Ka Un Lao **January 2022**

Contact Information

Virginia Commonwealth University
Department of Chemistry
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Career History

Assistant Professor, Virginia Commonwealth University (2019–present)

- Department of Chemistry

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

- 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)

Publications

***h*-index = 23, total citations = 4,013** (source: Google Scholar)

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. *Frontiers in Chemistry* **submitted**, (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* **in press**, (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. 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, and Featured on cover]

37. 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).

36. 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).

35. F. Ballesteros, S. Dunivan, 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).

34. M. K. Shehab, K. S. Weeraratne, T. Huang, **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).

33. **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]

32. 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).

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 for the duration of the week of May 16, 2016]

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).

ORAL PRESENTATIONS

- 2022 Jun. Midwest Theoretical Chemistry Conference, 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")
- 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. The 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

- 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

Invited Seminars

- 2021 May 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)

Teaching

- 2019–2021 CHEM 510: Atomic and Molecular Structure (Graduate), 3 credits
- 2020–2021 CHEM 314: Physical Chemistry I with Math Modules (Undergraduate), 4 credits
- 2020–2021 CHEM 313: Physical Chemistry I (Undergraduate), 3 credits

Funding

- 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.
- 2020–2022 Understanding and controlling the aggregation behavior of petroleum asphaltenes. ACS Petroleum Research Fund (Doctoral New Investigator Grant). $110,000. Single PI.

Fellowships and Funding for Students

- 2021 Altria Undergraduate Summer Research Fellowship. $5,000 (Tony Huang).
- 2020 Enhanced drug design through robust quantum chemistry calculation and machine learning. VCU Honors Summer Undergraduate Research Program (HSURP). $3,100 (Tony Huang).

Supercomputer Grants

- 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. Brian Fuglesta, VCU Chemistry
- Dr. Katharine Tibbetts, VCU Chemistry
- Dr. Xuewei Wang, VCU Chemistry
- Dr. Weining Wang , VCU Mechanical & Nuclear Engineering
- Dr. Heather Allen, OSU Chemistry & Biochemistry

Software Development

- Developer, Q-Chem Inc. (2011-present) [Theoretical methods developed by me may be available in Q-Chem]

Departmental and University Service

- 2019–present Graduate Admissions Committee of VCU Chemistry
- 2021 Search Committee, VCU High Performance Research Computing Core Facility Director, resulted in the appointment of Dr. Alberto Cano

Professional Service	◦ 2019–present	Peer reviewer for publications including *Physical Review Letters*, *Physical Review A*, *Chemical Science*, *The Journal of Chemical Physics*, *Physical Chemistry Chemical Physics*, *Journal of Materials Chemistry A*, *Journal of Computational Chemistry*, *International Journal of Quantum Chemistry*, *Journal of Theoretical and Computational Chemistry*, *Journal of Molecular Modeling*, *International Journal of Molecular Sciences*, and others
	◦ 2020	Peer reviewer for the American Chemical Society Petroleum Research Fund
	◦ 2020–2022	Reviewer for NSF Graduate Research Fellowship Program
	◦ 2018	Presider, ACS National Meeting, Boston, MA (Symposium on "Quantum Mechanics")
	◦ 2017–2016	Participated in Cornell GIAC outreach program
	◦ 2016	Local Organizing Committee Member, 10th International Conference on Computational Physics (ICCP10)