

Alexander Yu. Sokolov

Curriculum Vitae

(Last updated: December 29, 2024)

CONTACT INFORMATION

ADDRESS: Department of Chemistry & Biochemistry
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PROFESSIONAL EXPERIENCE

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| <i>Current</i> 5/2023 | <i>Associate Professor</i> The Ohio State University , Columbus, OH (USA) Department of Chemistry & Biochemistry |
| 8/2017–5/2023 | <i>Assistant Professor</i> The Ohio State University , Columbus, OH (USA) Department of Chemistry & Biochemistry |
| 7/2016–8/2017 | <i>Postdoctoral Scholar</i> California Institute of Technology , Pasadena, CA (USA) Advisor: Professor Garnet K.-L. Chan |
| 8/2014–6/2016 | <i>Postdoctoral Research Associate</i> Princeton University , Princeton, NJ (USA) Advisor: Professor Garnet K.-L. Chan |

EDUCATION

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| 2009–2014 | <i>Doctor of Philosophy</i> University of Georgia , Center for Computational Quantum Chemistry, Athens, GA (USA) Advisor: Professor Henry F. Schaefer III Thesis: “Development of density cumulant functional theory” |
| 2004–2009 | <i>Specialist Degree (M.S.)</i> St. Petersburg State University , St. Petersburg (Russia) <i>Diploma with Distinction</i> Major: Chemistry Advisor: Professor Olga V. Sizova Thesis: “Valence structure analysis of heavy transition metal complexes with electronic configurations d^6 , d^7 , d^8 , and d^{10} ” |

ACADEMIC AWARDS AND FELLOWSHIPS

- 2024 | Dirac Medal from the World Association of Theoretical and Computational Chemists (WATOC)
- 2023 | OpenEye Outstanding Junior Faculty Award in Computational Chemistry
- 2021 | National Science Foundation CAREER Award
- 2016 | American Chemical Society Physical Chemistry Division Postdoctoral Award
- 2015 | IBM-Löwdin Award for Postdoctoral Associates, 55th Sanibel Symposium, St. Simons' Island, GA (USA)
- 2014 | Martin Reynolds Smith Award, University of Georgia, Athens, GA (USA)
- 2013 | Dissertation Completion Award, University of Georgia, Athens, GA (USA)
- 2013 | Best Graduate Student Poster Award, 53rd Sanibel Symposium, St. Simons' Island, GA (USA)
- 2012 | James L. Carmon Award, University of Georgia, Athens, GA (USA)
- 2009 | Charles Coulson Fellowship, Center for Computational Quantum Chemistry, Athens, GA (USA), 5 years
- 2009 | Best Alumnus of St. Petersburg 2009 Award, St. Petersburg (Russia)
- 2008 | Special Scholarship of the Government of Russian Federation (Russia), 1 year
- 2008 | Summer Fellowship, Center for Computational Quantum Chemistry, Athens, GA (USA)
- 2004 | Full Scholarship, St. Petersburg State University (Russia), 5 years

PUBLICATIONS (H-INDEX: 21)

* Corresponding authors are denoted with asterisk.

- [56] C. E. V. d. Moura and **A. Yu. Sokolov***. "Efficient Spin-Adapted Implementation of Multireference Algebraic Diagrammatic Construction Theory. I. Core-Ionized States and X-ray Photoelectron Spectra." *J. Phys. Chem. A* **128**, 5816–5831 (2024).
- [55] N. P. Gaba, C. E. V. d. Moura, R. Majumder, and **A. Yu. Sokolov***. "Simulating transient X-ray photoelectron spectra of Fe(CO)₅ and its photodissociation products with multireference algebraic diagrammatic construction theory." *Phys. Chem. Chem. Phys.* **26**, 15927–15938 (2024).
- [54] R. Majumder and **A. Yu. Sokolov***. "Consistent Second-Order Treatment of Spin–Orbit Coupling and Dynamic Correlation in Quasidegenerate N-Electron Valence Perturbation Theory." *J. Chem. Theory Comput.* **20**, 4676–4688 (2024).
- [53] T. L. Stahl and **A. Yu. Sokolov***. "Quantifying spin contamination in algebraic diagrammatic construction theory of electronic excitations." *J. Chem. Phys.* **160**, 204104 (2024).

