
CONTACT INFORMATION	Virginia Commonwealth University Department of Chemistry 3046 Oliver Hall Richmond, VA 23284	Tel: (804) 828-3071 laoku@vcu.edu Google Scholar Group Website
RESEARCH INTERESTS	Developing novel methodologies to accelerate quantum chemistry calculations via <ul style="list-style-type: none">◦ Grassmannians◦ Fragmentation◦ Machine Learning Exploring noncovalent interactions in large and/or complex systems	
CAREER HISTORY	Associate Professor, Virginia Commonwealth University (2025–present) Assistant Professor, Virginia Commonwealth University (2019–2025) <ul style="list-style-type: none">◦ Department of Chemistry Member <ul style="list-style-type: none">◦ VCU Center for Drug Discovery (2024–present)◦ VCU Institute for Sustainable Energy and Environment (2022–present) Postdoctoral Associate, Cornell University (2016–2019) <ul style="list-style-type: none">◦ Department of Chemistry and Chemical Biology◦ Advisor: Professor Robert A. DiStasio Jr.	
EDUCATION	Ph.D., The Ohio State University , Columbus, OH (2011–2016) <ul style="list-style-type: none">◦ Advisor: Professor John M. Herbert◦ Thesis: <i>Accurate and Efficient Quantum Chemistry Calculations for Noncovalent Interactions in Many-Body Systems</i>◦ GPA: 4.0/4.0 M.S., National Tsing Hua University , Hsinchu, Taiwan (2007–2009) <ul style="list-style-type: none">◦ Advisor: Professor Chin-Hui Yu◦ Thesis: <i>A Computational Study of Neutral Low Barrier Hydrogen Bonds: The Effect of Water Molecules and Peptide Bonds</i> B.S., National Tsing Hua University , Hsinchu, Taiwan (2003–2007) <ul style="list-style-type: none">◦ Chemistry major and Physics minor (Ranking: 1st/56, 3.95 GPA)	
AWARDS AND HONORS	<ul style="list-style-type: none">◦ 2026 JSPS Invitational Research Fellowship (Japan Society for the Promotion of Science)◦ 2025 Emerging Investigator (<i>The Journal of Chemical Physics</i>)◦ 2025 VCU National/International Recognition Award (NIRA)◦ 2025 VCU Outstanding Early Career Faculty Award◦ 2025 VCU ISEE Travel Grant◦ 2025 ACS COMP Division OpenEye Cadence Molecular Sciences Outstanding Junior Faculty Award◦ 2025 VCU CHS Excellence in Scholarship Award	

- 2025 Sanibel Symposium Young Investigator Award (University of Florida's Quantum Theory Project)
- 2025 Editors' Choice (*The Journal of Chemical Physics*, 2024)
- 2025 NSF CAREER Award
- 2024 Emerging Investigator (*The Journal of Chemical Physics*)
- 2024 Editors' Choice (*The Journal of Chemical Physics*, 2023)
- 2023 Emerging Investigator (*The Journal of Chemical Physics*)
- 2020 ACS Petroleum Research Fund Doctoral New Investigator Award
- 2019 Macau Excellent Talents Award Scheme (Macau Foundation)
- 2019 Top Ten Outstanding Chinese American Youth Award
- 2019 PCTC Postdoctoral Fellow Award (Penn Conference in Theoretical Chemistry)
- 2018 ACS COMP Division Wiley Computers in Chemistry Outstanding Postdoc Award
- 2016 1st place oral award in Mathematical and Physical Sciences area at The 30th Edward F. Hayes Graduate Research Forum (The Ohio State University)
- 2015 Phi Tau Phi (PTP) Mid-America Scholarship Award
- 2015 ACS COMP Division Chemical Computing Group Excellence Award for Graduate Students
- 2015 Presidential Fellowship Award (The Ohio State University)
- 2015 1st place award in Albert L. Henne Research Competition (The Ohio State University)
- 2013 Funding for attending the Telluride School of Theoretical Chemistry (Telluride Science Research Center)
- 2009–2012 Postgraduate Scholarships for Ph.D. (Macau Tertiary Education Services Office)
- 2009 The President's Scholarship (National Tsing Hua University)
- 2007–2009 Postgraduate Scholarships for Master (Macau Tertiary Education Services Office)
- 2007 Chemistry Department Fellowship (National Tsing Hua University)
- 2007 Visiting Scholarship to Texas A&M University
- 2007 Dr. I-Chi Mei Memorial Medal (highest honor to a graduate for achievement in both academic work and campus activities at National Tsing Hua University)
- 2007 Honorary member of Phi Tau Phi Scholastic Honor Society (Taiwan)
- 2006 Selected to attend Nobel Science Camp in The Conference of Trends in Chemical Dynamics: From Small Molecules to Biomolecules (Taiwan)
- 2006 Senior Student Research Grant (National Science Council of Taiwan 95-2815-C007-002)
- 2006 Ministry of Education Scholarship (Ministry of Education, Taiwan)
- 2006 The Zhu Shun Yi He Qin Scholarship (ZyXEL Communications Corp.)
- 2006 Overseas Chinese Association Scholarship (Overseas Chinese Association, Taiwan)

- 2005–2006 The Guangdong Association Scholarship (The Guangdong Association of Taipei)
- 2005–2006 UMC Scholarship (United Microelectronics Corp.)
- 2005 TASC0 Chemical Corporation Scholarship (TASC0 Chemical Corp.)
- 2005 Selected as “The Chun-Tsung Scholar” to Peking University
- 2004–2006 The College of Science Young Elite Scholarship (National Tsing Hua University)
- 2004–2007 The Overseas Student Scholarship (Overseas Community Affairs Council, Taiwan)
- 2003–2007 The Academic Achievement Award (given to students in the top 2%; received for seven consecutive semesters at National Tsing Hua University)
- 2003–2007 Higher Education Scholarships (Macau Education and Youth Affairs Bureau)

