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

- Worked on novel research projects at the intersection of astronomy, chemistry, and data science.
- CO-AUTHORED 22 PUBLICATIONS TO DATE WITH 89 CITATIONS, as a project leader and as part of large teams.
- Lead successful grant proposals as co-investigator from the Smithsonian Institution, National Science Foundation, and NASA; *raised over $500,000 USD* in public funding.
- Developed machine learning models and open-source frameworks for automated analysis of wide band spectroscopic data.
- Created productive collaborations between the Center for Astrophysics and international groups, facilitated with open-sourced tools I developed.
- Mentored early career researchers on scientific and numerical Python, and reproducibile workflows.
- Used quantum chemical calculations to guide microwave spectroscopy experiments of transient molecules.

Aug 2016—Feb 2017

University of New South Wales—Sydney, Australia

Postdoctoral Research Fellow

- Researched photochemistry of atmospheric molecules; destruction of pollutants under UV irradiation.
- Lead the experiments, analysis, and dissemination of multiple research projects through peer-reviewed publications and oral presentations at international conferences.
- 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 chemical calculations of photolytic reactions of pollutants; quasi-classical trajectory simulations of how molecules dissociate.

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

Computing	Distributed computing workflows on national and instituitional HPC platforms. Massively parallel quantum chemistry calculations. Efficient computational workflows with `numpy` and `julia`. Source control managment with `git` and `dvc`. Reproducible environments with `conda` and `docker`. Exploratory data analysis with Jupyter/Google Co-Labs. General object-oriented programming and development with Python 3.
Data analysis	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 model (e.g. Monte Carlo methods) development with `pymc3` and

	`Flux.jl`.
Writing	Review Editor of open-access journal "Frontiers of Astronomy and Space Science". 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	Reviewer for SciPy 2020. 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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