- [52] **A. Yu. Sokolov***. “Multireference perturbation theories based on the Dyll Hamiltonian.” *Adv. Quant. Chem* **90**, 121–155 (2024).
- [51] N. E. Sparks, C. Smith, T. Stahl, D. L. Amarasekara, C. Hamadani, E. Lambert, S. W. Tang, A. Kulkarni, B. M. Derbigny, G. S. Dasanayake, G. Taylor, M. Ghazala, N. I. Hammer, **A. Yu. Sokolov**, N. C. Fitzkee, E. E. L. Tanner, and D. L. Watkins*. “NIR-II emissive donor–acceptor–donor fluorophores for dual fluorescence bioimaging and photothermal therapy applications.” *J. Mat. Chem. C* **12**, 4369–4383 (2024).
- [50] S. Carter, W. Tao, R. Majumder, **A. Yu. Sokolov***, and S. Zhang. “Two-State Hydrogen Atom Transfer Reactivity of Unsymmetric $[\text{Cu}_2(\text{O})(\text{NO})]^{2+}$ Complexes.” *J. Am. Chem. Soc.* **145**, 17779–17785 (2023).
- [49] I. M. Mazin and **A. Yu. Sokolov***. “Core-Excited States and X-ray Absorption Spectra from Multireference Algebraic Diagrammatic Construction Theory.” *J. Chem. Theory Comput.* **19**, 4991–5006 (2023).
- [48] S. Banerjee and **A. Yu. Sokolov***. “Algebraic Diagrammatic Construction Theory for Simulating Charged Excited States and Photoelectron Spectra.” *J. Chem. Theory Comput.* **19**, 3037–3053 (2023). (**Highlight: invited review**).
- [47] S. Bandaranayake, A. Patnaik, E. Hruska, Q. Zhu, **A. Yu. Sokolov**, and L. R. Baker*. “Electronic Structure and Ultrafast Electron Dynamics in CuO Photocatalysts Probed by Surface Sensitive Femtosecond X-ray Absorption Near-Edge Structure Spectroscopy.” *J. Phys. Chem. Lett.* **14**, 3643–3650 (2023).
- [46] J. K. Bower, M. S. Reese, I. M. Mazin, L. M. Zarnitsa, A. D. Cypcar, C. E. Moore, **A. Yu. Sokolov***, and S. Zhang*. “C(sp³)–H cyanation by a formal copper(iii) cyanide complex.” *Chem. Sci.* (2023).
- [45] R. Majumder and **A. Yu. Sokolov***. “Simulating Spin–Orbit Coupling with Quasidegenerate N-Electron Valence Perturbation Theory.” *J. Phys. Chem. A* **127**, 546–559 (2023). (**Highlight: invited article, “Early-Career and Emerging Researchers in Physical Chemistry” special issue**).
- [44] S. Lin, S. Banerjee, M. T. Fortunato, C. Xue, J. Huang, **A. Yu. Sokolov***, and C. Turro*. “Electrochemical Strategy for Proton Relay Installation Enhances the Activity of a Hydrogen Evolution Electrocatalyst.” *J. Am. Chem. Soc.* **144**, 20267–20277 (2022).
- [43] S. Banerjee and **A. Yu. Sokolov***. “Non-Dyson Algebraic Diagrammatic Construction Theory for Charged Excitations in Solids.” *J. Chem. Theory Comput.* **18**, 5337–5348 (2022).
- [42] T. L. Stahl, S. Banerjee, and **A. Yu. Sokolov***. “Quantifying and reducing spin contamination in algebraic diagrammatic construction theory of charged excitations.” *J. Chem. Phys.* **157**, 044106 (2022).
- [41] C. E. V. de Moura and **A. Yu. Sokolov***. “Simulating X-ray photoelectron spectra with strong electron correlation using multireference algebraic diagrammatic construction theory.” *Phys. Chem. Chem. Phys.* **24**, 4769–4784 (2022). (**Highlight: PCCP HOT Article**).
- [40] I. M. Mazin and **A. Yu. Sokolov***. “Multireference Algebraic Diagrammatic Construction Theory for Excited States: Extended Second-Order Implementation and Benchmark.” *J. Chem. Theory Comput.* **17**, 6152–6165 (2021).

