KIN LONG KELVIN LEE

Postdoctoral Researcher — Center for Astrophysics | Harvard & Smithsonian

https://laserkelvin.github.io

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PROFESSIONAL EXPERIENCE

Since Feb 2017

Center for Astrophysics | Harvard & Smithsonian—Cambridge, MA

Postdoctoral Research Fellow

- Projects at the intersection of astronomy, chemistry, and data science.
- CO-AUTHORED 22 PUBLICATIONS TO DATE WITH 86 CITATIONS
- Lead successful grant proposals from the Smithsonian Institution, National Science Foundation, and NASA; *over $500,000 USD* in public funding.
- Enabled discovery of new molecules in the interstellar medium, as an active scientific member and observer in three large scale astronomy projects.
- Developed machine learning models and open-source frameworks for analyzing molecular spectra.
- Mentored early career researchers on scientific and numerical Python.
- Supervised undergraduate and graduate students on multiple published research projects.
- Curated multiple data sets for machine learning and statistics from quantum chemistry calculations.

Aug 2016—Feb 2017

University of New South Wales—Sydney, Australia

Postdoctoral Research Fellow

- Researched photochemistry of atmospheric molecules.
- Prepared manuscripts for publication in peer-reviewed chemistry journals.
- Experiments involved laser spectroscopy and ion imaging techniques.
- Mentored undergraduate students on theoretical and experimental research projects.
- Developed open-source tools for automated analysis of ion images and trajectory simulations.
- High accuracy quantum chemistry of photolytic reactions.

Mar 2013—Aug 2016

University of New South Wales—Sydney, Australia

Doctor of Philosophy in Chemistry

- Researched photodestruction of atmospheric pollutants under single-molecule

conditions.
- Experiments involved laser spectroscopy and ion imaging techniques.
- Developed open-source tools for automated analysis of ion images and trajectory simulations.
- Receipient of the *Australian Postgraduate Award*.
- Worked as postgraduate teaching fellow; lead weekly tutorials for undergraduate chemistry classes.

SELECTED OPEN-SOURCE CONTRIBUTIONS

Python	PySpecTools is a library I developed to help analyze broadband spectral data with an emphasis on reproducibility and collaboration. FTSpecViewer application written in Python and Qt5 to process Fourier-transform microwave data. Repro-repo cookie-cutter template I designed to promote simple reproducible projects. Spectron3000 web app written with Dash for viewing astronomical spectra. RMG Python program for graph-based generation of molecules.

My Github repository contains all of the coding projects I have worked on.

SELECTED RECENT PROJECTS

- Characterization of miniature spectrometer designed for spacecraft/rover missions
  - Spectrometer designed by the Jet Propulsion Laboratory for trace detection of salts and organic molecules using rotational spectroscopy.
- Identification of unknown molecules using probabilistic deep learning models
  - Developed high performance, probabilistic neural network architectures to identify unknown molecules with rotational spectroscopy.
- Accuracy and uncertainty benchmarking of quantum chemical methods with Bayesian methods.
  - Determined systematic uncertainties with low-cost electronic structure theory using Hamiltonian Monte Carlo models.
- Developed open-source tools for analyzing broadband spectral data
  - Founder of PySpectools, a Python library that helps manage analysis of rotational spectra consisting of hundreds of spectral features and distinct species.
- Spectroscopy and quantum chemistry expert of GOTHAM and ARKHAM observing projects of Taurus Molecular Cloud-1
  - Provided laboratory and theoretical critical for the analysis of large scale observing results.

SKILLS & EXPERTISE

High-performance computing	Distributed computing workflows on national and instituitional HPC platforms. Massively parallel quantum chemistry calculations.
Python	General object-oriented programming and development with Python 3. Exploratory data analysis and data pipeline design with `numpy`, `dask`, `pandas`.

	Data visualization using `matplotlib`, `plotly`, and `bokeh`.
	Baseline machine learning models with `scikit-learn`.
	Deep learning models with PyTorch and Tensorflow.
	Probabilstic Bayesian models with `pymc3`.
Writing	Author of 22 peer-reviewed articles for expert audiences.
	Review Editor of open-access journal "Frontiers of Astronomy and Space Science".
	Writer on Medium and TowardsDataScience for general audiences.
	Proficient in document workflows with LaTeX, `pandoc`, and Markdown.
Oral Presentations	Presented scientific results at over 18 international conferences in Chemistry and Astronomy.
	Presented workshops on reproducible Python and code practices to undergraduates at the Center for Astrophysics | Harvard & Smithsonian.
Experimental Techniques	Pulsed laser maintenance and operation.
	High vacuum technology.
	High speed radio and microwave electronics.

EDUCATION

2013—2016

University of New South Wales—Sydney, Australia

Doctor of Philosophy in Chemistry

Title: *Spectroscopy and Photodissociation of Small Atmospheric Molecules* under the supervision of Professor Scott Kable and Professor Meredith Jordan.

2008—2012

University of Sydney—Sydney, Australia

Bachelor of Science; First Class Honours in Chemistry & Plant Sciences

Title: *Roaming Reaction Dynamics in Small Aldehydes* under the supervision of Professor Scott Kable and Professor Meredith Jordan.

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