Lee Michael THOMPSON *Curriculum vitae*

Contact Information

Department of Chemistry
University of Louisville
Room 251, Chemistry Bld.
3230 S. Brook St. Louisville, KY
USA, 40208

Phone: +1 (502) 852-0730
Mobile: +1 (209) 201-2140
E-mail: lee.thompson.1@louisville.edu
Website: www.lmthompsongroup.com

Current Position

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

Previous Employment

Postdoctoral Scholar (Jan 2014 to May 2017)
Laboratory of Prof. Hrant P. Hratchian,
Chemistry and Chemical Biology, University of California, Merced

Education

Doctor of Philosophy in Chemistry (PhD) (Oct 2009 to Sep 2013)
Imperial College London
Supervisor: Prof. Michael J. Bearpark
Co-Supervisor: Dr. Jasper J. van Thor
Thesis Title: Molecular Vibrations and Chemical Reactivity in Complex Environments

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

Teaching Experience

Lecture Courses

- **University of Lousiville**: CHEM 202 *General Chemistry II* (Fall 2017); CHEM 660 *Advanced Physical Chemistry* (Fall 2018); CHEM 446 *Physical Chemistry II* (Spring 2019, Spring 2020); CHEM 555 *Theory and Application of Computational Chemistry* (Fall 2019)

Workshops

- **NSCCS**: Gaussian for Beginners (20-21th Sep 2016); Gaussian for Beginners (16-17th Sep 2015); Gaussian for Beginners (17-18th Sep 2014); Applied Computational Chemistry (23-24th Apr 2013); Gaussian for Beginners (11-12th Sep 2012); Applied Computational Chemistry (17-18th Apr 2012); Gaussian for Advanced Users (15th Sep 2011); Gaussian for Beginners (14th Sep 2011)
- **Gaussian**: New Delhi, India (6-10th Jan 2014); Wroclaw, Poland (24-28th Jun 2013); New Delhi, India (17-21th Dec 2012); Santiago de Compostela, Spain (11-15th Jul 2011)
- **Imperial College London**: Dynamics of Triatomic Systems - developed code and GUI for module (2011-2012); Transition States Modelling (2010-2012); Molecular Orbitals and Symmetry (2009-2012); 1st Year Physical Chemistry Lab (16-26th Nov 2009)

Skills

Language Skills:

- English (native), Spanish (B2), French (A1)

Computing Skills:

- Fortran 77, Fortran 90-08, OpenMP, MATLAB, Mathematica, Maple, Perl, Python, AWK, SED, UNIX shell scripting, TEX (LATEX, BIBTEX), Vim, Microsoft Office, Git, Gnuplot, Microsoft Windows, Apple OS X, Linux

Professional Membership

American Chemical Society (ACS); Royal Society of Chemistry (RSC) – Associate Member (AMRSC)

PUBLICATIONS

1. Kempfer-Robertson, E. M.; **Thompson, L. M.** Control of Photo and Thermal Isomerization Pathways in Azobenzene with Oriented External Electric Fields, *Journal of the American Chemical Society* **2019**, submitted for publication.

2. Mahler, A. D.; **Thompson, L. M.** Resonant Hartree-Fock Calculations of Excited States: Selection of Basis Functions and Conditions for Variational Behavior, *Journal of Chemical Physics* **2019**, submitted for publication.

3. 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.

4. 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* **2019**, 16(1), 154–163.

5. 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.

6. 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.

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

8. **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.

9. 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.

10. **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.

11. 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.

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

13. **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.

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

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

16. **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.

17. 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.

18. 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.

