physics (ISTCP-VI), Vancouver, Canada, 29-24 July, 2008.

119. Development of Force Fields using *Ab Initio* Electronic Structure Calculations, Telluride, Colorado, 6-11 July, 2008
120. Molecular Quantum Mechanics - Analytic Gradients and Beyond, an international conference in honor of Prof. Peter Pulay, Budapest, Hungary, 29 May - 3 June 2007
121. Department of Chemistry, University of Tennessee, Chattanooga, TN, November 2, 2007
122. Department of Chemistry, Middle Tennessee State University, Murfreesboro, TN, November 1, 2007
123. Biology and Chemistry Lecture Series, Trevecca University, Nashville, TN, October 31, 2007
124. 59th Southeastern Regional Meeting of the American Chemical Society, Greenville, SC, 25 October 2007
125. Solvay-COPE Symposium on Organic Electronics, Georgia Tech, 8 May 2007
126. Department of Chemistry, Michigan State University, 22 February 2007
127. XIth European Workshop on Quantum Systems in Chemistry and Physics (QSCP-XI), St. Petersburg, Russia, 20-25 August 2006
128. 35th Meeting of the Southeast Theoretical Chemistry Association, Emory University, 19-20 May 2000
129. Quantitative Quantum Chemistry, a conference in honor of Dr. Thom Dunning, Santa Fe, New Mexico, 17-20 March, 2006
130. Department of Chemistry, University of South Carolina, 30 January 2006
131. International Chemical Congress of Pacific Basin Societies (Pacifichem), Honolulu, Hawaii, 15-20 December 2005
132. 14th Conference on Current Trends in Computational Chemistry, Jackson, MS, 4-5 November 2005
133. Quantum Theory Project, University of Florida, 5 October 2005
134. Department of Chemistry, University of Florida, 4 October 2005
135. Highlands in Chemistry Seminar, Virginia Tech, 4 March 2005
136. 7th Congress of the World Association of Theoretically Oriented Chemists, Cape Town, South Africa, 16-21 January 2005
137. Department of Chemistry, University of North Dakota, 12 November 2004
138. Department of Chemistry, University of Southern California, 25 October 2004
139. Department of Chemistry, Rice University, 9 September 2004
140. Department of Chemistry, Imperial College, London, 23 July 2004
141. 228th National Meeting of the American Chemical Society, Philadelphia, 22-26 August 2004
142. Oak Ridge National Laboratory, 16 June 2004
143. 33rd Meeting of the Southeast Theoretical Chemistry Association, University of Mississippi, 21-22 May 2004
144. Department of Chemistry, Wake Forest University, 3 March 2004
145. Southeastern Regional Meeting of the ACS (SERMACS), Atlanta, 17 November 2003
146. 226th National Meeting of the American Chemical Society, New York, 8 September 2003
147. Symposium on Frontiers in Computational Chemistry, Emory University, 12 April 2003
148. 225th National Meeting of the American Chemical Society, New Orleans, 24 March 2003
149. Department of Chemistry, Hampton University, 30 January 2003
150. Department of Chemistry, Old Dominion University, 6 December 2002
151. Eastern Texas Section of the ACS, 24 October 2002
152. Department of Chemistry, Kilgore College, 24 October 2002
153. Department of Chemistry, Iowa State University, 20 September 2002
154. Gordon Research Conference on Computational Chemistry, Colby-Sawyer College, New London, NH, 1 July 2002
155. Atlanta Area Chemical Physics Seminar, 6 May 2002
156. University of Georgia Chemistry Graduate Student Organization, Athens, 26 April 2002
157. 223rd National Meeting of the American Chemical Society, Orlando, 9 April 2002
158. Department of Chemistry, University of Tennessee at Chattanooga, 15 February 2002
159. Quantum Theory Project, University of Florida, 17 October 2001
160. Department of Chemistry, University of Florida, 16 October 2001
161. 4th Harold Nations Symposium, Georgia Institute of Technology, 5 October 2001
162. Southeastern Regional Meeting of the ACS (SERMACS), Savannah, 24 September 2001
163. Department of Chemistry, University of Alabama, Birmingham, 6 September 2001

164. 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
165. 30th Meeting of the Southeast Theoretical Chemistry Association, Auburn University, 17-19 May 2001
166. 41st Sanibel Symposium, 24 February - 2 March 2001
167. APS Centennial Meeting, Atlanta, GA, 25 March 1999
168. NASA Ames, December 1998
169. Department of Chemistry, Yale University, 14 December 1998
170. School of Chemistry and Biochemistry, Georgia Institute of Technology, 23 November 1998
171. Department of Chemistry, University of Southern California, 9 November 1998
172. 18th Annual West Coast Theoretical Chemistry Conference, Berkeley, CA, 11 April 1997
173. Department of Chemistry, Massachusetts Institute of Technology, 12 January 1997
174. 25th Meeting of the Southeast Theoretical Chemistry Association, Florida State University, 25 May 1996
175. IX Strasbourg Seminar on Computational Chemistry, Girona, Spain, 14 July 1993

Upcoming Presentations:

1. From ab initio Computations to Conceptual Insights into Bonding, Telluride Science & Innovation Center, Telluride CO, 27-31 May 2025
2. World Association of Theoretical and Computational Chemists (WATOC), 21-27 June 2025, Oslo, Norway
3. International Academy of Quantum Molecular Science, 28-29 June 2025, Menton, France
4. 2025 Computer Aided Drug Design Gordon Research Conference, 13-18 July 2025, University of Southern Maine, Portland, ME
5. 3<sup>rd</sup> International Symposium on Machine Learning in Quantum Chemistry (SMLQC), University of Tennessee, Knoxville, 5-7 October 2025
6. Computational Quantum Chemistry: Synergy Between Theory and Experiment, International Chemical Congress of Pacific Basin Societies 2025 (Pacifichem), 15-20 December 2025
7. Machine Learning-Based Accelerated Discovery of Advanced Materials in Support of Green Energy Transition, International Chemical Congress of Pacific Basin Societies 2025 (Pacifichem), 15-20 December 2025

## **E. Grants and Contracts**

### **E1. As Principal Investigator**

Title of Project: Collaborative Research: Frameworks: Software Infrastructure for Next-Generation Quantum Chemistry

Agency/Company: NSF OAC (Software Institutes)

Project Period: 9/15/24-9/14/28

Total Dollar Amount: \$3,196,572 (\$1,569,071 to GT; \$683,700 to CDS)

Role: lead PI (Collaborative proposal involving E. Chow, J. Kretchmer, T. D. Crawford, J. Turney, D. Nascimento)

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  $\pi$ - $\pi$  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: POSE: Phase I: Sustainable Data Interchange for Quantum Chemistry and Beyond  
Agency/Company: NSF TI  
Project Period: 6/1/25 – 5/31/26  
Total Dollar Amount: \$238,519 (Planning grant, \$104k to CDS group personnel)  
Role: lead PI

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

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: 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	CHEM 6491	Quantum Mechanics (graduate)
F '22, '24		
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)

**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 – 5/24)  
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 Interactions 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 Substituent 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, Schrödinger, 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  $\pi$ - $\pi$  and Sulfur- $\pi$  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  $\pi$ - $\pi$  Interactions and Their Role in Molecular  
*1st Place, House-Flaschka-Ashby Student Awards Symposium, Georgia Tech, 2004*  
*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: $\pi$ - $\pi$ 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- $\pi$ interactions
Ryan Steele	5/02 - 7/02	NSF REU student: Cation- $\pi$ 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)