Kin Long Kelvin Lee

Specialties: Python, Deep Learning, Probabilistic Models, Chemistry, Spectroscopy, Grant Procurement

PhD in Chemistry, BSc (H1) in Chemistry/Plant Sciences

Professional Experience

Since Feb 2017 *Postdoctoral Researcher at Center for Astrophysics | Harvard & Smithsonian* (Cambridge, MA)

Worked on many diverse research projects at the intersection of Astronomy, Chemistry, and Data Science with Dr. Michael McCarthy. The general theme of my research has been on investigating the role of chemistry in astrophysical processes, and developing novel methods for automating data analysis. Over the last three years, I have **published 21 peer-reviewed articles** in high-impact journals. Three of my most recent projects include:

- Identification of unknown molecules using probabilistic deep learning models
  - Developed high performance, probabilistic neural network architectures that infer stochiometries and functionalization in unknown molecules.
- 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 Python library that helps manage analysis of rotational spectra consisting of hundreds of spectral features, and up to 100 distinct species.

I also actively took part in promoting programming literacy and mentoring programs, particularly with the NSF funded Latino Initiative. Each summer, I teach a workshop on reproducibile scientific workflows and coding practices in Python. I have also mentored four graduate students working on various projects in the laboratory, which have allowed me to build my leadership skills.

Over the last three years, I have played an active role in securing public funding; I am co-investigator on grants from the Smithsonian Institution and National Science Foundation worth over $500,000.

Aug 2016-Feb 2017 *Postdoctoral Researcher at University of New South Wales* (Kable group - Sydney, Australia)

Researched the photochemistry of atmospheric molecules using a combination of laser spectroscopy and velocity-mapped ion imaging techniques; how molecules in the atmosphere are destroyed by light. Part of my responsibilities included maintenance of ns-laser systems and high vacuum equipment, as well as preparation of manuscripts for publication. I also developed several Python tools for automated analysis of ion images and for analyzing trajectory simulations of chemical reactions.

Mar 2013-Aug 2016 *PhD in Chemistry at University of New South Wales* (Sydney, Australia)

Researched how molecules (pollutants) undergo photodissociation in the atmosphere; particularly acetone and nitrous oxide. Over the course of my PhD, I published four articles in major peer-reviewed journals. As part of my studies, I developed skills in academic/report writing, reproducible workflows in Python, and the operation of lasers and high vacuum equipment.

Over the course of my PhD studies, I presented my work at six international conferences, and won two early-career researcher awards. During this time I also worked as a Postgraduate Teaching Fellow, where I taught undergraduate tutorials.

Selected Open-source Contributions

Python PySpecTools is a library I developed to help analyze broadband spectral data with an emphasis on reproducibility and collaobration.
FTSpecViewer application written in Python and Qt5 to process Fourier-transform microwave data.
Repro-repo cookiecutter 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.

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 21 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.

Education

2013-2016	*PhD in Chemistry at University of New South Wales* (Sydney, Australia)
	Title: *Spectroscopy and Photodissociation of Small Atmospheric Molecules* under the supervision of Professor Scott Kable and Professor Meredith Jordan.
2008-2012	*Bachelor of Science, First Class Honours at University of Sydney* (Sydney, Australia)
	Title: *Roaming Reaction Dynamics in Small Aldehydes* under the supervision of Professor Scott Kable and Professor Meredith Jordan.

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