

# 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 16 PUBLICATIONS; SIX AS LEAD AUTHOR, one as project leader, and remainder 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 by open-sourced tools I developed.
- Mentored early career researchers on scientific and numerical Python, and reproducible workflows.
- Performed quantum chemical calculations to guide microwave spectroscopy experiments of transient molecules.
- Reviewed new research articles in major publications: role as referee/reviewer on 13 manuscripts.

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 by lasers.
- Lead the experiments, analysis, and dissemination of multiple research projects through peer-reviewed publications and oral presentations at international conferences.
- Published five publications in major peer-reviewed journals; three as lead author.
- Mentored undergraduate students on various 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 institutional HPC platforms. Massively parallel quantum chemistry calculations. Efficient computational workflows with <code>numpy</code> and <code>julia</code> . Source control management with <code>git</code> and <code>dvc</code> . Reproducible environments with <code>conda</code> and <code>docker</code> . Exploratory data analysis in notebook environments. General object-oriented programming and development with Python 3.
Data analysis	Exploratory data analysis and data pipeline design with <code>numpy</code> , <code>dask</code> , <code>pandas</code> . Data visualization using <code>matplotlib</code> , <code>plotly</code> , and <code>bokeh</code> . Baseline machine learning models with <code>scikit-learn</code> . Deep learning models with <code>PyTorch</code> and <code>Tensorflow</code> . Probabilistic model (e.g. Monte Carlo methods) development with <code>pymc3</code> , <code>pyro</code> , and <code>Flux.jl</code> .
Written communication	Author of 21 peer-reviewed articles for expert audiences; 94 citations to date. Review Editor of open-access journal “Frontiers of Astronomy and Space Science”. Writer on <a href="#">MEDIUM</a> and <a href="#">TowardsDataScience</a> for general audiences. Proficient in document workflows with <code>LaTeX</code> , <code>pandoc</code> , and <code>Markdown</code> .
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	Pulsed laser maintenance and operation.

Techniques                      High vacuum technology.  
   High speed radio and microwave electronics.

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EDUCATION

2020                              Coursera  
   *Deep Learning Specialization*

- Completed three out of five courses required for this specialization.
- Foundations for projects in machine learning and deep learning by [deeplearning.ai](https://www.deeplearning.ai)

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.