# Lee Michael THOMPSON *Curriculum vitae*


**Contact Information**

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**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)

**Workshops**

- **NSCCS Workshops**: Gaussian for Beginners (20-21$^{th}$ Sep 2016); Gaussian for Beginners (16-17$^{th}$ Sep 2015); Gaussian for Beginners (17-18$^{th}$ Sep 2014); Applied Computational Chemistry (23-24$^{th}$ Apr 2013); Gaussian for Beginners (11-12$^{th}$ Sep 2012); Applied Computational Chemistry (17-18$^{th}$ Apr 2012); Gaussian for Advanced Users (15$^{th}$ Sep 2011); Gaussian for Beginners (14$^{th}$ Sep 2011)
- **Gaussian Workshops**: New Delhi, India (6-10$^{th}$ Jan 2014); Wroclaw, Poland (24-28$^{th}$ Jun 2013); New Delhi, India (17-21$^{th}$ Dec 2012); Santiago de Compostela, Spain (11-15$^{th}$ Jul 2011)
- **Imperial College London**: 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 (16-26$^{th}$ 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); American Association for the Advancement of Science (AAAS)

PUBLICATIONS

1. Ogunwale, M.; Knipp, R.; Evrard, C.; **Thompson, L. M.**; Nantz, M.; Fu, X.-A. The Influence of $\beta$-Ammonium Substitution on the Reaction Kinetics of Aminooxy Condensations with Aldehydes and Ketones, *Journal of Physical Chemistry A* **2018**, submitted for publication.

2. **Thompson, L. M.**; Hratchian, H. P. On Approximate Projection Models, *Molecular Physics* **2018**, accepted for publication.

3. **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.

4. 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.

5. **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.

6. 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.

8. **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.

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

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

11. **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.

12. 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.

13. 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.** *Methods for localized electronic structure in photocatalytic mechanisms* Contributed talk presented at 256 ACS National Meeting & Exposition, 23rd August 2018, Boston, USA

2. **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

3. **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

4. **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

5. **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

6. **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

7. **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

8. **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

9. **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

10. **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

11. **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

12. **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

13. **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

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

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