Lee Michael THOMPSON *Curriculum vitae*

CONTACT INFORMATION

Department of Chemistry
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EMPLOYMENT

Associate Professor (July 2023 to present)
Department of Chemistry, University of Louisville

Assistant Professor (Aug 2017 to June 2023)
Department of Chemistry, University of Louisville

Postdoctoral Scholar (Jan 2014 to May 2017)
Chemistry and Chemical Biology, University of California, Merced

EDUCATION

Doctor of Philosophy in Chemistry (PhD) (Oct 2009 to Dec 2013)
Imperial College London

Master of Chemistry (MChem) (Oct 2004 to Jul 2008)
University of Southampton

TEACHING AND MENTORING

Courses Taught

General Chemistry II (undergraduate 200-level second semester, regular and honors sections taught)

Physical Chemistry I (undergraduate quantum mechanics and spectroscopy)

Physical Chemistry II (undergraduate statistical mechanics, thermodynamics and kinetics)

Advanced Physical Chemistry (graduate electronic structure theory)

Quantum Mechanics (graduate quantum mechanics)

Theory and Application of Computational Chemistry (graduate computational chemistry – new course)

Postdoctoral Researchers

Megan Mackintosh, 2024-current

Andrew D. Mahler, 2018-2020

Graduate Students

Peyton Simpson, 2023-current

An Tran, 2022-current

Zihui Song, 2022-current

Adam Kinyua, 2021-current

Emily M. Kempfer-Robertson, 2018-2023

2022 Arnos Spatola Fellowship
2023 John M. Houchens dissertation prize

Xinju (Spancer) Dong, 2018-2023

Clint N. Evrard, 2018-2023

Undergraduate Research Students

Erin Pidcock, 2023

Casandra Shaefer, 2023

Jayden Connelly, 2022

Jonathan Bersson, 2022

Meagan Haase, 2021-2022

Kushal Nellore, 2021

Irma Avdic, 2020-2021

Senior honors thesis
2021 best thesis award

Piper N. Roe, 2020

T. Dane Pike, 2020

High School Students

Demos Negash (duPont Manual High School, Louisville, KY), 2019 (Amazon Innovation Award)

Service

8. Member, University of Louisville College of Arts and Sciences Undergraduate Thesis Committee (2021-)
7. Director, University of Louisville Department of Chemistry graduate studies program (2021-)
6. Member, faculty search committee (2021)
5. Advisor, University of Louisville College Chemistry Graduate Student Association (2019-2020)
4. Member, University of Louisville College of Arts and Sciences Technology and Facilities Committee (2019-2020)
3. Organizer, University of Louisville Chemistry Department Seminar (2018-2020)
2. Member, University of Louisville Department of Chemistry graduate admissions committee (2017-2022)
1. Served on Ph.D. thesis defense committees of 10 students (2017-2022)

Awarded Grants

7. Attosecond electron dynamics modeled using a time-dependent resonant Hartree-Fock approach. Department of Energy. $480,000 (2023-2026). PI.
6. Exploring photon-initiated electron-neutral interactions in strongly correlated lanthanide complexes. Department of Energy. $1,356,131 (2023-2026). co-PI.
5. CC* Data Storage: Cardinal Academic Research Data Storage (CARDS). National Science Foundation. $500,000 (2023-2025). co-PI.
4. CAREER: Resonant Hartree-Fock inspired descriptions of excited state processes. National Science Foundation. $650,000 (2022-2027). PI.

3. REU: Interdisciplinary, multi-scale materials modeling (I3M). National Science Foundation. $397,130 (2021-2024). Senior-personnel.

2. Elucidation and design of metallophotocatalytic pathways for partial oxidation of methane. ACS petroleum research fund (DNI grant). $110,000 (2019-2022). PI.

1. Nonorthogonal configuration interaction in a symmetry-broken basis for examining the role of defects in semiconductor photocatalysis. EVPRI internal grant program (RII grant). $10,000 (2018-2019). PI.

