
CONTACT INFORMATION	Virginia Commonwealth University Department of Chemistry 3046 Oliver Hall Richmond, VA 23284	Tel: (804) 828-3071 laoku@vcu.edu kaunlao@gmail.com http://www.kaunlaolab.com
CAREER HISTORY	Assistant Professor, Virginia Commonwealth University (2019–present) <ul style="list-style-type: none">Department of Chemistry Postdoctoral Associate, Cornell University (2016–2019) <ul style="list-style-type: none">Department of Chemistry and Chemical BiologyAdvisor: 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. HerbertThesis: <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 YuThesis: <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">2020 ACS Petroleum Research Fund Doctoral New Investigator Award2019 Macau Excellent Talents Award Scheme (Macau Foundation)2019 Top Ten Outstanding Chinese American Youth Award2019 PCTC Postdoctoral Fellow Award (Penn Conference in Theoretical Chemistry)2018 ACS COMP Division Wiley Computers in Chemistry Outstanding Postdoc Award2016 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 Award2015 ACS COMP Division Chemical Computing Group Excellence Award for Graduate Students2015 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 TASCOC Chemical Corporation Scholarship (TASCOC 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 = 21, total citations = 2,912** (source: [Google Scholar](#))

34. M. K. Shehab, S. Weeraratne, T. Huang, **K. U. Lao**, and H. M. El-Kaderi. Aza-covalent organic framework as a cathode in sodium ion batteries for high capacity, energy, and power performance. **to be submitted**, (2020).
33. **K. U. Lao**, Y. Yang, and R. A. DiStasio Jr. Confinement meet electron delocalization: Non-additivity and finite-size effects in the polarizabilities and dispersion coefficients of the fullerenes. **submitted**, (2020).
32. 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).
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 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
- o 2021 Jun. Midwest Theoretical Chemistry Conference, Columbus, OH
 - o 2019 Aug. Penn Conference in Theoretical Chemistry, Philadelphia, PA
 - o 2018 Aug. ACS National Meeting, Boston, MA (Symposium on “Quantum Mechanics”)
 - o 2017 Mar. APS National Meeting, New Orleans, LA (Symposium on “Van der Waals Bonding in Advanced Materials III”)
 - o 2017 Jan. 10th International Conference on Computational Physics (ICCP10), Macao (Symposium on “Computational Chemistry”)
 - o 2016 Oct. ACS Northeast Regional Meeting, Binghamton, NY (Symposium on “Theoretical & Computational Chemistry”)
 - o 2016 Feb. The 30th Edward F. Hayes Graduate Research Forum, Columbus, OH
 - o 2015 Aug. Q-Chem Workshop, Boston, MA
 - o 2015 Aug. ACS National Meeting, Boston, MA (Symposium on “Electronic Structure Methods for Large Systems”)
 - o 2015 Jun. Midwest Theoretical Chemistry Conference, Ann Arbor, MI
 - o 2014 Nov. Quantum Systems in Chemistry, Physics and Biology, QSCP XIX, Taipei, Taiwan (Flash Talk)
 - o 2013 Sep. ACS National Meeting, Indianapolis, IN (Symposium on “Quantum Chemistry”)
 - o 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 4th Cross-Strait Theoretical and Computational Chemistry Conference (CTCC-4), Kinmen, Taiwan
- INVITED SEMINARS
- 2019 Oct. Virginia Commonwealth University
 - 2019 Jun. University of Macau
 - 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
- 2019–2020 CHEM 510: Atomic and Molecular Structure (Graduate), 3 credits
 - 2020 CHEM 314: Physical Chemistry I with Math Modules (Undergraduate), 4 credits
 - 2020 CHEM 313: Physical Chemistry I (Undergraduate), 3 credits
- EXTERNAL FUNDING
- 2020–2022 Understanding and controlling the aggregation behavior of petroleum asphaltene. ACS Petroleum Research Fund (Doctoral New Investigator Grant). \$110,000.
- INTERNAL FUNDING
- 2020 Enhanced drug design through robust quantum chemistry calculation and machine learning. VCU Honors Summer Undergraduate Research Program (HSURP). \$3,100.

- SUPERCOMPUTER GRANTS
- 2020 DOE Mission Science award, 1,500,000 CPU hours (An Effective Fragmentation Approach for High-Throughput Screening in Materials Design)
 - 2019 DOE Mission Science 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)
- SOFTWARE DEVELOPMENT
- Developer, Q-Chem Inc. (2011-present) [Theoretical methods developed by me may be available in [Q-Chem](#)]
- JOURNAL REVIEWER
- 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
- PROFESSIONAL SERVICE
- 2020 Reviewer for the ACS Petroleum Research Fund
 - 2020–2021 Reviewer for the NSF Graduate Research Fellowship Program
 - 2019– Graduate Admissions Committee of VCU Chemistry
 - 2018 Aug. 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)
- PROFESSIONAL MEMBERSHIPS
- American Chemical Society (ACS)
 - ACS Division of Computers in Chemistry (COMP)
 - American Physical Society (APS)
 - American Association for the Advancement of Science (AAAS)