Ka Un Lao **November 2025**

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
- 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)

- Department of Chemistry

Member

- VCU Center for Drug Discovery (2024–present)
- VCU Institute for Sustainable Energy and Environment (2022–present)

Postdoctoral Associate, Cornell University (2016–2019)

- Department of Chemistry and Chemical Biology
- Advisor: Professor Robert A. DiStasio Jr.

EDUCATION

Ph.D., The Ohio State University, Columbus, OH (2011–2016)

- Advisor: Professor John M. Herbert
- Thesis: *Accurate and Efficient Quantum Chemistry Calculations for Noncovalent Interactions in Many-Body Systems*
- GPA: 4.0/4.0

M.S., National Tsing Hua University, Hsinchu, Taiwan (2007–2009)

- Advisor: Professor Chin-Hui Yu
- Thesis: *A Computational Study of Neutral Low Barrier Hydrogen Bonds: The Effect of Water Molecules and Peptide Bonds*

B.S., National Tsing Hua University, Hsinchu, Taiwan (2003–2007)

- Chemistry major and Physics minor (Ranking: 1st/56, 3.95 GPA)

AWARDS AND HONORS

- 2025 JCP Emerging Investigators Collection
- 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 Excellence in Scholarship Award (VCU College of Humanities and Sciences)
- 2025 Sanibel Symposium Young Investigator Award (University of Florida's Quantum Theory Project)

- 2025 The Journal of Chemical Physics Editors' Choice 2024
- 2025 NSF CAREER Award
- 2024 JCP Emerging Investigators Collection (Three Times)
- 2024 The Journal of Chemical Physics Editors' Choice 2023
- 2023 JCP Emerging Investigators Collection
- 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 TASCO Chemical Corporation Scholarship (TASCO 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 ultrafast 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

- 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 = 32, total citations = 8,002;** 13 papers with ≥ 100 citations
69 publications (source: Google Scholar)

36 Independently Published Papers at VCU + 1 in Review
6 Co-Authored with Undergraduates
*__**corresponding author**__, __undergraduate student__[U]

70. X. Ma, B. Huang, J. Zhu, **K. U. Lao**, and L.-H. Cai. An injectable antifibrotic supramolecular bottlebrush hydrogel crosslinked via unexpected *s*-tetrazine π–π stacking. *ACS Cent. Sci.* **in review**, (2025).

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 $Fe_{2-x}Mo_xP$ 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 $Si_{1-x}Ge_x$ 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 Editor's 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. Pearcy, **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 $Ni_{2-x}Zn_xP$ 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 CO_2 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 Ni_5P_4 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 $FeCl_3$ 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 C_{60} dimer, DNA−ellipticine, and HIV−indinavir. *J. Phys. Chem. A* **126**, 4326 (2022). [Featured on cover]

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. Pearcy, **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 noncovalent 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-π 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

- 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. Pacifichem 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 4^{th} Cross-Strait Theoretical and Computational Chemistry Conference (CTCC-4), Kinmeni, 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 Ph.D. Students

- Kalana Wickramasinghe
- Luke Conley
- Tammam El Kadri

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)

Collaborators

- Dr. Indika Arachchige, VCU Chemistry
- Dr. Hani El-Kaderi, 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. Ümit Özgür, VCU Electrical & Computer Engineering
- Dr. Weining Wang, VCU Mechanical & Nuclear Engineering
- Dr. Liheng Cai, UVA Materials Science and Engineering & Chemical Engineering

Software Development

- Developer, Q-Chem Inc. (2011-present) [Theoretical methods developed by my research group may be available in Q-Chem]
- Machine learning models developed by my research group are available on Github

Scholarship Development Activities

- 2022 Selected to attend the NSF Chemistry Early Career Investigator Workshop
- 2021–2022 Selected to attend the VCU Grant Academy

Departmental and University Service

- 2025–present VCU Chemistry, Physical Faculty Coordinator
- 2025–present VCU Chemistry, Graduate Recruiting Committee
- 2024–present VCU Chemistry, Curriculum and Undergrad affairs Committee
- 2024–present VCU Chemistry, Graduate Evaluation and Advising Committee
- 2023 VCU Chemistry, Graduate Curriculum Redesign Committee
- 2022–present VCU Chemistry, Faculty Awards Committee
- 2022–present Peer reviewer/Panelist, VCU internal funding
- 2022–2023 Search Committee, VCU Department of Chemistry, Physical Chemistry Term Faculty, resulted in the appointment of Dr. Michael Crawford
- 2022–2023 Panelist, VCU NSF-GRFP Campus Review Panels
- 2021 Search Committee, VCU High Performance Research Computing Core Facility Director, resulted in the appointment of Dr. Alberto Cano
- 2020–2021 VCU Chemistry, Recording of Faculty Meeting Minutes
- 2019–2023 VCU Chemistry, Graduate Recruitment and Admissions Committee
- 2020–2025 VCU Chemistry, Seminar Committee
- 2019–2023 VCU Chemistry, Physical Chemistry Cumulative Exam

National Professional Service

- 2025–present: Co-organizer, National ACS COMP Division Symposium on "Quantum Mechanics"
- 2023: Co-organizer, Virginia Clean Energy and Catalysis Club Summit
- 2025: Judge, ACS COMP Division Award
- 2025: Peer reviewer for Poland National Science Centre
- 2024: Peer reviewer for Swiss National Science Foundation
- 2023–present: Peer reviewer for DOE
- 2020–present: Peer reviewer/Panelist for NSF
- 2020–present: Peer reviewer for the American Chemical Society Petroleum Research Fund
- 2019–present: Peer reviewer for publications including *Nature Computational Science*, *Nature Communications*, *Physical Review Letters*, *Physical Review A*, *Chemical Science*, *Journal of the American Chemical Society*, *The Journal of Chemical Physics*, *Journal of Chemical Theory and Computation*, *The Journal of Physical Chemistry*, *Physical Chemistry Chemical Physics*, *ChemPhysChem*, *Journal of Materials Chemistry*, *Journal of Computational Chemistry*, *International Journal of Quantum Chemistry*, and others
- 2023: Presider, ACS Southeastern Regional Meeting, Durham, NC (Symposium on "Physical Chemistry: Theory Development and Experimental Frontiers")
- 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)