Publications at University of Louisville

29. Dong, X.; **Thompson, L. M.** Time Propagation of Electronic Wavefunctions Using Nonorthogonal Determinant Expansions, *Journal of Chemical Physics*, **2024**, 160(2), 024106.

28. **Thompson, L. M.**; Kempfer-Robertson, E. M.; Parmar, S.; Saha, S.; Kozlowski, P. M. Nonorthogonal Multireference Wavefunction Description of Triplet-Triplet Energy Transfer Couplings, *Journal of Chemical Theory and Computation*, **2023**, 19(21), 7685–7694.

27. Evrard, E. N.; **Thompson, L. M.** Reactivity of Group 5 and 6 Single-Site Photocatalysts for Partial Oxidation of Methane: Comparison of Chromium, Niobium, and Tungsten-Doped Mesoporous Amorphous Silica., *Journal of Physical Chemistry A*, **2023**, 127(33), 6974–6988.

26. Evrard, E. N.; **Thompson, L. M.** Mechanistic Origin of Selective Methane to Methanol Oxidation on Vanadium-Doped Mesoporous Amorphous Silica Photocatalyst., *Journal of Physical Chemistry C*, **2023**, 127(22), 10488-10498.

25. Kempfer-Robertson, E. M.; E. M.; Avdic, I.; Haase, M. N.; Pike, T. D.; **Thompson, L. M.** Protonation State Control of Electric Field Induced Molecular Switching Mechanisms, *Physical Chemistry Chemical Physics*, **2023**, 25(6), 5251-5261.

24. Kempfer-Robertson, E. M.; Mahler, A. D.; Haase, M. N.; Roe, P.; **Thompson, L. M.** Nonorthogonal Active Space Decomposition of Wave Functions With Multiple Correlation Mechanisms, *Journal of Physical Chemistry Letters*, **2022**, 13(51), 12041-12048.

23. Kempfer-Robertson, E. M.; Haase, M. N.; Avdic, I.; **Thompson, L. M.** Role of Exact Exchange in Difference Projected Double-Hybrid Density Functional Theory for Treatment of Local, Charge-Transfer, and Rydberg Excitations, *Journal of Physical Chemistry A*, **2022**, 126(43), 8058-8069.

22. Avdic, I.; Kempfer-Robertson, E. M.; **Thompson, L. M.** Oriented External Electric Field Tuning of Unsubstituted Azoheteroarene Thermal Isomerization Half-Lives, *Journal of Physical Chemistry A* **2021**, 125(37), 8238-8248.

21. Rahaman, M. S.; Tulaphol, S.; Hossain, M. A.; Evrard, C. N.; **Thompson, L. M.**; Sathitsuksanoh, N. Kinetics of Phosphotungstic Acid Catalyzed Condensation of Levulinic Acid With Phenol to Diphenolic Acid: Temperature-Controlled Regioselectivity, *Molecular Catalysis* **2021**, 514, 111848.

20. Mahler, A. D.; **Thompson, L. M.** Orbital Optimization in Resonant Hartree-Fock Applied to the Study of Conical Intersections and Avoided Crossings, *Journal of Chemical Physics* **2021**, 154(24), 244101.

19. Kempfer-Robertson, E. M.; Pike, T. D.; **Thompson, L. M.** Difference Projection-After-Variation Double-Hybrid Density Functional Theory Applied to the Calculation of Vertical Excitation Energies, *Journal of Chemical Physics* **2020**, 153(7), 074103.

18. Dong, X.; Mahler, A. D.; Kempfer-Robertson, E. M.; **Thompson, L. M.** Global Elucidation of Self-Consistent Field Solution Space Using Basin Hopping, *Journal of Chemical Theory and Computation* **2020**, 16(9), 5635–5644.

