
Professional Experience

Position	Institution	From	To
Postdoctoral Researcher	Center for Astrophysics, Harvard & Smithsonian (USA)	06/02/2017	Present
Postgraduate Teaching Fellow	University of New South Wales (AUS)	01/03/2014	01/03/2016
Laboratory Demonstrator	University of Sydney (AUS)	01/03/2013	01/11/2013
Laboratory Demonstrator	University of Sydney (AUS)	01/03/2012	01/11/2012

Education

Degree	Institution	From	To
Doctor of Philosophy	University of New South Wales (AUS)	08/03/2013	16/01/2017
Bachelor of Science (Honours)	University of Sydney (AUS)	08/03/2009	12/04/2013

Prizes and awards

Year	Award
2019	IAU Laboratory Astrophysics Travel Grant
2016	ATA Young Scientist Prize
2014	RACI Physical Chemistry Division Poster Prize
2014	RACI Physical Chemistry Division Best Questions Prize
2014	University of New South Wales Postgraduate Research Student Scholarship
2013–2016	Australian Postgraduate Award Scholarship
2013	University of Sydney Postgraduate Research Student Scholarship

Year	Program	Status	Value
<i>TITLE: Understanding Interstellar Aromatic Chemistry: An Integrated Experimental, Theoretical, and Astronomical Approach</i>			
2019 – 2022	National Science Foundation – AST Division	Co-investigator (PI: M. C. McCarthy)	\$435,367
<i>TITLE: Scholarly Studies – Understanding Interstellar Aromatic Chemistry</i>			
2018	Smithsonian Institution	Co-investigator (PI: M. C. McCarthy)	\$73,916

Publications

21 publications in peer-reviewed scientific journals; total citations: 98; h-index: 5

1. Lee, K. L. K. & McCarthy, M. Bayesian Analysis of Theoretical Rotational Constants from Low-Cost Electronic Structure Methods. *The Journal of Physical Chemistry A* **5**, 898–910 (2020).
2. McCarthy, M. & Lee, K. L. K. Molecule Identification with Rotational Spectroscopy and Probabilistic Deep Learning. *The Journal of Physical Chemistry A* **124**, 3002–3017 (2020).
3. Raymond, A. W., Lee, K. L. K., McCarthy, M. C., Drouin, B. J. & Mazur, E. Detecting Laser-Volatilized Salts with a Miniature 100-GHz Spectrometer. *The Journal of Physical Chemistry A* (2020).
4. Lee, K. L. K. & McCarthy, M. Study of Benzene Fragmentation, Isomerization, and Growth Using Microwave Spectroscopy. *The Journal of Physical Chemistry Letters* **10**, 2408–2413 (2019).
5. Lee, K. L. K., McGuire, B. A. & McCarthy, M. C. Gas-phase synthetic pathways to benzene and benzonitrile: a combined microwave and thermochemical investigation. *Physical Chemistry Chemical Physics* **21**, 2946–2956 (2019).
6. Lee, K. L. K., Thorwirth, S., Martin-Drumel, M.-A. & McCarthy, M. C. Generation and structural characterization of Ge carbides GeC. *Physical Chemistry Chemical Physics* **21**, 18911–18919 (2019).
7. Martin-Drumel, M.-A., Lee, K. L. K., Belloche, A., Zingsheim, O., Thorwirth, S., Müller, H. S. P., Lewen, F., Garrod, R. T., Menten, K. M., McCarthy, M. C. & Schlemmer, S. Submillimeter spectroscopy and astronomical searches of vinyl mercaptan, C₂H₃SH. *Astronomy & Astrophysics* **623**, A167 (2019).
8. McGuire, B. A., Shingledecker, C. N., Willis, E. R., Kelvin Lee, K. L., Martin-Drumel, M.-A., Blake, G. A., Brogan, C. L., Burkhardt, A. M., Caselli, P., Chuang, K.-J., El-Abd, S., Hunter, T. R., Ioppolo, S., Linnartz, H., Remijan, A. J., Xue, C. & McCarthy, M. C. Searches for Interstellar HCCSH and H₂ CCS. *The Astrophysical Journal* **883**, 201 (2019).
9. Porterfield, J. P., Lee, K. L. K., Dell’Isola, V., Carroll, P. B. & McCarthy, M. C. Characterization of the simplest hydroperoxide ester, hydroperoxymethyl formate, a precursor of atmospheric aerosols. *Physical Chemistry Chemical Physics* **21**, 18065–18070 (2019).
10. Decin, L., Danilovich, T., Gobrecht, D., Plane, J. M. C., Richards, A. M. S., Gottlieb, C. A. & Lee, K. L. K. Constraints on Metal Oxide and Metal Hydroxide Abundances in the Winds of AGB Stars: Potential Detection of FeO in R Dor. *The Astrophysical Journal* **855**, 113 (2018).
11. Harrison, A. W., Kharazmi, A., Shaw, M. F., Quinn, M. S., Lee, K. L. K., Nauta, K., Rowell, K. N., Jordan, M. J. T. & Kable, S. H. Dynamics and quantum yields of H₂ + CH₂CO as a primary photolysis channel in CH₃CHO. *Physical Chemistry Chemical Physics* **21**, 14284–14295 (2018).