- [39] S. Banerjee and **A. Yu. Sokolov***. “Efficient implementation of the single-reference algebraic diagrammatic construction theory for charged excitations: Applications to the TEMPO radical and DNA base pairs.” *J. Chem. Phys.* **154**, 074105 (2021). (**Highlight: Invited article, 2021 JCP Emerging Investigators Special Collection**).
- [38] J. P. Misiewicz, J. M. Turney, H. F. Schaefer*, and **A. Yu. Sokolov**. “Assessing the orbital-optimized unitary Ansatz for density cumulant theory.” *J. Chem. Phys.* **153**, 244102 (2020).
- [37] K. Chatterjee and **A. Yu. Sokolov***. “Extended Second-Order Multireference Algebraic Diagrammatic Construction Theory for Charged Excitations.” *J. Chem. Theory Comput.* **16**, 6343–6357 (2020).
- [36] Q. Sun, X. Zhang, S. Banerjee, P. Bao, M. Barbry, N. S. Blunt, N. A. Bogdanov, G. H. Booth, J. Chen, Z.-H. Cui, J. J. Eriksen, Y. Gao, S. Guo, J. Hermann, M. R. Hermes, K. Koh, P. Koval, S. Lehtola, Z. Li, J. Liu, N. Mardirossian, J. D. McClain, M. Motta, B. Mussard, H. Q. Pham, A. Pulkin, W. Purwanto, P. J. Robinson, E. Ronca, E. R. Sayfutyarova, M. Scheurer, H. F. Schurkus, J. E. T. Smith, C. Sun, S.-N. Sun, S. Upadhyay, L. K. Wagner, X. Wang, A. F. White, J. D. Whitfield, M. J. Williamson, S. Wouters, J. Yang, J. M. Yu, T. Zhu, T. C. Berkelbach, S. Sharma, **A. Yu. Sokolov**, and G. K.-L. Chan*. “Recent developments in the PySCF program package.” *J. Chem. Phys.* **153**, 024109 (2020).
- [35] 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. S. 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 III, U. Bozkaya, R. A. King, F. A. Evangelista, J. M. Turney, T. D. Crawford, and C. D. Sherrill*. “PSI4 1.4: Open-source software for high-throughput quantum chemistry.” *J. Chem. Phys.* **152**, 184108 (2020).
- [34] S. Banerjee and **A. Yu. Sokolov***. “Third-order algebraic diagrammatic construction theory for electron attachment and ionization energies: Conventional and Green’s function implementation.” *J. Chem. Phys.* **151**, 224112 (2019).
- [33] K. Chatterjee and **A. Yu. Sokolov***. “Second-order multireference algebraic diagrammatic construction theory for photoelectron spectra of strongly correlated systems.” *J. Chem. Theory Comput.* **15**, 5908–5924 (2019).
- [32] J. K. Bower, **A. Yu. Sokolov**, and S. Zhang*. “Four-coordinate copper halonitrosyl (CuNO)¹⁰ complexes.” *Angew. Chem. Int. Ed.* **58**, 10225–10229 (2019).
- [31] R. Peng, A. V. Copan, and **A. Yu. Sokolov***. “Simulating X-ray absorption spectra with linear-response density cumulant theory.” *J. Phys. Chem. A* **123**, 1840–1850 (2019). (**Highlight: Invited article, “Young Scientists” virtual special issue**).
- [30] **A. Yu. Sokolov***. “Multi-reference algebraic diagrammatic construction theory for excited states: General formulation and first-order implementation.” *J. Chem. Phys.* **149**, 204113 (2018). (**Highlight: JCP Editors’ Pick article**).
- [29] A. V. Copan and **A. Yu. Sokolov***. “Linear-response density cumulant theory for excited electronic states.” *J. Chem. Theory Comput.* **14**, 4097–4108 (2018).

