Dr Keiran Rowell | Curriculum Vitæ

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Employment

Bioinformatician
Australian Proteomics Analysis Facility *2022–present*
Working with R code for mass spectrometry proteomics analysis. Refactoring an existing experiment-specific codebase to be more modular, allowing easy addition of new analysis functions. Mentoring a final-year PhD candidate in refactoring code, while learning how to clean-up terse R scripts. Retiring legacy systems.

Research Computing Support Officer
Research Technology Services, UNSW *2021–2022*
HPC and research computing support, including day-to-day system administration. Installation and troubleshooting of scientific software. HPC outreach and uptake, including weekly 'Hacky Hour' sessions.

Postdoctoral Research Associate
School of Chemistry, USYD *2020–2021*
Continuation of my PhD research. Multiconfigurational quantum chemistry calculations (CASSCF & CASPT2). Mentoring PhD candidates to submission and employment. Preparing research papers.

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.

Postgraduate Teaching Fellow & Tutor
School 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.

Education

PhD - Computational 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: Structure-activity relationships for carbonyl UV photochemistry were comprehensively elucidated for 38 molecules across seven structural classes, for ten unique reaction mechanisms, on all relevant ground (S_0) and excited (S_1 & T_1) states. Theoretical protocols for photolysis thresholds and excitation energies were extensively validated to the available spectroscopic and kinetic data for $\pm$ 10 kJ/mol accuracy.
B.Sc. (Adv.) - Chemistry - Honours Class 1 - Angyal Prize (Top Performance)
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
  - 'Rising Star' award for introducing Jupyter Notebooks interactive coding lessons
  - Wrote 'Intro to Python and plotting' lessons for physical science students

- Molecular rotational constants calculator; exploratory data analysis with `pandas` and `matplotlib`
- Developed code to process, search, and plot 1000s of pair-wise energies between DNA fragments

High Performance Computing

- 5+ years experience running within Linux and high performance computing environments
  - Bash scripting, environment modules, basic sys. admin., schedulers (PBS Pro)
  - Fundamental command line tools, compilers: `vim, git, awk, ch(mod|own|grp)`, *etc.*
  - Attended regular ResTech seminars on computational research methods and data management

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Undergraduate coursework

- Bioinformatics (BINF3020, **HD**)
  - String alignment (DNA and protein sequences), Statistical modelling (HMM, Bayes net)
  - Collaborated to develop a web app for *saccharomyces cerevisiae* regulatory networks
- Computer science (COMP1917, **DN**)
  - Memory allocation, alogrithms and data structures.
  - Object-oriented programming, classes, inheritance from COMP1927 recordings

Fortran

- Worked with 'Grow' in-house Fortran code for potential energy surface interpolation

Teaching and Mentorship

Postgraduate Teaching Fellowship

- 3 year tenure, 75 hours commitment per year, tutorials, developed physical chemistry resources

University Subjects Taught

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

Academic Mentorship

- Mentored theoretical chemistry Honours students in performing computational chemistry research
- Mentored newer Teaching Fellows in effective chemistry tutorials and pedagogical techniques

Presentation Highlights

Group & 'Super-group' organiser: Organised weekly group and monthly 'super-group' meetings: sourcing academic speakers, coordinating schedules. Ran computing & 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*

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

Awards

Rising Star - PhD Casual Teacher
School of Chemistry UNSW *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 undergraduates to gain early research experience

Computer Skills

Programming: Python, Bash, C
Documents: Word, LaTeX, Overleaf
Analysis: Excel, Python, Pandas
Figures: Matplotlib, Inkscape, GNU IMP

Publications (refer to my Google Scholar page)

1. — **Rowell, K.**; Kable, S.; Jordan, M., "An assessment of the tropospherically accessible photo-initiated ground state chemistry of carbonyls", *Atmospheric Chemistry and Physics*, **(2022)**, doi:10.5194/acp-22-929-2022

2. — Juan, C.Z.T; Syme, A-M.; **Rowell, K**.; *et al.*, "Infrared Spectroscopy of Phosphorus-containing Molecules", *Frontiers in Astronomy and Space Science*, **(2021)**, doi:10.3389/fspas.2021.639068

3. — **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

4. — **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

5. — 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

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