EXTERNAL
FUNDING

Secured 7 External Funding Awards Totaling \$2.6 Million

- 2025–2029 CAREER: Integrating Grassmannians with electronic structure theory for next-generation quantum chemistry. NSF CAREER, CTMC program. \$653,043. Single PI (CHE-2441101).
- 2025–2027 Understanding the impact of conformational isomerism on ultra-fast molecular dynamics. NSF-CHE, CSD program. \$480,000. Co-PI (CHE-2426037).
- 2023–2026 Equipment: MRI: Track 1 Acquisition of NVIDIA DGX H100 GPU system for research and education at VCU. NSF-OAC, MRI program. \$299,621. Co-PI (OAC-2316003).
- 2022–2026 CAS: Bimetallic transition metal phosphide nanostructures as high-efficiency, earth-abundant, and durable catalysts for electrochemical water splitting. NSF-CHE, CAT program. \$429,412. Co-PI (CHE-2154747).
- 2022–2026 Low-dimensional Si-Sn and Si-Ge-Sn nanoalloys as high-efficiency, direct-gap nanostructures for visible to infrared optoelectronics. NSF-DMR, EPM program. \$499,912. Co-PI (DMR-2211606).
- 2020–2024 Understanding and controlling the aggregation behavior of petroleum asphaltenes. ACS Petroleum Research Fund (Doctoral New Investigator Grant). \$110,000. Single PI (61654-DNI6).
- 2019–2020 Huge-memory nodes with ultra-fast solid-state drives for high-performance computing. Higher Education Equipment Trust Fund (HEETF). \$117,000. Single PI.

INTERNAL
FUNDING

- 2026 Advancing drug discovery through quantum-chemically accurate machine learning potentials. The VCU College of Humanities and Sciences Dean’s Research Grant. \$3,225. Single PI.
- 2024–2026 Direct-gap group IV alloy quantum dots as low-cost and high-efficiency nanostructures for generation-III photovoltaics. The VCU Breakthroughs Fund. \$200,000. Co-PI.

- 2024–2025 Grassmannian-augmented strategies for accelerated materials design. The VCU College of Humanities and Sciences Seed Awards program. \$5,000. Single PI.
- 2023–2024 First-principles quantum-crystallographic X-ray structure refinement. The VCU College of Humanities and Sciences Seed Awards program. \$5,000. Single PI.
- 2021–2022 Bimetallic transition metal phosphide nanostructures as high-efficiency earth abundant catalysts for electrochemical water splitting. The VCU Presidential Research Quest Fund (PeRQ). \$50,000. Co-PI.
- 2020 Enhanced drug design through robust quantum chemistry calculation and machine learning. VCU Honors Summer Undergraduate Research Program (HSURP). \$3,100. Single PI.

PUBLICATIONS ***h*-index = 33, total citations = 8,606**; 13 papers with ≥ 100 citations
72 publications (source: [Google Scholar](#))

39 Independently Published Papers at VCU + 3 in Review
6 Co-Authored with Undergraduates
*corresponding author, undergraduate student^U

75. K. Wickramasinghe and **K. U. Lao***. Grassmann-DIIS extrapolation for accelerating two-dimensional potential energy surface scans. *Chem. Phys. Lett.* **in review**, (2026).
74. X. Ma, B. Huang, J. Zhu, **K. U. Lao**, and L.-H. Cai. Injectable antifibrotic bottlebrush hydrogels from unexpected architecture-driven supramolecular assembly. *Mater. Horiz.* **in review**, (2026).
73. Z. Song and **K. U. Lao***. Accelerating geometry optimization via Grassmann-DIIS extrapolation. *Phys. Chem. Chem. Phys.* **in revision**, (2026). [Themed collection: PCCP 2025 Emerging Investigators]
72. **K. U. Lao***. [Benchmarking nanoscale noncovalent complexes at the two-hundred-atom scale with converged local CCSD\(T\)](#). *J. Phys. Chem. A* **130**, 4136 (2026). [Special issue: Steve Scheiner Festschrift VSI, [Featured on cover](#)]
71. M. K. Alam, D. Wang, J. Baker, **K. U. Lao**, and I. U. Arachchige. [Crystal structure and morphology-controlled synthesis of \$\text{Co}_{1-x}\text{Mn}_x\text{P}\$ nanocrystals and their composition-dependent electrocatalytic activity for hydrogen evolution reaction](#). *ACS Appl. Mater. Interfaces* **18**, 28612 (2026).
70. J. Saunier, Z. A. Christensen, K. A. Mason, **K. U. Lao**, and M. S. El-Shall. [Water-mediated isomerization in the stepwise hydration of the nitrobenzene radical cation with 1–6 water molecules](#). *J. Phys. Chem. A* **130**, 2968 (2026). [Special issue: Michael A. Duncan Festschrift VSI, [Featured on cover](#)]
69. **K. U. Lao***, K. Wickramasinghe, and J. A. Tan. [Grassmann extrapolation via direct inversion in the iterative subspace](#). *J. Chem. Phys.* **163**, 144114 (2025). [2025 JCP Emerging Investigators Special Collection]