- [28] 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. Evangelista, J. M. Turney, T. D. Crawford, and C. D. Sherrill*. “Psi4 1.1: An open-source electronic structure program emphasizing automation, advanced libraries, and interoperability.” *J. Chem. Theory Comput.* **13**, 3185–3197 (2017).
- [27] **A. Yu. Sokolov***, S. Guo, E. Ronca, and G. K.-L. Chan*. “Time-dependent N-electron valence perturbation theory with matrix product state reference wavefunctions for large active spaces and basis sets: Applications to the chromium dimer and all-trans polyenes.” *J. Chem. Phys.* **146**, 244102 (2017).
- [26] X. Wang, **A. Yu. Sokolov***, J. M. Turney, and H. F. Schaefer*. “Spin-adapted formulation and implementation of density cumulant functional theory with density-fitting approximation: Application to transition metal compounds.” *J. Chem. Theory Comput.* **12**, 4833–4842 (2016).
- [25] **A. Yu. Sokolov*** and G. K.-L. Chan*. “A time-dependent formulation of multi-reference perturbation theory.” *J. Chem. Phys.* **144**, 064102 (2016). (**Highlight: JCP 2016 Editors’ Choice article**).
- [24] J. W. Mullinax, **A. Yu. Sokolov**, and H. F. Schaefer*. “Can density cumulant functional theory describe static correlation effects?” *J. Chem. Theory Comput.* **11**, 2487–2495 (2015).
- [23] **A. Yu. Sokolov*** and G. K.-L. Chan*. “A transformed framework for dynamic correlation in multireference problems.” *J. Chem. Phys.* **142**, 124107 (2015).
- [22] **A. Yu. Sokolov***, H. F. Schaefer, and W. Kutzelnigg. “Density cumulant functional theory from a unitary transformation: N-representability, three-particle correlation effects, and application to O_4^+ .” *J. Chem. Phys.* **141**, 074111 (2014).
- [21] J. W. Mullinax*, **A. Yu. Sokolov**, and H. F. Schaefer. “Conical intersections and low-lying electronic states of tetrafluoroethylene.” *ChemPhysChem* **15**, 2359–2366 (2014).
- [20] A. V. Copan*, **A. Yu. Sokolov**, and H. F. Schaefer. “Benchmark study of density cumulant functional theory: thermochemistry and kinetics.” *J. Chem. Theory Comput.* **10**, 2389–2398 (2014).
- [19] **A. Yu. Sokolov*** and H. F. Schaefer. “Orbital-optimized density cumulant functional theory.” *J. Chem. Phys.* **139**, 204110 (2013).
- [18] **A. Yu. Sokolov***, D. B. Magers, J. I. Wu, W. D. Allen*, P. v. R. Schleyer, and H. F. Schaefer. “Free cyclooctatetraene dianion: planarity, aromaticity, and theoretical challenges.” *J. Chem. Theory Comput.* **9**, 4436–4443 (2013).
- [17] Y. Qiu, **A. Yu. Sokolov**, Y. Yamaguchi, and H. F. Schaefer*. “BeCH₂: the simplest metal carbene. High levels of theory.” *J. Phys. Chem. A* **117**, 9266–9273 (2013).
- [16] S. Vogt-Geisse, **A. Yu. Sokolov**, S. R. McNew, Y. Yamaguchi, and H. F. Schaefer*. “Structures and transition states of Ge₂CH₂.” *J. Phys. Chem. A* **117**, 5765–5774 (2013).