17. Kempfer-Robertson, E. M.; **Thompson, L. M.** The Effect of Oriented External Electric Fields on the Photo and Thermal Isomerization of Azobenzene, *Journal of Physical Chemistry A* **2020**, 124(18), 3520–3529.

16. Sheng, X.; **Thompson, L. M.**; Hratchian, H. P. Assessing the Calculation of Exchange Coupling Constants and Spin Crossover Gaps Using the Approximate Projection Model to Improve Density Function Calculations, *Journal of Chemical Theory and Computation* **2020**, 16(1), 154–163.

15. Evrard, C. N..; Mahler, A. D.; **Thompson, L. M.** Excited State Electronic Structure of Single-Site Vanadium Oxide Photocatalysts Supported on Mesoporous Silica, In *Computational Photocatalysis: Modeling of Photophysics and Photochemistry at Interfaces*, Kilin, D., Kilina, S., Han, Y., Eds.; ACS Symposium Series, American Chemical Society, Washington, DC, **2019**, Vol. 1331, 327-341.

14. Harb, H.; **Thompson, L. M.**; Hratchian, H. P. On the Linear Geometry of Lanthanide Hydroxide (LnOH, Ln=La-Lu), *Chemical Physics Physical Chemistry* **2019**, 21, 21890–21897.

13. Ogunwale, M.; Knipp, R.; Evrard, C.; **Thompson, L. M.**; Nantz, M.; Fu, X.-A. The Influence of β-Ammonium Substitution on the Reaction Kinetics of Aminooxy Condensations with Aldehydes and Ketones, *ChemPhysChem* **2019**, 20(6), 815–822.

12. **Thompson, L. M.**; Hratchian, H. P. On Approximate Projection Models, *Molecular Physics* **2019**, 117(9-12), 1421–1429.

11. **Thompson, L. M.** Global Elucidation of Broken Symmetry Solutions to the Independent Particle Model Through a Lie Algebraic Approach, *Journal of Chemical Physics* **2018**, 149(19), 194106.

10. Angnes, R.A.; **Thompson, L. M.**; Mashuta, M. S.; Correia, C.R.; Hammond, G. B. Non-Covalent Substrate Directed Enantioselective Heck Desymmetrization of *cis*-Cyclohex-4-ene-1,2-diol: Synthesis of All *cis* Chiral 5-Aryl-cyclohex-3-ene-1,2-diols and Mechanistic Investigation, *Advanced Synthesis & Catalysis* **2018**, 360(19), 3760– 3767.

Publications Prior to University of Louisville

9. **Thompson, L. M.**; Jarrold, C. C.; Hratchian, H. P. Explaining the $MoVO_4^-$ Photoelectron Spectrum: Rationalization of Geometric and Electronic Structure *Journal of Chemical Physics* **2017**, 146(10), 104301.

8. Abdullahi, M. H.; **Thompson, L. M.**; Bearpark, M. J.; Vinader, V.; Afarinkia, K. The Role of Substituents in Retro Diels-Alder Extrusion of CO_2 from 2(H)-pyrone Cycloadducts *Tetrahedron* **2016**, 72(40), 6021–6024.

7. **Thompson, L. M.**; Hratchian, H. P. Natural Ionization Orbitals for Interpreting Electron Photodetachment Processes *Journal of Chemical Physics* **2016**, 144(20), 204117.

6. **Thompson, L. M.**; Hratchian, H. P. $MoNbO_2^-$ Theoretical Photoelectron Spectra Accounting for Spin Contamination in Density Functional Theory *Journal of Physical Chemistry A* **2015**, 119(32), 8744–8751.

5. **Thompson, L. M.**; Hratchian, H. P. Second Derivatives for Approximate Spin Projection Methods *Journal of Chemical Physics* **2015**, 142(5), 054106.

4. **Thompson, L. M.**; Hratchian, H. P. Spin Projection with Double Hybrid Density Functional Theory *Journal of Chemical Physics* **2014**, 141(3), 034108.