68. **K. U. Lao*** and D. Wang. [Accurate and rapid ranking of protein–ligand binding affinities using density matrix fragmentation and physics-informed machine learning dispersion potentials](#). *ChemPhysChem* **26**, e202500094 (2025). [Special issue: Physical Chemistry in North America]
67. J. Baker, D. Wang, M. K. Alam, **K. U. Lao**, and I. U. Arachchige. [Dopant-induced hexagonal to orthorhombic phase transition in \$\text{Fe}_{2-x}\text{Mo}_x\text{P}\$ nanorods and its influence on the electrocatalytic hydrogen evolution reaction](#). *Chem. Mater.* **37**, 3260 (2025).
66. G. C. Spence, D. S. Pate, C. Villot, R. M. Fouzie, L. S. Graves, **K. U. Lao**, U. Özgür, and I. U. Arachchige. [Solid-state synthesis of \$\text{Si}_{1-x}\text{Ge}_x\$ nanoalloys with composition-tunable energy gaps and visible to near infrared optical properties](#). *Nanoscale* **17**, 3306 (2025).
65. E. Britt, H. A. L. Peña, J. M. Shusterman, K. Sangroula,^U **K. U. Lao**, and K. M. Tibbetts. [Ultrafast dissociation dynamics of the sensitive explosive ethylene glycol dinitrate](#). *J. Phys. Chem. Lett.* **16**, 882 (2025).
64. **K. U. Lao***. [Accurate computation of gas binding in the nanoscale porous organic cage CC3 via coupled cluster theory](#). *Nanotechnology* **36**, 095704 (2025). [Special issue: Focus on Virginia Commonwealth University (VCU)]
63. **K. U. Lao***. [Canonical coupled cluster binding benchmark for nanoscale non-covalent complexes at the hundred-atom scale](#). *J. Chem. Phys.* **161**, 234103 (2024). [Selected as a “JCP and CPR Editors’ Choice 2024”, Selected in 2024 JCP Emerging Investigators Special Collection, Selected as a Featured Article, and Highlighted on the JCP Homepage]
62. P. Sutton, J. Saunier, K. A. Mason, A. C. Percy, **K. U. Lao**, and M. S. El-Shall. [Formation of complex organics by covalent and non-covalent interactions of the sequential reactions of 1-4 acrylonitrile molecules with the benzonitrile radical cation](#). *Phys. Chem. Chem. Phys.* **26**, 29708 (2024). [Featured on cover]
61. P. Sutton, J. Saunier, **K. U. Lao**, and M. S. El-Shall. [Sequential reactions of acetylene with the benzonitrile radical cation: New insights into structures and rate coefficients of the covalent ion products](#). *J. Phys. Chem. Lett.* **15**, 11067 (2024). [Featured on cover]
60. L. S. Graves, R. Sarkar, J. Baker, **K. U. Lao**, and I. U. Arachchige. [Structure- and morphology-controlled synthesis of hexagonal \$\text{Ni}_{2-x}\text{Zn}_x\text{P}\$ nanocrystals and their composition-dependent electrocatalytic activity for hydrogen evolution reaction](#). *ACS Appl. Energy Mater.* **7**, 5679 (2024).
59. C. Villot and **K. U. Lao***. [Accurate and efficient prediction of optical gaps in silicon and germanium nanoparticles using a high-local-exchange density functional](#). *Chem. Phys. Lett.* **850**, 141460 (2024).
58. **K. U. Lao*** and C. Villot. [Improving second-order Møller–Plesset perturbation theory for noncovalent interactions with the machine learning-corrected *ab initio* dispersion potential](#). *J. Chem. Phys.* **160**, 184108 (2024). [Selected in 2024 JCP Emerging Investigators Special Collection]

57. C. Villot and **K. U. Lao***. *Ab initio* dispersion potentials based on physics-based functional forms with machine learning. *J. Chem. Phys.* **160**, 184103 (2024). [Selected in 2024 JCP Emerging Investigators Special Collection, Selected as a JCP Editor's Pick, Highlighted on the JCP Homepage, and the model is freely available on [GitHub](#)]
56. H. A. L. Peña, J. M. Shusterman, C. Dalkiewicz,^U S. L. McPherson, C. Dunstan,^U K. Sangroula,^U **K. U. Lao**, and K. M. Tibbetts. Photodissociation dynamics of the highly stable *ortho*-nitroaniline cation. *J. Phys. Chem. A* **128**, 1634 (2024).
55. J. Chen, M. R. Ahasan, J.-S. Oh, J. A. Tan, S. Hennessey,^U M. M. Kaid, H. M. El-Kaderi, L. Zhou, **K. U. Lao**, R. Wang, and W.-N. Wang. Highly efficient CO₂ electrochemical reduction on dual metal (Co-Ni)-nitrogen sites. *J. Mater. Chem. A* **12**, 4601 (2024).
54. F. Ballesteros and **K. U. Lao***. Analysis of two overlapping fragmentation approaches in density matrix construction: GMBE-DM vs. ADMA. *Phys. Chem. Chem. Phys.* **26**, 4386 (2024).
53. J. A. Tan and **K. U. Lao***. Mapping spin contamination-free potential energy surfaces using restricted open-shell methods with Grassmannians. *Phys. Chem. Chem. Phys.* **26**, 1436 (2024).
52. D. Spera, D. Pate, G. C. Spence, C. Villot, C. J. Onukwughara, D. White, **K. U. Lao**, U. Özgür, and I. U. Arachchige. Colloidal synthesis of homogeneous Ge_{1-x-y}Si_ySn_x nanoalloys with composition-tunable visible to near IR optical properties. *Chem. Mater.* **35**, 9007 (2023).
51. L. S. Graves, R. Sarkar, **K. U. Lao**, and I. U. Arachchige. Composition-dependent electrocatalytic activity of Zn-doped Ni₅P₄ nanocrystals for the hydrogen evolution reaction. *Chem. Mater.* **35**, 6966 (2023).
50. F. Ballesteros, J. A. Tan, and **K. U. Lao***. An accurate and efficient fragmentation approach via the generalized many-body expansion for density matrices. *J. Chem. Phys.* **159**, 074107 (2023). [Selected as a "JCP Editor's Choice 2023", Selected in 2023 JCP Emerging Investigators Special Collection, Selected as a JCP Editor's Pick, and Highlighted on the JCP Homepage]
49. C. Villot, T. Huang,^U and **K. U. Lao***. Accurate prediction of global-density-dependent range-separation parameters based on machine learning. *J. Chem. Phys.* **159**, 044103 (2023). [The model is freely available on [GitHub](#)]
48. J. A. Tan and **K. U. Lao***. The Grassmann interpolation method for spin-unrestricted open-shell systems. *J. Chem. Phys.* **158**, 214104 (2023).
47. C. Villot and **K. U. Lao***. Electronic structure theory on modeling short-range noncovalent interactions between amino acids. *J. Chem. Phys.* **158**, 094301 (2023).
46. J. A. Tan and **K. U. Lao***. Generating accurate density matrices on the tangent space of a Grassmann manifold. *J. Chem. Phys.* **158**, 051101 (2023).