- [15] **A. Yu. Sokolov***, A. C. Simmonett, and H. F. Schaefer. “Density cumulant functional theory: the DC-12 method, an improved description of the one-particle density matrix.” *J. Chem. Phys.* **138**, 024107 (2013).
- [14] **A. Yu. Sokolov***, S. Mittal, A. C. Simmonett, and H. F. Schaefer III. “Characterization of the t-butyl radical and its elusive anion.” *J. Chem. Theory Comput.* **8**, 4323–4329 (2012).
- [13] **A. Yu. Sokolov***, J. J. Wilke, A. C. Simmonett, and H. F. Schaefer III. “Analytic gradients for density cumulant functional theory: the DCFT-06 model.” *J. Chem. Phys.* **137**, 054105 (2012).
- [12] **A. Yu. Sokolov*** and H. F. Schaefer III. “Ground and excited state properties of photoactive platinum(IV) diazido complexes: theoretical considerations.” *Dalton Trans.* **40**, 7571–7582 (2011).
- [11] **A. Yu. Sokolov*** and H. F. Schaefer III. “Coordination properties of bridging diazene ligands in unusual diiron complexes.” *Organometallics* **29**, 3271–3280 (2010).
- [10] **A. Yu. Sokolov** and O. V. Sizova*. “Quantum-chemical study of trans-influence in gold(I) linear complexes.” *Russ. J. Gen. Chem.* **80**, 1223–1231 (2010).
- [9] V. V. Pakal’nis*, **A. Yu. Sokolov**, A. A. Slisenko, M. E. Borovitev, S. P. Tunik, and O. V. Sizova. “Synthesis and spectral characteristics of a novel heterometallic binuclear complex on the basis of 3,6-bis(2-pyridyl)-1,2,4,5-tetrazine.” *Russ. J. Gen. Chem.* **79**, 980–984 (2009).
- [8] O. V. Sizova*, L. V. Skripnikov, **A. Yu. Sokolov**, and V. V. Sizov. “Atomic-orbital-symmetry based σ -, π -, and δ -decomposition analysis of bond orders.” *Int. J. Quant. Chem.* **109**, 2581–2590 (2009).
- [7] O. V. Sizova*, L. V. Skripnikov, and **A. Yu. Sokolov**. “Calculation of σ -, π -, and δ -components of quantum-chemical bond orders.” *Russ. J. Gen. Chem.* **78**, 2146–2147 (2008).
- [6] O. V. Sizova*, L. V. Skripnikov, and **A. Yu. Sokolov**. “Symmetry decomposition of quantum-chemical bond orders.” *J. Mol. Struct. (THEOCHEM)* **870**, 1–9 (2008).
- [5] **A. Yu. Sokolov**, N. J. Stibrich, and H. F. Schaefer* III. “BO₃ molecular structures: examples of the importance of electron correlation.” *Coll. Czech. Chem. Commun.* **73**, 1495–1508 (2008).
- [4] O. V. Sizova*, **A. Yu. Sokolov**, and L. V. Skripnikov. “Quantum-chemical study of donor-acceptor interactions in chelate dicarbonyl complexes of rhodium(I).” *Russ. J. Coord. Chem.* **33**, 800–808 (2007).
- [3] O. V. Sizova*, **A. Yu. Sokolov**, L. V. Skripnikov, and V. I. Baranovski. “Quantum chemical study of the bond orders in the ruthenium, diruthenium and dirhodium nitrosyl complexes.” *Polyhedron* **26**, 4680–4690 (2007).
- [2] O. V. Sizova*, L. V. Skripnikov, **A. Yu. Sokolov**, and N. V. Ivanova. “Rhodium and ruthenium tetracarboxylate nitrosyl complexes: electronic structure and metal-metal bond.” *Russ. J. Coord. Chem.* **33**, 588–593 (2007).
- [1] O. V. Sizova*, L. V. Skripnikov, **A. Yu. Sokolov**, and O. O. Lyubimova. “Features of the electronic structure of ruthenium tetracarboxylates with axially coordinated nitric oxide (II).” *J. Struct. Chem.* **48**, 28–36 (2007).

