Keiran Rowell | Résumé

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Employment

Postdoctoral Research Assistant
School of of Chemistry USYD *2020–current*
Performing analytics on the data generated during my PhD to develop generalisable photoreaction models. Building a framework to automatically detect photoreactive motifs in molecules and apply theoretical chemistry predictions, allowing users to enter an arbitrary molecular structure and receive a best-estimate reaction rate backed by theoretical chemistry.

Casual Science Teacher
Matrix Education *2016–2020*
Student experience questionnaire 2-year average : **4.7/5**
Top quality high school curriculum tuition. Classroom lessons, quiz marking, workbook development. Development work for the Matrix+ online lessons, and the chemistry 'Max Series' exam preparation books.

Postgraduate Teaching Fellow & Tutor
School of of Chemistry UNSW *2016–2018, 2019–2020*
1st year tutorials, mentoring, 3rd year physical chemistry resource development, exam marking, outreach.

Laboratory Demonstrator
School of Chemistry UNSW *2014–2015, 2020*
Laboratory teaching, supervision, and marking, for 1st, 2nd and 3rd year chemistry students.

Casual Science Tutor
Scholani Education College *2011–2012*
Primary and high school 10–20 student classes. Marking duties. Assisting students in homework room.

Education

PhD - Theoretical Chemistry
University of New South Wales *2016–2020*
Thesis Title: Structure–Activity Relationships for Carbonyl Photolysis
Supervisors: Prof. Scott Kable, Prof. Meredith Jordan
Assessment: **A,A** — All categories 'Outstanding' — Nominated for a Dean's Award
Thesis Summary
Using high performance computing to run quantum chemistry calculations, I simulated the ultraviolet (UV) light-initiated chemical reactions that break down molecules in the atmosphere. The use of 'from the ground up' computational modelling allowed me to predict all of the possible reactions pathways of 38 different molecules, for which hundreds of reactive geometries and energies needed to be calculated. For comparison there are only 19 well validated experimental rates included in the entire Master Chemical Mechanism; a long-running multi-university initiative to generate a detailed model of atmospheric chemistry. Through the calculations of my PhD work, I was able to develop 'structure-activity relationships' that predicted chemical reactivity from the structural motifs in a molecule.

The end users of my PhD research would be the atmospheric modelling and UV degradation community. The modelling protocols developed in my PhD can accurately predict experimental photoreaction energies, and the structural relationships I found provide a cost-free and comprehensive estimate of reaction energies wherever experimental data are missing.

B.Sc. (Adv.) Honours Class 1 - Angyal Prize - Chemistry
University of New South Wales *2011–2014*
Dissertation Title: Computational Studies on the Basis of 'Neighbour Exclusion' in a Series of Diacridine and Di-(terpy)Pt(II) Thiol Bisintercalators: combined MD & FMO approaches
Supervisors: A/Prof. Graham Ball, A/Prof. Larry Wakelin, Dr Donald Thomas

Programming Experience

Python

- Developed resources for Python and Jupyter Notebooks instruction in 3rd year chemistry
  - Received 'Rising Star' award for introduction of Jupyter Notebooks into UNSW's 3rd year physical chemistry course. The Notebooks format is now adopted in some 1st and 2nd year chemistry courses
  - Wrote 'Intro to Python and Plotting' lessons for physical science students
- Command line tools for physical chemistry and spectroscopy
  - Rotational constant calculator
  - Exploratory datasets; visualisation and correlation of spectroscopic data with pandas and matplotlib
  - Automated transition state searches, and parsing output to create several-hundred line input files
- Updating Python interfacing code for Fortran in-house 'Grow' software
  - Added support for more recent quantum chemistry packages and formatting
- Developed code to process, search, and plot 1000s of pair-wise energies between DNA fragments
  - Energies from fragment-based quantum chemistry calculations parsed with Python into data structures that were queryable and then automatically plotted with matplotlib
  - Pair-wise DNA fragment interactions could be decomposed into energy types to yield physical insight

High Performance Computing

- 5+ years experience in Linux and high performance computing environments
  - Bash scripting, Python scripts, Linux system management
  - Batch scheduling systems (PBS Pro), module and enviroment management
  - Command line tools: vim, grep, wc, awk, sed, regex, chmod, tar, *etc.*
  - Attended regular UNSW ResTech seminars on computational research methods and data management

C

- Bioinformatics (BINF3020, **HD**) coursework
  - Efficient string alignment and matching (DNA and protein sequences)
  - Statistical modelling (Hidden Markov models, Bayesian networks)
  - Wrote pair-wise sequence alignment code, amino acid mutator for protein evolution simulation
- Computer science (COMP1917, **DN**) undergraduate instruction
  - Memory allocation/management, debugging, makefiles
  - Pointers, linked lists, stacks, queues, heaps
  - Sorting algorithms, search trees
  - Object-oriented programming, classes, inheritance from COMP1927 recordings

Fortran

- Worked with 'Grow' in-house Fortran code for potential energy surface interpolation
  - Added a module to randomise initial velocity directions and magnitude while conserving total energy, in order to efficiently sample the phase space of the dynamics
  - Modified variables, data, printing, and formatting as required for new chemical systems
  - Managed compilation, debugging and some performance profiling with ifort and gfort

Version Control

- Initiated and implemented code management for the Jordan research group
  - Migrated codebases stored in disparate locations to central USYD GitHub Enterprise repository
  - Data from my Honours and PhD work stored on data DVDs and UNSW Research Data Archive