45. W. Li, D. Wang, **K. U. Lao**^{*}, and X. Wang. [Inclusion complexation of *S*-nitrosoglutathione for sustained nitric oxide release from catheter surfaces: A strategy to prevent and treat device-associated infections.](#) *ACS Biomater. Sci. Eng.* **9**, 1694 (2023). [Featured on cover]
44. K. C. Ng, T. Adel, **K. U. Lao**, M. Varmecky, Z. Liu, M. Arrad, and H. C. Allen. [Iron \(III\) chloro complexation at the air-aqueous FeCl₃ interface via second harmonic generation spectroscopy.](#) *J. Phys. Chem. C* **126**, 15386 (2022).
43. C. Villot, F. Ballesteros, D. Wang, and **K. U. Lao**^{*}. [Coupled cluster benchmarking of large noncovalent complexes in L7 and S12L as well as the C₆₀ dimer, DNA–ellipticine, and HIV–indinavir.](#) *J. Phys. Chem. A* **126**, 4326 (2022). [Featured on cover, Selected for Inclusion in the Collection “Celebrating 25 Years of Scientific Discoveries in Physical Chemistry Supported by the ACS Petroleum Research Fund”]
42. H. A. L. Peña, J. M. Shusterman, D. A. Boateng, **K. U. Lao**, and K. M. Tibbetts. [Coherent control of molecular dissociation by selective excitation of nuclear wave packets.](#) *Front. Chem.* **10**, 859095 (2022).
41. M. D. Word, H. A. L. Peña, D. A. Boateng, S. L. McPherson, G. L. Gutsev, L. G. Gutsev, **K. U. Lao**, and K. M. Tibbetts. [Ultrafast dynamics of nitro-nitrite rearrangement and dissociation in nitromethane cation.](#) *J. Phys. Chem. A* **126**, 879 (2022).
40. F. Ballesteros and **K. U. Lao**^{*}. [Accelerating the convergence of self-consistent field calculations using the many-body expansion.](#) *J. Chem. Theory Comput.* **18**, 179 (2022).
39. W. Li, D. Wang, **K. U. Lao**, and X. Wang. [Buffer concentration dramatically affects the stability of *S*-nitrosothiol in aqueous solutions.](#) *Nitric Oxide* **118**, 59 (2022).
38. K. Carter-Fenk, **K. U. Lao**, and J. M. Herbert. [Predicting and understanding noncovalent interactions using novel forms of symmetry-adapted perturbation theory.](#) *Acc. Chem. Res.* **54**, 3679 (2021).
37. E. Epifanovsky *et al.* [Software for the frontiers of quantum chemistry: An overview of developments in the Q-Chem 5 package.](#) *J. Chem. Phys.* **155**, 084801 (2021).
36. F. Ballesteros, [S. Dunivan](#)^U, and **K. U. Lao**^{*}. [Coupled cluster benchmarks of large noncovalent complexes: The L7 dataset as well as DNA-ellipticine and buckycatcher-fullerene.](#) *J. Chem. Phys.* **154**, 154104 (2021).
35. M. K. Shehab, K. S. Weeraratne, [T. Huang](#)^U, **K. U. Lao**, and H. M. El-Kaderi. [Exceptional sodium-ion storage by aza-covalent organic framework for high energy and power destiny sodium-ion batteries.](#) *ACS Appl. Mater. Interfaces* **13**, 15083 (2021).

34. K. A. Mason, A. C. Percy, **K. U. Lao**, Z. A. Christensen, and M. S. El-Shall. [Non-covalent interactions of hydrogen cyanide and acetonitrile with the quinoline radical cation via ionic hydrogen bonding](#). *Chem. Phys. Lett.* **754**, 137744 (2020).

Postdoc and Graduate Work

33. Z. M. Sparrow, B. G. Ernst, P. T. Joo, **K. U. Lao**, and R. A. DiStasio Jr. [NENCI-2021 part I: A large benchmark database of non-equilibrium non-covalent interactions emphasizing close intermolecular contacts](#). *J. Chem. Phys.* **155**, 184303 (2021). [Selected as a Feature Article, Highlighted on the JCP Homepage, [Featured on cover](#), and selected as an “Editor’s Choice for 2021”]
32. **K. U. Lao**, Y. Yang, and R. A. DiStasio Jr. [Electron confinement meet electron delocalization: Non-additivity and finite-size effects in the polarizabilities and dispersion coefficients of the fullerenes](#). *Phys. Chem. Chem. Phys.* **23**, 5773 (2021). [Selected as a [2021 PCCP HOT Article](#)]
31. B. G. Ernst, **K. U. Lao**, A. G. Sullivan, and R. A. DiStasio Jr. [Attracting opposites: Promiscuous ion- \$\pi\$ binding in the nucleobases](#). *J. Phys. Chem. A* **124**, 4128 (2020).
30. T. Suh, Y. Yang, P. Zhao, **K. U. Lao**, H.-Y. Ko, J. Wong, R. A. DiStasio Jr., and J. R. Engstrom. [Competitive adsorption as a route to area-selective deposition](#). *ACS Appl. Mater. Interfaces* **12**, 9989 (2020).
29. Y. Yang, **K. U. Lao**, D. M. Wilkins, A. Grisafi, M. Ceriotti, and R. A. DiStasio Jr. [Quantum mechanical static dipole polarizabilities in the QM7b and AlphaML showcase databases](#). *Sci. Data* **6**, 152 (2019).
28. K. Carter-Fenk, **K. U. Lao**, K.-Y. Liu, and J. M. Herbert. [Accurate and efficient *ab initio* calculations for supramolecular complexes: Symmetry-adapted perturbation theory with many-body dispersion](#). *J. Phys. Chem. Lett.* **10**, 2706 (2019).
27. D. M. Wilkins, A. Grisafi, Y. Yang, **K. U. Lao**, R. A. DiStasio Jr., and M. Ceriotti. [Accurate molecular polarizabilities with coupled-cluster theory and machine learning](#). *Proc. Natl. Acad. Sci. USA* **116**, 3401 (2019).
26. Y. Yang, **K. U. Lao**, and R. A. DiStasio Jr. [Influence of pore size on the van der Waals interaction in two-dimensional molecules and materials](#). *Phys. Rev. Lett.* **122**, 026001 (2019). (Also read: [Cornell Chronicle feature](#); [Phys.org](#))
25. **K. U. Lao**, J. Jia, R. Maitra, and R. A. DiStasio Jr. [On the geometric dependence of the molecular dipole polarizability in water: A benchmark study of higher-order electron correlation, basis set incompleteness error, core electron effects, and zero-point vibrational contributions](#). *J. Chem. Phys.* **149**, 204303 (2018). [Selected as a Feature Article, Highlighted on the JCP Homepage, and [Featured on cover](#)]
24. **K. U. Lao** and J. M. Herbert. [A simple correction for nonadditive dispersion within extended symmetry-adapted perturbation theory \(XSAPT\)](#). *J. Chem. Theory Comput.* **14**, 5128 (2018).