INVITED CONFERENCE PRESENTATIONS

- 06/2025 | WATOC 2025 Congress, Oslo (Norway)
- 06/2025 | Symposium “Frontiers in Quantum Chemistry”, Ottawa (Canada)
- 06/2023 | Conference “Quantum International Frontiers”, Lodz (Poland)
- 06/2023 | Symposium “Advances in Theoretical and Computational Chemistry”, Vancouver (Canada)
- 04/2023 | Workshop on Excited-State Methodologies, Toulouse (France)
- 03/2023 | COMP Awards Symposium, ACS National Meeting, Indianapolis, IN (USA)
- 06/2022 | 10th Molecular Quantum Mechanics (MQM) Congress, Blacksburg, VA (USA)
- 06/2022 | International Workshop on Reduced Density Matrix Theory for Quantum Many-Fermion Systems, San Sebastian (Spain)
- 02/2022 | Sanibel Symposium, St. Simon’s Island, GA (USA)
- 12/2021 | Symposium “Computational Quantum Chemistry: Synergism Between Theory and Experiment” (virtual), Pacificchem 2020, Honolulu, HI (USA)
- 07/2021 | Workshop “New Developments in Coupled-Cluster Theory” (virtual), Telluride, CO (USA)
- 06/2021 | Conference “New Frontiers in Electron Correlation” (virtual), Telluride, CO (USA)
- 06/2020 | Conference “Low-scaling and Unconventional Electronic Structure Techniques” (LUEST) (virtual), Telluride, CO (USA)
- 08/2019 | Symposium “Computational Quantum Chemistry: From Promise to Prominence”, 258th ACS National Meeting, San Diego, CA (USA)
- 07/2019 | 32nd Midwest Undergraduate Computational Chemistry Consortium Conference, Columbus, OH (USA)
- 06/2019 | Workshop “Fundamental Challenges of Electron-Density-Based Approaches to Time-Dependent Processes and Open Quantum Systems”, ETH Zürich (Switzerland)
- 03/2019 | Symposium “Quantum Mechanics: Strong Correlation”, 257th ACS National Meeting, Orlando, FL (USA)
- 11/2018 | Psi4 Annual Developer’s Conference (PsiCon), Atlanta, GA (USA)
- 06/2018 | 50th Midwest Theoretical Chemistry Conference, Chicago, IL (USA)
- 08/2017 | Workshop “New Developments in Coupled-Cluster Theory”, Telluride, CO (USA)
- 05/2017 | Symposium “Electronic Structure Theory”, 100th Canadian Chemistry Conference, Toronto (Canada)
- 04/2017 | Symposium “Strong Electron Correlation & Nonadiabatic Dynamics”, 253rd ACS National Meeting, San Francisco, CA (USA)

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| 08/2016 | Symposium “Metal & Semiconductor Nanoclusters with Atomic Precision: Fundamentals & Applications”, <i>ACS Physical Chemistry Division Postdoctoral Award Talk</i> , 252 nd ACS National Meeting, Philadelphia, PA (USA) |
| 06/2016 | 8 th Molecular Quantum Mechanics (MQM) Congress, Uppsala University, Uppsala (Sweden) |
| 03/2016 | Symposium “Towards Predictive Calculations in Strongly Correlated Molecules and Materials”, 251 st ACS National Meeting, San Diego, CA (USA) |
| 08/2015 | Workshop on Quantum Marginals and Numerical Ranges, University of Guelph, Guelph (Canada) |
| 05/2014 | Annual Meeting of the Southeast Theoretical Chemistry Association (SETCA 2014), Atlanta, GA (USA) |
| 09/2013 | Quantum Mechanics in Many Dimensions, 246 th ACS National Meeting, Indianapolis, IN (USA) |

INVITED SEMINARS

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| 02/2024 | Stuttgart University, Stuttgart (Germany) |
| 01/2024 | Heidelberg University, Heidelberg (Germany) |
| 10/2023 | Akron University, Akron, OH (USA) |
| 10/2022 | John’s Hopkins University, Baltimore, MD (USA) |
| 10/2022 | Northeastern University, Boston, MA (USA) |
| 04/2022 | Emory University, Atlanta, GA (USA) |
| 04/2022 | University of Michigan, Ann Arbor, MI (USA) |
| 04/2022 | University of Washington, Seattle, WA (USA) |
| 03/2022 | University of California, Berkeley, CA (USA) |
| 02/2022 | University of Florida, Gainesville, FL (USA) |
| 02/2022 | Florida State University, Tallahassee, FL (USA) |
| 01/2022 | University of Chicago, Chicago, IL (USA) |

STUDENTS AND POSTDOCS SUPERVISED

Graduate students:

- Pallavi Panthakkal Das (2024 – present)
- Lakshan Weerasinghe (2024 – present)
- Haden Dickerson (2024 – present)
- Nicholas Chiang (2023 – present)