3. **Thompson, L. M.**; Lasoroski A.; Champion, P. M.; Sage, J. T.; Frisch, M. J.; van Thor, J. J.; Bearpark, M. J. Analytical Harmonic Vibrational Frequencies for the Green Fluorescent Protein Computed with ONIOM: Chromophore Mode Character and its Response to Environment *Journal of Chemical Theory and Computation* **2014**, 10(2), 751–766.

2. Vreven, T.; **Thompson, L. M.**; Larkin, S. M.; Kirker, I.; Bearpark, M. J. Deconstructing the ONIOM Hessian: Investigating Method Combinations for Transition Structures *Journal of Chemical Theory and Computation* **2012**, 8(12), 4907–4914.

1. Van Thor, J. J.; Lincoln, C. N.; Kellner, B.; Bourdakos, K. N.; **Thompson L. M.**; Bearpark, M. J.; Champion, P. M.; Sage, J. T. Ultrafast Vibrational Dynamics of Parallel Excited State Proton Transfer Reactions in the Green Fluorescent Protein *Vibrational Spectroscopy* **2012**, 61, 1–6.

Presentations While at University of Louisville

Invited Seminars

6. University of Louisville, Department of Chemistry (2nd September 2022).

5. Indiana State University, Department of Chemistry (1st February 2022).

4. Murray State University, Department of Chemistry (4th October 2021).

3. Dalhousie University, Department of Chemistry (16th April 2021).

2. University of Louisville, Department of Chemical Engineering (5th April 2019).

1. University of Louisville, Department of Physics (29th March 2019).

Invited Conference Presentations

7. Canadian Symposium on Theoretical and Computational Chemistry (CSTCC), Halifax, Canada (scheduled for July 2024).

6. ACS National Meeting, Indianapolis, IN, symposium on 'Electrooxidation of Organic Molecules for Energy and Sustainability' (26th March 2023).

5. ACS National Meeting, Chicago, IL, symposium on '40 Years of Exploring Potential Energy Surfaces. A Symposium Honoring H. Bernhard Schlegel' (21st August 2022).

4. 12th Triennial Congress of the World Association of Theoretical and Computational Chemists (WATOC), Vancouver, Canada (2nd July 2022).

3. ACS National Meeting, San Diego, CA, symposium on 'Atomic-level Understanding & Design of Materials & Processes for Energy Applications' (28th August 2019).

2. South East Theoretical Chemistry Association Meeting, Knoxville, TN (17th May 2019).

1. South Eastern Regional ACS Meeting, Charlotte, NC, symposium on 'Contemporary Computational Chemistry' (9th November 2017).

Contributed Conference Presentations

7. ACS National Meeting, New Orleans, LA, symposium on 'Quantum Mechanics' (20^{th} March 2024).

6. South Eastern Regional ACS Meeting, Durham, NC, symposium on 'Physical Chemistry: Theory Development and Experimental Frontiers' (25^{th} October 2023).

5. South Eastern Regional ACS Meeting, San Juan, PR, symposium on 'Physical Chemistry' (22^{nd} October 2022).

4. South Eastern Regional ACS Meeting, Birmingham, AL, symposium on 'Theoretical Chemistry: Method Development and Applications' (scheduled for 12^{th} November 2021).

3. ACS National Meeting, Online, symposium on 'Quantum Mechanics' (14^{th} April 2021).

2. ACS National Meeting, Online, COMP broadcast symposium, (20^{th} August 2020).

1. ACS National Meeting, Boston, MA, symposium on 'Computational Photocatalysis: Modeling of Photophysics & Photochemistry at Interfaces' (23^{rd} August 2018).