23. X. Yu, J. Jia, S. Xu, **K. U. Lao**, M. J. Sanford, R. K. Ramakrishnan, S. I. Nazarenko, T. R. Hoye, G. W. Coates, and R. A. DiStasio Jr. [Unraveling substituent effects on the glass transition temperatures of biorenewable polyesters](#). *Nat. Commun.* **9**, 2880 (2018).
22. **K. U. Lao** and J. M. Herbert. [Atomic orbital implementation of extended symmetry-adapted perturbation theory \(XSAPT\) and benchmark calculations for large supramolecular complexes](#). *J. Chem. Theory Comput.* **14**, 2955 (2018).
21. S. Xie, L. Tu, Y. Han, L. Huang, K. Kang, **K. U. Lao**, P. Poddar, C. Park, D. A. Muller, R. A. DiStasio Jr., and J. Park. [Coherent atomically-thin superlattices with engineered strain](#). *Science* **359**, 1131 (2018). (Also read: [Cornell Chronicle feature](#); [Inverse feature](#); [ZME Science](#))
20. **K. U. Lao**, K.-Y. Liu, R. M. Richard, and J. M. Herbert. [Understanding the many-body expansion for large systems. II. Accuracy considerations](#). *J. Chem. Phys.* **144**, 164105 (2016). [Selected as a JCP Editors' Pick and Highlighted on the JCP Homepage]
19. **K. U. Lao** and J. M. Herbert. [Energy decomposition analysis with a stable charge-transfer term for interpreting intermolecular interactions](#). *J. Chem. Theory Comput.* **12**, 2569 (2016).
18. **K. U. Lao**, R. Schäffer, G. Jansen, and J. M. Herbert. [Accurate description of intermolecular interactions involving ions using symmetry-adapted perturbation theory](#). *J. Chem. Theory Comput.* **11**, 2473 (2015).
17. **K. U. Lao** and J. M. Herbert. [Accurate and efficient quantum chemistry calculations for non-covalent interactions in many-body systems: The XSAPT family of methods](#). *J. Phys. Chem. A* **119**, 235 (2015). [Feature Article, ACS Editors' Choice, and [Featured on cover](#)]
16. Y. Shao *et al.* [Advances in molecular quantum chemistry contained in the Q-Chem 4 program package](#). *Mol. Phys.* **113**, 184 (2015).
15. R. M. Richard, **K. U. Lao**, and J. M. Herbert. [Understanding the many-body expansion for large systems. I. Precision considerations](#). *J. Chem. Phys.* **141**, 014108 (2014).
14. R. M. Richard, **K. U. Lao**, and J. M. Herbert. [Aiming for benchmark accuracy with the many-body expansion](#). *Acc. Chem. Res.* **47**, 2828 (2014).
13. **K. U. Lao** and J. M. Herbert. [Symmetry-adapted perturbation theory with Kohn-Sham orbitals using non-empirically tuned, long-range-corrected density functionals](#). *J. Chem. Phys.* **140**, 044108 (2014). [Selected by JCP as an "Editor's Choice for 2014"]
12. R. M. Richard, **K. U. Lao**, and J. M. Herbert. [Approaching the complete-basis limit with a truncated many-body expansion](#). *J. Chem. Phys.* **139**, 224102 (2013).