- James Serna (2023 – present)
- Donna Odhiambo (2022 – present)
- Abdelrahman Ahmed (2020 – present)
- Rajat Majumder (Ph.D., 2024)
- Terrence Stahl (Ph.D., 2024)
- Ilia Mazin (Ph.D., 2023)
- Samraghi Banerjee (Ph.D., 2022)

Undergraduate students:

- Xinyu Liu (2024 – present)
- Bryce Pickett (2023 – present)
- Guowei (Peter) Qu (2022 – 2024)
- Mallard Woodward (B.S., 2024)
- Yichen Fan (B.S., 2021)
- Ruoqing Peng (B.S., 2019)

Postdocs:

- Carlos Eduardo Vieira de Moura (2021 – 2023)
- Koushik Chatterjee (2018 – 2020)

TEACHING EXPERIENCE

Since 2023 | Quantum Mechanics and Spectroscopy (CHEM 6510), *Instructor*, OSU

Since 2019 | Physical Chemistry I (CHEM 4300), *Instructor*, OSU

2018 – 2021 | Advanced Quantum Mechanics and Spectroscopy (CHEM 7520), *Instructor*, OSU

2011 – 2014 | Advanced Quantum Chemistry (CHEM 8950), *Teaching Assistant*, UGA

2011, 2012 | Summer Undergraduate Fellowship Program, *Instructor and Mentor*, Center for Computational Quantum Chemistry, UGA

PROFESSIONAL SERVICE (EXTERNAL)

- Co-organizer, National ACS Meeting Symposium “Quantum Chemistry: Current and Future Frontiers”, Chicago, IL, USA (08/2022)
- Co-organizer, Midwest Theoretical Chemistry Conference, Columbus, OH, USA (06/2022)
- Reviewer for the funding agencies and computing facilities (2017 – present): National Science Foundation, Department of Energy, American Chemical Society Petroleum Research Fund, German Research Foundation, Swiss National Science Foundation, The Ohio Supercomputer Center

- Reviewer for the scientific journals (2014 – present): Journal of Chemical Theory and Computation, Journal of Chemical Physics, Journal of American Chemical Society, Journal of Physical Chemistry Letters, Journal of Physical Chemistry A, Physical Chemistry Chemical Physics, Dalton Transactions, International Journal of Quantum Chemistry, WIREs Computational Molecular Science, Theoretical Chemistry Accounts, New Journal of Chemistry, Acta Physica Polonica A

PROFESSIONAL SERVICE (OSU)

- Coordinator, Physical Chemistry Seminar Series (2020 – present)
- Graduate Student Admissions Committee (2019 – present)
- Center for Quantum Information Science and Engineering Advisory Board (2022 – 2024)
- Physical Division Faculty Search Committee (2023 – 2024)
- Temporary Advisor for the First-Year Graduate Students (2020 – 2022)
- Graduate Student Recruitment Committee (2018 – 2019)

PROFESSIONAL ORGANIZATIONS

- Member, Center for Quantum Information Science and Engineering (since 2022)
- Member, PySCF Board of Directors (since 2019)
- Member, Institute for Optical Science, OSU, Columbus, OH, USA (since 2019)
- Member of the COMP and PHYS divisions of American Chemical Society (since 2012, member # 30196915)

RESEARCH FUNDING

- “Flexible Embedding Framework for Efficient and Accurate Spectroscopic Simulations of Crystalline Defects With Applications in Quantum Science”, NMS Exploratory Grant Program, \$48,000 (1/2024 – 12/2024).
- “Efficient and Reliable Electronic Structure Theories for Spectroscopic Properties of Strongly Correlated Systems”, National Science Foundation CAREER Award, \$650,000 (5/2021 – 4/2026).
- “Elucidating Spectroscopic Properties of Heterogeneous Transition Metal Oxide Catalysts with Accurate Electronic Structure Theory”, American Chemical Society Petroleum Research Fund, \$110,000 (9/2022 – 8/2024).
- “Creating quantum bits based on rare-earth ions for quantum networking”, The Ohio State University President’s Research Excellence Program, \$200,000, (1/2022 – 12/2023). Co-PI with Ronald M. Reano, Daniel Gauthier, Ezekiel Johnston-Halperin, Roland Kawakami, Gregory Lafyatis.