
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.lmthompsonsgroup.com
CURRENT POSITION	Assistant Professor Department of Chemistry, University of Louisville	(Aug 2017 to present)
PREVIOUS EMPLOYMENT	Postdoctoral Scholar Laboratory of Prof. Hrant P. Hratchian, Chemistry and Chemical Biology, University of California, Merced	(Jan 2014 to May 2017)
EDUCATION	Doctor of Philosophy in Chemistry (PhD) 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) University of Southampton First Class Honours	(Oct 2009 to Sep 2013) (Oct 2004 to Jul 2008)
PROFESSIONAL DEVELOPMENT	Advanced OpenMP University of Edinburgh, Edinburgh 13th European Summer School in Quantum Chemistry Hotel Torre Normanna, Sicily UK Theoretical Chemistry Summer School University of Oxford, Oxford Graduate School Development Courses Imperial College, London	(5-8 th Dec 2011) (18-30 th Sep 2011) (5-17 th Sep 2010) (2009-2010)
TEACHING EXPERIENCE	NSCCS Workshops <ul style="list-style-type: none"><i>Courses:</i> 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 Workshops <ul style="list-style-type: none"><i>Courses:</i> 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 <ul style="list-style-type: none"><i>Courses:</i> Dynamics of Triatomic Systems Workshop - developed code and GUI for module (2011-2012); Transition States Modelling Workshop (2010-2012); Molecular Orbitals and Symmetry Workshop (2009-2012); 1st Year Physical Chemistry Lab (16-26th Nov 2009)	(2011-2016) (2011-2014) (2009-2012)

SKILLS

Foreign Language Skills:

- Spanish (B2), French (A1)

Computer Programming:

- Fortran 77, Fortran 90-08, OpenMP, MATLAB, Mathematica, Maple, Perl, Python, AWK, SED, UNIX shell scripting

Productivity Applications:

- \TeX (\LaTeX , \BibTeX), Vim, Microsoft Office, Git, GNUPlot

Operating Systems:

- Microsoft Windows, Apple OS X, Linux

PROFESSIONAL MEMBERSHIP

[American Chemical Society \(ACS\)](#)

[Royal Society of Chemistry \(RSC\)](#)

- Membership Grade: Associate Member, Royal Society of Chemistry (AMRSC)

[American Association for the Advancement of Science \(AAAS\)](#)

PUBLICATIONS

1. Sheng, X.; **Thompson, L. M.**; Hratchian, H. P. Predicting Spin Crossover Gaps and Exchange Coupling Constants for Transition Metal Complexes: Improving Density Functional Theory with Approximate Projection, to be submitted for publication.
2. **Thompson, L. M.**; Hratchian, H. P. An Analysis of the Strengths and Weaknesses of Approximate Projection Theories, submitted for publication, 2016.
3. **Thompson, L. M.**; Jarrold, C. C.; Hratchian, H. P. [Explaining the \$\text{MoVO}_4^-\$ Photoelectron Spectrum: Rationalization of Geometric and Electronic Structure](#) *Journal of Chemical Physics* **2017**, 146(10), 104301.
4. Abdullahi, M. H.; **Thompson, L. M.**; Bearpark, M. J.; Vinader, V.; Afarinkia, K. [The Role of Substituents in Retro Diels-Alder Extrusion of \$\text{CO}_2\$ from 2\(H\)-pyrone Cycloadducts](#) *Tetrahedron* **2016**, 72(40), 6021–6024.
5. **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. [\$\text{MoNbO}_2^-\$ Theoretical Photoelectron Spectra Accounting for Spin Contamination in Density Functional Theory](#) *Journal of Physical Chemistry A* **2015**, 119(32), 8744–8751.
7. **Thompson, L. M.**; Hratchian, H. P. [Second Derivatives for Approximate Spin Projection Methods](#) *Journal of Chemical Physics* **2015**, 142(5), 054106.
8. **Thompson, L. M.**; Hratchian, H. P. [Spin Projection with Double Hybrid Density Functional Theory](#) *Journal of Chemical Physics* **2014**, 141(3), 034108.
9. **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.

TALKS AND
POSTERS

10. 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.
11. 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.
1. **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
2. **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
3. **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
4. **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
5. **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
6. **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
7. **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
8. **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
9. **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
10. **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
11. **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

12. **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
13. **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
14. **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