11. L. D. Jacobson, R. M. Richard, **K. U. Lao**, and J. M. Herbert. [Efficient monomer-based quantum chemistry methods for molecular and ionic clusters.](#) *Annu. Rep. Comput. Chem.* **9**, 25 (2013).
10. R. M. Richard, **K. U. Lao**, and J. M. Herbert. [Achieving the CCSD\(T\) basis-set limit in sizable molecular clusters: Counterpoise corrections for the many-body expansion.](#) *J. Phys. Chem. Lett.* **4**, 2674 (2013).
9. **K. U. Lao** and J. M. Herbert. [An improved treatment of empirical dispersion and a many-body energy decomposition scheme for the explicit polarization plus symmetry-adapted perturbation theory \(XSAPT\) method.](#) *J. Chem. Phys.* **139**, 034107 (2013). [Erratum: *J. Chem. Phys.* **140**, 119901 (2014).]
8. **K. U. Lao** and J. M. Herbert. [Accurate intermolecular interactions at dramatically reduced cost: XPol+SAPT with empirical dispersion.](#) *J. Phys. Chem. Lett.* **3**, 3241 (2012).
7. J. M. Herbert, L. D. Jacobson, **K. U. Lao**, and M. A. Rohrdanz. [Rapid computation of intermolecular interactions: Self-consistent polarization plus symmetry-adapted perturbation theory.](#) *Phys. Chem. Chem. Phys.* **14**, 7679 (2012).
6. **K. U. Lao** and J. M. Herbert. [Breakdown of the single-exchange approximation in third-order symmetry-adapted perturbation theory.](#) *J. Phys. Chem. A* **116**, 3042 (2012).
5. C.-Y. Chiu, P.-J. Chung, **K. U. Lao**, C.-W. Liao, and M. H. Huang. [Facet-dependent catalytic activity of gold nanocubes, octahedra, and rhombic dodecahedra toward 4-nitroaniline reduction.](#) *J. Phys. Chem. C* **116**, 23757 (2012).
4. **K. U. Lao**, P.-K. Tsou, T. Lankau, and C.-H. Yu. [A computational study of organic polyradicals stabilized by chromium atoms.](#) *Phys. Chem. Chem. Phys.* **14**, 138 (2012).
3. **K. U. Lao**, T. Lankau, T.-I Fang, J.-W. Zou, and C.-H. Yu. [Interstitial water and the formation of low barrier hydrogen bonds: A computational model study.](#) *Int. J. Quantum Chem.* **112**, 1460 (2012).
2. H.-L. Wu, H.-R. Tsai, Y.-T. Hung, **K. U. Lao**, C.-W. Liao, P.-J. Chung, J.-S. Huang, I.-C. Chen, and M. H. Huang. [A comparative study of gold nanocubes, octahedra, and rhombic dodecahedra as highly sensitive SERS substrates.](#) *Inorg. Chem.* **50**, 8106 (2011).
1. **K. U. Lao** and C.-H. Yu. [A computational study of unique properties of pillar\[n\]quinones: Self-assembly to tubular structures and potential applications as electron acceptors and anion recognizers.](#) *J. Comput. Chem.* **32**, 2716 (2011).

INVITED
SEMINARS

- 2026 Jan. Iowa State University, Department of Chemistry
- 2025 Nov. University of Maryland—College Park, Department of Chemistry and Biochemistry
- 2025 Sep. Loyola University Chicago, Department of Chemistry and Biochemistry
- 2025 Feb. Wayne State University, Department of Chemistry
- 2024 Sep. University of Richmond, Department of Chemistry

- 2024 Jul. University of Macau, Department of Physics and Chemistry
 - 2024 Jun. National Center for Theoretical Sciences, Taiwan
 - 2024 Jun. Institute of Chemistry, Academia Sinica, Taiwan
 - 2024 May Trinity College Dublin, School of Physics, Ireland (virtual format)
 - 2024 May National Institutes of Health, National Heart, Lung, and Blood Institute (NHLBI)
 - 2024 Apr. Rutgers University–Newark, Department of Physics
 - 2024 Feb. Virginia Commonwealth University, Department of Physics
 - 2023 Nov. University of New Haven, Department of Chemistry
 - 2023 Jun. Institute of Atomic and Molecular Sciences, Academia Sinica, Taiwan
 - 2023 Mar. Virginia Commonwealth University, Department of Medicinal Chemistry
 - 2019 Oct. Virginia Commonwealth University, Department of Physics
 - 2019 Jun. University of Macau, Department of Physics and Chemistry
 - 2018 Oct. Cornell University (Graduate and Postdoc Seminar)
 - 2017 Oct. Cornell University (Graduate and Postdoc Seminar)
 - 2016 Mar. The Ohio State University (Physical Chemistry Student Lecture Series)
 - 2013 Apr. The Ohio State University (Physical Chemistry Student Lecture Series)
- INVITED
CONFERENCE
PRESENTATIONS
- 2025 Oct. 3rd International Symposium on Machine Learning in Quantum Chemistry (SMLQC), Knoxville, TN
 - 2025 Apr. Fifty Years of Computational Medicinal Chemistry Research at VCU, Richmond, VA
 - 2025 Mar. ACS National Meeting, San Diego, CA (Symposium on “OpenEye Cadence Molecular Sciences Outstanding Junior Faculty Award”)
 - 2024 May 52nd meeting of the Southeastern Theoretical Chemistry Association (SETCA), Blacksburg, VA
 - 2023 Apr. 8th Virginia Soft Matter Workshop, Richmond, VA
 - 2022 Jun. 52nd Midwest Theoretical Chemistry Conference (MWTCC), Columbus, OH
 - 2022 Mar. ACS National Meeting, San Diego, CA (Symposium on “New Developments in Hybrid QM/QM, QM/MM, and Fragmentation Methods”)
 - 2021 Nov. ACS Southeastern Regional Meeting, Birmingham, AL (Symposium on “Theoretical Chemistry: Method Development and Applications”)
- CONTRIBUTED
CONFERENCE
PRESENTATIONS
- 2025 Aug. ACS National Meeting, Washington, DC (Symposium on “Quantum Mechanics”)
 - 2024 Oct. ACS Southeastern Regional Meeting, Atlanta, GA (Symposium on “Quantum-Based Modeling of Complex Environments: Methods, Software, and Applications” in Honor of Herty Medalist David Sherrill)
 - 2024 Aug. ACS National Meeting, Denver, CO (Symposium on “Quantum Mechanics”)