12. Lattanzi, V., Spezzano, S., Laas, J. C., Chantzios, J., Bizzocchi, L., Lee, K. L. K., McCarthy, M. C. & Caselli, P. HSCO⁺ and DSCO⁺: a multi-technique approach in the laboratory for the spectroscopy of interstellar ions. *Astronomy & Astrophysics* **620**, A184 (2018).
13. Lee, K. L. K., Gottlieb, C. A. & McCarthy, M. C. Laboratory Rotational Spectra of Silyl Isocyanide. *The Astrophysical Journal* **860**, 63 (2018).
14. Lee, K. L. K., Martin-Drumel, M.-A., Lattanzi, V., McGuire, B. A., Caselli, P. & McCarthy, M. C. Gas phase detection and rotational spectroscopy of ethynethiol, HCCSH. *Molecular Physics* **6**, 1–11 (2018).
15. Lee, K. L. K., Quinn, M. S., Kolmann, S. J., Kable, S. H. & Jordan, M. J. T. Zero-point energy conservation in classical trajectory simulations: Application to H₂CO. *The Journal of Chemical Physics* **148**, 194113 (2018).
16. McGuire, B. A., Martin-Drumel, M.-A., Lee, K. L. K., Stanton, J. F., Gottlieb, C. A. & McCarthy, M. C. Vibrational satellites of C₂S, C₃S, and C₄S: microwave spectral taxonomy as a stepping stone to the millimeter-wave band. *Physical Chemistry Chemical Physics* **20**, 13870–13889 (2018).
17. Lee, K. L. K., Nauta, K. & Kable, S. H. Photodissociation of acetone from 266 to 312 nm: Dynamics of CH₃ + CH₃CO channels on the S₀ and T₁ states. *The Journal of Chemical Physics* **146**, 044304 (2017).
18. McCarthy, M. C., Lee, K. L. K. & Stanton, J. F. Detection and structural characterization of nitrosamide H₂NNO: A central intermediate in deNO_x processes. *The Journal of Chemical Physics* **147**, 134301 (2017).
19. Lee, K. L. K., Rabidoux, S. M. & Stanton, J. F. Cation States of Ethane: HEAT Calculations and Vibronic Simulations of the Photoelectron Spectrum of Ethane. *The Journal of Physical Chemistry A* **120**, 7548–7553 (2016).
20. Lee, K. L. K., Quinn, M. S., Maccarone, A. T., Nauta, K., Houston, P. L., Reid, S. A., Jordan, M. J. T. & Kable, S. H. Two roaming pathways in the photolysis of CH₃CHO between 328 and 308 nm. *Chemical Science* **5**, 4633–4638 (2014).
21. Krechkivska, O., Liu, Y., Lee, K. L. K., Nauta, K., Kable, S. H. & Schmidt, T. W. Triple-Resonance Spectroscopy Reveals the Excitation Spectrum of Very Cold, Isomer-Specific Protonated Naphthalene. *The Journal of Physical Chemistry Letters* **4**, 3728–3732 (2013).

Invited Talks & Conference Presentations

5. Lee, K. L. K. *An Experimentalist's Guide to Rotational Constants With Low-Cost Theory* 74th International Symposium on Molecular Spectroscopy: June 19-23, 2019 at The University of Illinois at Urbana-Champaign. (2019).
1. Lee, K. L. K. *Analysis of Benzene Discharge Chemistry with Rotational Spectroscopy* 26th Colloquium on High Resolution Molecular Spectroscopy (Dijon, France, 2019).
6. Lee, K. L. K. *Benzene's Inferno, Part II: Automated Analysis and Identification* 74th International Symposium on Molecular Spectroscopy: June 19-23, 2019 at The University of Illinois at Urbana-Champaign. (2019).
2. Lee, K. L. K. *Computer Assisted Spectral Analysis* **Invited seminar** (Green Bank Observatory, WV, 2019).
7. Lee, K. L. K. *Detection of C₃H⁺ Toward W49N: Elucidating The Molecular Complexity of The Diffuse Interstellar Gas* 74th International Symposium on Molecular Spectroscopy: June 19-23, 2019 at The University of Illinois at Urbana-Champaign. (2019).
3. Lee, K. L. K. *Interstellar Aromatic Chemistry* (Institute des Sciences Moléculaires d'Orsay, France, 2019). **Invited seminar**.
4. Lee, K. L. K. *Rotational Constants from Low-Cost Electronic Structure Theory* 26th Colloquium on High Resolution Molecular Spectroscopy Poster presentation. (Dijon, France, 2019).

