

---

CONTACT INFORMATION	Virginia Commonwealth University Department of Chemistry 3046 Oliver Hall Richmond, VA 23284	Tel: (804) 828-3071 <a href="mailto:laoku@vcu.edu">laoku@vcu.edu</a> <a href="#">Google Scholar</a> <a href="#">Group Website</a>
CAREER HISTORY	<b>Assistant Professor, Virginia Commonwealth University</b> (2019–present) <ul style="list-style-type: none"><li>Department of Chemistry</li></ul> <b>Postdoctoral Associate, Cornell University</b> (2016–2019) <ul style="list-style-type: none"><li>Department of Chemistry and Chemical Biology</li><li>Advisor: Professor Robert A. DiStasio Jr.</li></ul>	
EDUCATION	<b>Ph.D., The Ohio State University</b> , Columbus, OH (2011–2016) <ul style="list-style-type: none"><li>Advisor: Professor John M. Herbert</li><li>Thesis: <i>Accurate and Efficient Quantum Chemistry Calculations for Noncovalent Interactions in Many-Body Systems</i></li><li>GPA: 4.0/4.0</li></ul> <b>M.S., National Tsing Hua University</b> , Hsinchu, Taiwan (2007–2009) <ul style="list-style-type: none"><li>Advisor: Professor Chin-Hui Yu</li><li>Thesis: <i>A Computational Study of Neutral Low Barrier Hydrogen Bonds: The Effect of Water Molecules and Peptide Bonds</i></li></ul> <b>B.S., National Tsing Hua University</b> , Hsinchu, Taiwan (2003–2007) <ul style="list-style-type: none"><li>Chemistry major and Physics minor (Ranking: 1st/56, 3.95 GPA)</li></ul>	
AWARDS AND HONORS	<ul style="list-style-type: none"><li>2020 ACS Petroleum Research Fund Doctoral New Investigator Award</li><li>2019 Macau Excellent Talents Award Scheme (Macau Foundation)</li><li>2019 Top Ten Outstanding Chinese American Youth Award</li><li>2019 PCTC Postdoctoral Fellow Award (Penn Conference in Theoretical Chemistry)</li><li>2018 ACS COMP Division Wiley Computers in Chemistry Outstanding Postdoc Award</li><li>2016 1st place oral award in Mathematical and Physical Sciences area at The 30th Edward F. Hayes Graduate Research Forum (The Ohio State University)</li><li>2015 Phi Tau Phi (PTP) Mid-America Scholarship Award</li><li>2015 ACS COMP Division Chemical Computing Group Excellence Award for Graduate Students</li><li>2015 Presidential Fellowship Award (The Ohio State University)</li><li>2015 1st place award in Albert L. Henne Research Competition (The Ohio State University)</li><li>2013 Funding for attending the Telluride School of Theoretical Chemistry (Telluride Science Research Center)</li><li>2009–2012 Postgraduate Scholarships for Ph.D. (Macau Tertiary Education Services Office)</li></ul>	

- 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 = 26, total citations = 5,064** (source: [Google Scholar](#))

#### VCU Independent Work

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<sub>3</sub> 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<sub>60</sub> 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, 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, **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 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 | <ul style="list-style-type: none"> <li>○ 2023 Apr. 8th Virginia Soft Matter Workshop, Richmond, VA</li> <li>○ 2022 Aug. ACS National Meeting, Chicago, IL (Symposium on “Quantum Chemistry: Current &amp; Future Frontiers”)</li> <li>○ 2022 Aug. ACS National Meeting, Chicago, IL (Symposium on “Quantum Mechanics”)</li> <li>○ 2022 Jun. 52nd Midwest Theoretical Chemistry Conference, Columbus, OH</li> <li>○ 2022 Mar. ACS National Meeting, San Diego, CA (Symposium on “New Developments in Hybrid QM/QM, QM/MM, and Fragmentation Methods”)</li> <li>○ 2021 Nov. ACS Southeastern Regional Meeting, Birmingham, AL (Symposium on “Theoretical Chemistry: Method Development and Applications”)</li> <li>○ 2019 Aug. Penn Conference in Theoretical Chemistry, Philadelphia, PA</li> </ul> |
|--------------------|--|

- 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<sup>th</sup> Cross-Strait Theoretical and Computational Chemistry Conference (CTCC-4), Kinmen, Taiwan

INVITED  
SEMINARS

- 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)

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

- MENTORING
- Current Postdocs Jake Tan
  - Current Graduate Students Francisco Ballesteros  
Corentin Villot  
Danyang Wang  
Arthur Wang  
Nicole Sadler  
Kalana Wickramasinghe
  - Current Undergraduates Tong Huang  
Stephen Hennessey
  - Former Graduate Students Mi'Kayla Word (Postdoc at Sandia National Lab)
  - Former Undergraduates Shelbie Dunivan (VCU Pharm.D. Student)  
Brian Hua  
Christy Bouhaidar  
Henry Childs (Chemistry Ph.D. at Duke Univ.)

- FUNDING
- 2023–2024 First-principles quantum-crystallographic X-ray structure refinement. The VCU College of Humanities and Sciences Seed Awards program. \$5,000. Single PI.
  - 2022–2025 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).
  - 2022–2025 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).
  - 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.
  - 2020–2023 Understanding and controlling the aggregation behavior of petroleum asphaltene. ACS Petroleum Research Fund (Doctoral New Investigator Grant). \$110,000. Single PI (61654-DNI6).

- AWARDS,  
FELLOWSHIPS,  
AND FUNDING  
FOR STUDENTS
- 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).
  - 2020 VCU Honors Summer Undergraduate Research Program (HSURP). \$3,100 (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. Soma Dhakal, 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. Ümit Özgür, VCU Electrical & Computer Engineering
  - 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 my research group may be available in [Q-Chem](#)]
- 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
- 2023 VCU Chemistry, Graduate Curriculum Committee
  - 2022–2023 Search Committee, VCU Department of Chemistry, Physical Chemistry Term Faculty

- 2022 Panelist, VCU NSF GRFP Workshop
  - 2022 Peer reviewer/Panelist, VCU internal funding
  - 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
  - 2022–present VCU Chemistry, Faculty awards committee
  - 2019–present VCU Chemistry, Graduate Recruitment and Admissions Committee
  - 2019–present VCU Chemistry, Seminar Committee
  - 2019–present VCU Chemistry, Physical Chemistry Cumulative Exam
- NATIONAL PROFESSIONAL SERVICE
- 2023 Co-organizer, Virginia Clean Energy and Catalysis Club Summit
  - 2019–present Peer reviewer for publications including *Physical Review Letters*, *Physical Review A*, *Chemical Science*, *The Journal of Chemical Physics*, *The Journal of Physical Chemistry*, *ChemPhysChem*, *Physical Chemistry Chemical Physics*, *Journal of Materials Chemistry*, *Journal of Computational Chemistry*, *International Journal of Quantum Chemistry*, *Journal of Theoretical and Computational Chemistry*, *Journal of Molecular Modeling*, and others
  - 2020–present Peer reviewer/Panelist for NSF
  - 2020 Peer reviewer for the American Chemical Society Petroleum Research Fund
  - 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)
  - American Physical Society (APS)
  - American Association for the Advancement of Science (AAAS)