- 2024 Mar. ACS National Meeting, New Orleans, LA (Symposium on “Quantum Mechanics”)
- 2023 Oct. ACS Southeastern Regional Meeting, Durham, NC (Symposium on “Physical Chemistry: Theory Development and Experimental Frontiers”)
- 2023 Aug. ACS National Meeting, San Francisco, CA (Symposium on “Quantum Mechanics”)
- 2022 Aug. ACS National Meeting, Chicago, IL (Symposium on “Quantum Chemistry: Current & Future Frontiers”)
- 2022 Aug. ACS National Meeting, Chicago, IL (Symposium on “Quantum Mechanics”)
- 2019 Aug. Penn Conference in Theoretical Chemistry, Philadelphia, PA
- 2018 Aug. ACS National Meeting, Boston, MA (Symposium on “Quantum Mechanics”)
- 2017 Mar. APS National Meeting, New Orleans, LA (Symposium on “van der Waals Bonding in Advanced Materials III”)
- 2017 Jan. 10th International Conference on Computational Physics (ICCP10), Macao (Symposium on “Computational Chemistry”)
- 2016 Oct. ACS Northeast Regional Meeting, Binghamton, NY (Symposium on “Theoretical & Computational Chemistry”)
- 2016 Feb. 30th Edward F. Hayes Graduate Research Forum, Columbus, OH
- 2015 Aug. Q-Chem Workshop, Boston, MA
- 2015 Aug. ACS National Meeting, Boston, MA (Symposium on “Electronic Structure Methods for Large Systems”)
- 2015 Jun. Midwest Theoretical Chemistry Conference, Ann Arbor, MI
- 2014 Nov. Quantum Systems in Chemistry, Physics and Biology, QSCP XIX, Taipei, Taiwan (Flash Talk)
- 2013 Sep. ACS National Meeting, Indianapolis, IN (Symposium on “Quantum Chemistry”)
- 2013 Jun. 68th International Symposium on Molecular Spectroscopy, Columbus, OH
- 2011 Feb. Theoretical and Computational Chemistry Conference, Taipei, Taiwan
- 2007 Mar. ChuMei Theoretical Chemistry Seminar, Hsinchu, Taiwan

POSTERS

- 2025 Dec. Pacificchem 2025, Honolulu, HI (Symposium on “Computational Quantum Chemistry: Synergy Between Theory and Experiment”)
- 2025 Mar. ACS National Meeting, San Diego, CA (Symposium on “OpenEye Cadence Molecular Sciences Outstanding Junior Faculty Award”)
- 2025 Feb. 64th Sanibel Symposium, St. Augustine, FL
- 2023 Aug. ACS National Meeting, San Francisco, CA
- 2023 May. MolSSI workshop on Machine Learning and Chemistry, College Park, MD
- 2018 Aug. ACS National Meeting, Boston, MA (Symposium on “The Wiley Computers in Chemistry Outstanding Postdoc Award”)
- 2018 Aug. ACS National Meeting, Boston, MA (Symposium on “Sci-Mix”)
- 2015 Aug. ACS National Meeting, Boston, MA (Symposium on “The Chemical Computing Group Excellence Award for Graduate Students”)

- 2014 Nov. Quantum Systems in Chemistry, Physics and Biology, QSCP XIX, Taipei, Taiwan
- 2014 Sep. William Lloyd Evans Lecture-Dow Poster Session, Columbus, OH
- 2014 Jul. American Conference on Theoretical Chemistry, Telluride, CO
- 2014 Jun. Midwest Theoretical Chemistry Conference, Evanston, IL
- 2013 May. Midwest Theoretical Chemistry Conference, Urbana-Champaign, IL
- 2013 Jan. Gordon Research Conferences: Molecular Energy Transfer, Ventura, CA
- 2012 Jan. Gordon Research Conferences: Molecular & Ionic Clusters, Ventura, CA
- 2011 Jan. The 4th Cross-Strait Theoretical and Computational Chemistry Conference (CTCC-4), Kinmen, Taiwan

TEACHING Incorporating Python programming into chemistry education to **promote both programming skills and computational chemistry** among chemistry students:

- CHEM 510: Graduate Atomic & Molecular Structure, 3 credits
- CHEM 314: Undergraduate Physical Chemistry I with Math Modules, 4 credits
- CHEM 313: Undergraduate Physical Chemistry I, 3 credits

MENTORING Current Postdocs

- Zihui Song

Current Ph.D. Students

- Kalana Wickramasinghe
- Tammam El Kadri
- Luke Conley

Former Postdocs

- Jake Tan (Assistant Professor at the University of West Florida)

Former Ph.D. Students

- Mi'Kayla Word (Postdoc at Sandia National Laboratories)
- Francisco Ballesteros (Postdoc at the University of Zürich)
- Corentin Villot (Research Scientist at Qubit Pharmaceuticals)
- Danyang Wang

Former Master's Students

- Arthur Wang

Former Undergraduates

- Shelbie Dunivan (Graduated with a Pharm.D. from VCU)
- Brian Hua
- Christy Bouhaidar (Medical School at Virginia Tech)
- Henry Childs, 2021 NSF-REU (Chemistry Ph.D. at Duke University)
- Tong Huang
- Stephen Hennessey
- Ashelyn Kyne (Master of Chemistry at the University of Manchester)

Former High School Students

- Asia Fairley, 2023 ACS Project SEED
- Isis Olds, 2024 ACS Project SEED
- Diamilatou Ba, 2025 ACS Project SEED
- Cadence Tang, 2025

AWARDS,
FELLOWSHIPS,
AND FUNDING
FOR STUDENTS

- 2024 VCU Graduate School Dissertation Assistantship. University tuition and \$9,375 stipend for Spring semester (Corentin Villot).
- 2023 The Distinguished Chemist Fund. \$1,200 (Corentin Villot).
- 2023 Drs. Billy L. Stump and Raphael M. Ottenbrite Fellowship in Chemistry. \$1,600 (Francisco Ballesteros).
- 2022 Honorable Mention to the Poster Presentation at 52nd MWTCC. (Francisco Ballesteros).
- 2022 Drs. Billy L. Stump and Raphael M. Ottenbrite Fellowship in Chemistry. \$1,500 (Francisco Ballesteros).
- 2021 Altria Undergraduate Summer Research Fellowship. \$5,000 (Tony Huang).