Teaching and Mentorship

Postgraduate Teaching Fellowship

- Selected for the first cohort of Postgraduate teaching fellows to teach first year UNSW Chemistry tutorials
- 3 year tenure, 75 hours commitment per year, **resource development specialisation**
- Structured mentorship, feedback, weekly teaching brief and debrief meetings

- Developed physical chemistry resources for a 1st year and a 3rd year chemistry course
- One of first two tutors to deliver online Blackboard Collaborate tutorials for UNSW's COVID response

University Subjects Taught

- 3rd year physical chemistry – class demonstrator and coding facilitator — **satisfaction rose 65% to 94%**
- 2nd year physical chemistry – laboratory demonstrator
- 1st year chemistry – tutor and laboratory demonstrator — tutor feedback form average **4.6/5**

Academic Mentorship

- Mentored theoretical chemistry Honours student in performing quantum chemistry calculations
  - This included understanding of the fundamental principles of molecular electronic structure, scientific computing, gaussian functions and basis sets, algorithms, bra–ket notation, and molecular spectroscopy
  - Additional mentorship of Honours research students in literature searching, academic writing, document management, presentation skills
- Mentored several experimental PhD students in how to perform chemistry calculations
  - Most had little-to-no computing background so this included familiarisation with the command line, SSH, data management, resource allocation, big $\mathcal{O}(n)$ notation for estimating computational expense
- Mentored newer Teaching Fellows in delivering chemistry tutorials and pedagogical technique

Presentation Highlights

Group and 'Super-group' organiser: Organised weekly group meetings, and monthly four-group 'super-group' meetings, sourcing speakers (including external academics), coordinating schedules.
Ran my own workshops on quantum chemistry calculations, and chemical visualisation masterclasses.

APATCC 2019 (*volunteer, poster*) — USYD - Sydney
Asia-Pacific Association of Theoretical and Computational Chemists — *Sep. 2019*

ISTCP-X (*poster*) — UiT - Tromsø
10th Triennial Congress of the International Society of Theoretical Chemical Physics — *Jul. 2019*

QUACCS 3.0 (*talk*) — ANU Campus - Kioloa
Computational chemistry workshops & student 'chalk 'n talk' presentations — *Dec. 2018*
Workshops attended: Global Optimisation, Stationary point search, Write your own HF & MP2, QM/MM

ACCOMC 2018 (*poster*) — CSIRO - Aspendale
Atmospheric composition & modelling conference for Australasian region — *Dec. 2018*

Awards

Rising Star - PhD Casual Teacher
UNSW Faculty of Science — *2018*
Awarded to two casual PhD tutors who have demonstrated educational excellence in a single year

Poster presenter prize
Association of Molecular Modellers of Australia — *2015*
Best Honours-level poster presenter

Angyal prize
School of Chemistry UNSW — *2014*
Top mark in Chemistry Honours

Bosworth prize
School of Chemistry UNSW — *2013*
Equal 1st in third year Physical Chemistry

Summer Vacation Research Scholarship
School of Chemistry UNSW — *2012*
UNSW Science competitive scholarships for enrolled undergraduates to gain early research experience

Publications

1. — **Rowell, K.**; Thomas, D.; Ball, G.; Wakelin, L., "Molecular Dynamic Simulations of Diacridine Binding to DNA: Indications that C6 Diacridine can Bisintercalate Spanning Two Base Pairs", *Biopolymers*, **(2020)**, doi:10.1002/bip.23409

2. — **Rowell, K.**; Kable, S; Jordan, M., "Substituent Effects on the Norrish Type I α-bond Cleavage of Tropospheically Important Carbonyls", *The Journal of Physical Chemistry A*, **(2020)**, doi:10.1021/acs.jpca.9b05534

3. — Harrison, A.; Kharazmi, A.; Shaw, M.; Quinn, M.; Lee, K.; Klaas, N.; **Rowell, K.**; Jordan, M.; Kable, S., "Dynamics and Quantum Yields of $H_2 + CH_2CO$ as a Primary Photolysis Channel in CH_3CHO", *Physical Chemistry Chemical Physics*, **(2019)**, doi:10.1039/C8CP06412A

Pre-prints

Juan, C.Z.T; Syme, A-M.; **Rowell, K**.; *et al.*, "Infrared Spectroscopy of Phosphorus-containing Molecules", *Frontiers in Astronomy and Space Science* [submitted]

Rowell, K.; Kable, S.; Jordan, M., "Predicting Carbonyl Excitation Energies Efficiently Using EOM-CC Trends", doi:10.26434/chemrxiv.12917369.v2

Rowell, K.; Kable, S.; Jordan, M., "Structural Causes of the Singlet/Triplet Preferences of Norrish Type II Reactions in Carbonyls", doi:10.26434/chemrxiv.12941702.v1

Rowell, K.; Kable, S.; Jordan, M., "The Under-Explored Possibilities of Ground State Carbonyl Photochemistry", doi:10.26434/chemrxiv.12950822.v1

Computer Skills

Programming: Python, Bash, C, Fortran

Documents: LaTeX, Overleaf, Word, LibreOffice

Quantum Chemistry: ORCA, G16, DALTON

Analysis: Excel, Python, Pandas

Figures: Matplotlib, Inkscape, GNU IMP

Molecular Dynamics: Amber, VMD

References (details upon request)

Supervisors

- Prof. Scott Kable (Supervisor - HoS Chem UNSW)
- Prof. Meredith Jordan (Co-supervisor - USYD)
- Dr Kim Lapere (Teaching Fellow Coordinator)

Tutoring Employment

- Dr Alex Argyros (Head of Science)
- Dr Peter Jurd (Head of Junior Science)
- Vivian Law (Head of Chemistry)