Coauthored Presentations

17. Dong, X., ACS National Meeting, San Francisco, CA, symposium on 'Quantum Mechanics' (2023).

16. Song, Z., ACS National Meeting, San Francisco, CA (2023).

15. Dong, X., ACS National Meeting, Indianapolis, IN, symposium on 'Quantum Mechanics' (2023).

14. Kempfer-Robertson, E. M., ACS National Meeting, Chicago, IL, symposium on 'Quantum Mechanics' (2022).

13. Dong, X., ACS National Meeting, Chicago, IL, symposium on 'Quantum Mechanics' (2022).

12. Kempfer-Robertson, E. M., Oak Ridge National Laboratory, Oak Ridge, TN (2022).

11. Kempfer-Robertson, E. M., 12th Triennial Congress of the World Association of Theoretical and Computational Chemists (WATOC), Vancouver, Canada (2022).

10. Kempfer-Robertson, E. M., South Eastern Regional ACS Meeting, Birmingham, AL, symposium on 'Theoretical Chemistry: Method Development and Applications' (2021).

9. Dong, X., South Eastern Regional ACS Meeting, Birmingham, AL, symposium on 'Theoretical Chemistry: Method Development and Applications' (2021).

8. Evrard E. N., South Eastern Regional ACS Meeting, Birmingham, AL, symposium on 'Photocatalysis, Electrocatalysis, and Electrochemistry Methods for Clean Energy Harvesting, Conversion and Storage' (2021).

7. Evrard E. N., ACS National Meeting, Online, symposium on 'Physical and Computational Chemistry' (2021).

6. Kempfer-Robertson, E. M., ACS National Meeting, Online, symposium on 'Quantum Mechanics' (2021).

5. Dong, X., ACS National Meeting, Online, symposium on 'Quantum Mechanics' (2021).

4. Kempfer-Robertson, E. M., Graduate Student Region Research Conference, Online (2021).

3. Dong, X., South East Theoretical Chemistry Association Meeting, Knoxville, TN (2019).

2. Evrard E. N., South East Theoretical Chemistry Association Meeting, Knoxville, TN (2019).

1. Kempfer-Robertson, E. M., South East Theoretical Chemistry Association Meeting, Knoxville, TN (2019).

Presentations Prior to University of Louisville

Invited Seminars

1. University of Louisville, Department of Chemistry (27th January 2017).

Invited Presentations

2. NSCCS Applied Computational Chemistry Workshop for Synthetic Chemists, London, UK (24th April 2014).

1. NSCCS Gaussian Workshop for Beginners, London, UK (12th September 2012).

Contributed Conference Presentations

10. Theory and Application of Computational Chemistry Meeting, Seattle, WA (29th August 2016).

9. Canadian Chemistry Conference, Halifax, Canada (9th June 2016).

8. ACS National Meeting, San Diego, CA (14th March 2016).

7. ACS National Meeting, Boston, MA (20th August 2015).

6. ACS National Meeting, Boston, MA (19th August 2015).

5. ACS National Meeting, San Francisco, CA (13th August 2014).

4. ACS National Meeting, Dallas, TX (16th March 2014).

3. Computational Molecular Science Meeting, Cirencester, UK (15th June 2012).

2. Modelling of Biologically-Inspired Photoactive Systems Meeting, Marseilles, France (31st March 2011).

1. Computational Molecular Science Meeting, Cirencester, UK (28th June 2010).

Awards

4. Student Champion Award, 2022.

3. College of Arts & Sciences Award for Outstanding Graduate Mentor, 2022.

2. National Science Foundation CAREER Award, 2021.

1. Student Champion Award, 2021.

Synergistic Activities

5. Reviewer for Journal of the American Chemical Society, Journal of Chemical Theory and Computation, Journal of Physical Chemistry, Industrial and Engineering Chemistry Research, Applied Nano Materials, Langmuir, Department of Energy, American Chemical Society Petroleum Research Fund.

4. Louisville area American Chemical Society section board-member.

3. Membership of the American Chemical Society.

2. Developer of MQCPack library (https://github.com/MQCPack/mqcpack) and contributor to the Gaussian suite of electronic structure programs (www.gaussian.com).

1. ACS Scholars Program mentor (2018-2020).