Talks and Posters

1. **Thompson, L. M.** *Excited state resonating Hartree-Fock models of excited state processes in methane activation applications* (Abstract #473) Invited talk presented at 258th ACS National Meeting & Exposition, 28th August 2019, San Diego, USA

2. **Thompson, L. M.** *Resonant Hartree-Fock description of multistate reaction pathways* Invited talk presented at South East Theoretical Chemistry Association Meeting 2019, 17th May 2019, Knoxville, USA

3. **Thompson, L. M.** *Single-reference wavefunctions as first-order approximations for efficient variational and orthogonal description of multistate reaction pathways* Department of Chemical Engineering Seminar, University of Louisville, 5th April 2019, Louisville, USA

4. **Thompson, L. M.** *Single-reference wavefunctions as first-order approximations for efficient variational and orthogonal description of multistate reaction pathways* Department of Physics Colloquium, University of Louisville, 29th March 2019, Louisville, USA

5. **Thompson, L. M.** *Methods for localized electronic structure in photocatalytic mechanisms* (Abstract #562) Contributed talk presented at 256th ACS National Meeting & Exposition, 23rd August 2018, Boston, USA

6. **Thompson, L. M.** *Computational Methodologies for Assignment of Transition-Metal-Oxide Cluster Species in Photoelectron Detachment Spectra* Invited talk presented at the Contemporary Computational Chemistry Symposium held during SERMACS 2017, 9th November 2017, Charlotte, USA

7. **Thompson, L. M.** *Exploring the Structure of Transition Metal Oxide Clusters* Invited talk presented at the Brown and Williamson Departmental Seminar, 27th January 2017, Louisville, USA

8. **Thompson, L. M.**; Hratchian, H. P. *Simulation of Transition Metal Oxide Cluster Photodetachment Spectra* (Abstract #M38) Poster presented at Theory and Application of Computational Chemistry, 29th August 2016, Seattle, USA

9. **Thompson, L. M.**; Hratchian, H. P. *Efficient Simulation of Transition Metal Cluster Photoelectron Spectra Using Approximate Projection* (Abstract #01758) Contributed talk presented at 99th Canadian Chemistry Conference & Exhibition, 9th June 2016, Halifax, Canada

10. **Thompson, L. M.**; Hratchian, H. P. *Efficient Modelling of Transition Metal Systems Using Approximate Projection: Development and Applications* (Abstract #141) Contributed talk presented at 251st ACS National Meeting & Exposition, 14th March 2016, San Diego, USA

11. **Thompson, L. M.**; Hratchian, H. P. *Transition Metal Oxide Clusters: Accounting for Spin Contamination* (Abstract #639) Contributed talk presented at 250th ACS National Meeting & Exposition, 20th August 2015, Boston, USA

12. **Thompson, L. M.**; Hratchian, H. P. *Resolving Multiple Spin Contaminants Using Approximate Projection* (Abstract #362) Contributed talk presented at 250th ACS National Meeting & Exposition, 19th August 2015, Boston, USA

13. **Thompson, L. M.**; Hratchian, H. P. *Metal oxide clusters: The need for spin pure states* (Abstract #610) Poster presented at 248th ACS National Meeting & Exposition, 13th August 2014, San Francisco, USA

14. **Thompson, L. M.**; Champion, P. M.; Sage, J. T.; Frisch, M. J.; van Thor, J. V.; Bearpark, M. J. *Analytical Harmonic Modes of GFP: Chromophore Response to Environment* (Abstract #48) Contributed talk presented at 247th ACS National Meeting & Exposition, 16th March 2014, Dallas, USA

15. **Thompson, L. M.** *Using the ONIOM Method in the Study of Large Molecules* Invited Talk presented at NSCCS Applied Computational Chemistry Workshop for Synthetic Chemists, 24th April 2014, London, UK

16. **Thompson, L. M.** *Vibrational Frequencies of Large Molecules Using the ONIOM method* Invited Talk presented at NSCCS Gaussian Workshop for Beginners, 12th September 2012, London, UK

17. **Thompson, L. M.**; Forester, A.; Vreven T.; Bearpark, M. J. *Computing and Analysing Vibrational Frequencies of Large Molecules Using the ONIOM method* Poster presented at Computational Molecular Science 2012, 25th June 2012, Cirencester, UK

18. **Thompson, L. M.**; Bearpark, M. J. *Vibrational Analysis of Photoactive Proteins using ONIOM* Contributed talk presented at Modelling of Biologically-Inspired Photoactive Systems, 31st March 2011, Marseilles, France

19. **Thompson, L. M.**; Forester, A.; Bearpark, M. J. *Vibrational Analysis of Photoactive Proteins using ONIOM* Poster presented at Computational Molecular Science 2010, 28th June 2010, Cirencester, UK