SUPERCOMPUTER
GRANTS

- 2023 DOE Mission Science Allocation Award, 2,240 CPU node hours (A Low-Cost Wavefunction-Based Method for Nanoscale Systems)
- 2022 DOE Mission Science Allocation Award, 5,000 CPU node hours (A Low-Cost Wavefunction-Based Method for Nanoscale Systems)
- 2021 DOE Mission Science Allocation Award, 850,000 CPU hours (A Low-Cost Wavefunction-Based Method for Nanoscale Systems)
- 2020 DOE Mission Science Allocation Award, 1,500,000 CPU hours (An Effective Fragmentation Approach for High-Throughput Screening in Materials Design)
- 2019 DOE Mission Science Allocation Award, 3,500,000 CPU hours (Quantum Chemical Study of Area-Selective Atomic Layer Deposition)
- 2018 NERSC Production Allocation Award, 500,000 CPU hours (Quantum Chemical Study of Area-Selective Atomic Layer Deposition)
- 2017 NERSC Production Allocation Award, 800,000 CPU hours (Dipole Polarizability of a Condensed-Phase Water Molecule)

CURRENT
COLLABORATORS

- Dr. Indika Arachchige, VCU Chemistry
- Dr. Samy El-Shall, VCU Chemistry
- Dr. Katharine Tibbetts, VCU Chemistry
- Dr. Xuewei Wang, VCU Chemistry
- Dr. Ram Gupta, VCU Chemical & Life Science Engineering
- Dr. Liheng Cai, UVA Materials Science and Engineering & Chemical Engineering

SOFTWARE
DEVELOPMENT

- Developer, Q-Chem Inc. (2011–present); developed theoretical methods implemented in [Q-Chem](#)
- Open-source machine learning models developed by my research group are available on [GitHub](#)

SCHOLARSHIP DEVELOPMENT ACTIVITIES	<ul style="list-style-type: none"> ○ 2022 ○ 2021–2022 	<p>Selected to attend the NSF Chemistry Early Career Investigator Workshop</p> <p>Selected to attend the VCU Grant Academy</p>
DEPARTMENTAL AND UNIVERSITY SERVICE	<ul style="list-style-type: none"> ○ 2026 ○ 2025–2026 ○ 2025–present ○ 2025–present ○ 2024–present ○ 2024–present ○ 2023 ○ 2022–present ○ 2022–present ○ 2022–2023 ○ 2022–2023 ○ 2021 ○ 2020–2021 ○ 2019–2023 ○ 2020–2025 ○ 2019–2023 	<p>Chair, VCU Chemistry Pre-Promotion Committee</p> <p>VCU CHS, Faculty Awards Committee</p> <p>VCU Chemistry, Physical Faculty Coordinator</p> <p>VCU Chemistry, Graduate Recruiting Committee</p> <p>VCU Chemistry, Curriculum and Undergrad affairs Committee</p> <p>VCU Chemistry, Graduate Evaluation and Advising Committee</p> <p>VCU Chemistry, Graduate Curriculum Redesign Committee</p> <p>VCU Chemistry, Faculty Awards Committee</p> <p>Peer reviewer/Panelist, VCU internal funding</p> <p>Search Committee, VCU Department of Chemistry, Physical Chemistry Term Faculty, resulted in the appointment of Dr. Michael Crawford</p> <p>Panelist, VCU NSF-GRFP Campus Review Panels</p> <p>Search Committee, VCU High Performance Research Computing Core Facility Director, resulted in the appointment of Dr. Alberto Cano</p> <p>VCU Chemistry, Recording of Faculty Meeting Minutes</p> <p>VCU Chemistry, Graduate Recruitment and Admissions Committee</p> <p>VCU Chemistry, Seminar Committee</p> <p>VCU Chemistry, Physical Chemistry Cumulative Exam</p>
NATIONAL PROFESSIONAL SERVICE	<ul style="list-style-type: none"> ○ 2025–present ○ 2023 ○ 2025 ○ 2025 ○ 2024 ○ 2023–present ○ 2020–present ○ 2020–present ○ 2019–present ○ 2023 	<p>Co-organizer, National ACS COMP Division Symposium on “Quantum Mechanics”</p> <p>Co-organizer, Virginia Clean Energy and Catalysis Club Summit</p> <p>Judge, ACS COMP Division Award</p> <p>Peer reviewer for Poland National Science Centre</p> <p>Peer reviewer for Swiss National Science Foundation</p> <p>Peer reviewer for DOE</p> <p>Peer reviewer/Panelist for NSF</p> <p>Peer reviewer for the American Chemical Society Petroleum Research Fund</p> <p>Peer reviewer for publications including <i>Nature Computational Science</i>, <i>Nature Communications</i>, <i>Physical Review Letters</i>, <i>Physical Review A</i>, <i>Chemical Science</i>, <i>Journal of the American Chemical Society</i>, <i>The Journal of Chemical Physics</i>, <i>Journal of Chemical Theory and Computation</i>, <i>The Journal of Physical Chemistry</i>, <i>Physical Chemistry Chemical Physics</i>, <i>ChemPhysChem</i>, <i>Journal of Materials Chemistry</i>, <i>Journal of Computational Chemistry</i>, <i>International Journal of Quantum Chemistry</i>, and others</p> <p>Presider, ACS Southeastern Regional Meeting, Durham, NC (Symposium on “Physical Chemistry: Theory Development and Experimental Frontiers”)</p>

- 2018 Presider, ACS National Meeting, Boston, MA (Symposium on “Quantum Mechanics”)
- 2016–2017 Participated in Cornell GIAC outreach program
- 2016 Local Organizing Committee Member, 10th International Conference on Computational Physics (ICCP10)

PROFESSIONAL
MEMBERSHIPS

- American Chemical Society (ACS)
- ACS Division of Computers in Chemistry (COMP)
- ACS Division of Physical Chemistry (PHYS)