8. Lee, K. L. K. *Rotational Spectroscopy of Silicon-Nitrogen Molecules: SiH₃NC and NH₂Si* 74th International Symposium on Molecular Spectroscopy: June 19-23, 2019 at The University of Illinois at Urbana-Champaign. (2019).
9. Lee, K. L. K. *Interstellar aromatic chemistry: a combined laboratory, observational, and theoretical perspective* IAUS 350 Laboratory Astrophysics: from Observations to Interpretation (Cambridge, UK, 2019).
10. Lee, K. L. K. *Astrochemistry in the Laboratory - Combining Theory and Experiment* (Brookhaven National Laboratories, USA, 2018). **Invited seminar.**
14. Lee, K. L. K. *Investigation of thioketene isomers: microwave spectroscopy and formation chemistry of HCCSH* 73rd International Symposium on Molecular Spectroscopy: June 19-23, 2018 at The University of Illinois at Urbana-Champaign. Talk TJ03 (2018).
11. Lee, K. L. K. *Laboratory Studies into Aromatic Molecule Formation in the Interstellar Medium* (University of Bristol, UK, 2018). **Invited seminar.**
12. Lee, K. L. K. & McCarthy, M. C. *High accuracy thermochemistry and kinetics of the HCN/HNC system* Quantum Chemistry, Dynamics and Reaction Modeling for Molecules and Materials in Astrophysical Environments at the 255th American Chemical Society National Meeting (2018).
13. Lee, K. L. K. & McCarthy, M. C. *High accuracy thermochemistry and kinetics of the HCN/HNC system* 73rd International Symposium on Molecular Spectroscopy: June 19-23, 2018 at The University of Illinois at Urbana-Champaign. Talk WL10 (2018).
15. McCarthy, M. C. & Lee, K. L. K. *Carbon-13 studies of sulfur-terminated carbon chains: chemical bonding, molecular structures and formation pathways* 73rd International Symposium on Molecular Spectroscopy: June 19-23, 2018 at The University of Illinois at Urbana-Champaign (2018).
16. Lee, K. L. K., McCarthy, M. C. & Stanton, J. F. *On the Relative Stability of Cumulenone and Aldehyde Isomers: when we HEAT345(Q) Things UP* 72nd International Symposium on Molecular Spectroscopy: June 19-23, 2017 at The University of Illinois at Urbana-Champaign. Talk WF10 (2017).
17. Lee, K. L. K. *Photodissociation of nitrous oxide and friends* Royal Australian Chemical Institute PhysChem Student Conference (Adelaide, Australia, 2016).
18. Lee, K. L. K. *Acetone photodissociation: what the fragments tell us* The International Chemical Congress of Pacific Basin Societies (Pacifichem) Poster presentation. (Hawaii, USA, 2015).
19. Lee, K. L. K. *Acetone photodissociation dynamics: three mechanisms, one radical* Royal Australian Chemical Institute PhysChem Conference (Hobart, Australia, 2014).
20. Lee, K. L. K. *Near Threshold Photodissociation Dynamics of Acetone* Royal Australian Chemical Institute National Congress Poster presentation (Adelaide, Australia, 2014).
21. Lee, K. L. K. *Quasi-Classical Trajectories on a Zero-Point Energy Corrected Potential Energy Surface* Royal Australian Chemical Institute PhysChem Student Conference (Blue Mountains, Australia, 2013).
22. Lee, K. L. K. *Zero-Point Energy Corrections to Quasi-Classical Trajectory Simulations in Roaming Reactions* 59th Western Spectroscopy Conference (Asilomar, USA, 2013).

Year	Activity
2020	Undergraduate supervision; Ms Jacqueline Patterson (Indiana University, Bloomington) on machine learning approaches to automated spectral analysis methods as part of the Center for Astrophysics Harvard & Smithsonian Research Experiences for Undergraduates (REU) program.
2019	Undergraduate supervision; Mr Alex MacLeod (UMass, Lowell) on neural network analysis of rotational spectra as part of the NSF funded Latino Initiative at the Center for Astrophysics Harvard & Smithsonian.
2019	Presented workshop on optimizing Python code for readability and speed to undergraduate students part of the NSF funded Latino Initiative at the Center for Astrophysics Harvard & Smithsonian
2019	Undergraduate supervision; Ms Valentina Dell'isola (U. Bologna) on high-resolution microwave spectroscopy of carbon-sulfur molecules as part of her Master's thesis work.
2018	Presented workshop on reproducible scientific workflows to undergraduate students part of the NSF funded Latino Initiative at the Center for Astrophysics Harvard & Smithsonian.
2017	Undergraduate supervision; Ms Jasmine Oliveira (UMass, Boston) on the SpecDATA project as part of the NSF funded Latino Initiative at the Center for Astrophysics Harvard & Smithsonian.
2016	Undergraduate supervision; mentored two undergraduate students on a machine learning and a laboratory project respectively, at the University of New South Wales.
