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.
- 22 PUBLICATIONS TO DATE; 86 CITATIONS.
- Experiments with high-resolution rotational spectroscopy of transient molecules.
- Data analysis includes probabilistic machine learning models, quantum chemistry, and distributed computing.
- Developed open-source tools for analyzing broadband spectra.
- Public outreach and mentoring activities with the NSF Latino Initiative; taught workshops on Python each summer.
- Co-investigator on grants from the Smithsonian Institution, National Science Foundation, and NASA; *over $500,000 USD* in public funding.

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.
- 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*.
- 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

- SUPERVISED 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 that infer stochiometries and functionalization in unknown molecules from rotational spectroscopy parameters.
- 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
  - Developed PYSPECTOOLS, A PYTHON LIBRARY that helps manage analysis of rotational spectra consisting of hundreds of spectral features and distinct species.

SKILLS & EXPERTISE

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.

	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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