# Dr Keiran Rowell | Curriculum Vitæ

+(61) 422 774 330 • keiran.rowell@gmail.com • keiran-rowell
orcid.org/0000-0001-6955-1167

## Research Interests

### Topics

Electronic structure calculations, Photochemistry, Atmospheric chemistry, Carbonyl reactions, Structure–activity relationships, Gas-phase reactions, Code development, Spectrosopic experiments

### Methods

DFT (*including double-hybrid*), Excited state methods (*TD-DFT, EOM-CC*), Multiconfigurational methods (*CASSCF, CASPT2*), Composite methods, PES construction & dynamics (*'Grow' – modified Shepard interpolation*), Reaction rate constants (*RRKM & $\mu$VTST*), Kinetics (*MultiWell*)

## Education

**PhD - Computational Atmospheric Photochemistry**
*The 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

A comprehensive study of the photochemistry of 38 carbonyl species across seven structural classes, for ten unique reaction mechanisms, on all ground ($S_0$) and excited ($S_1$ & $T_1$) electronic states relevant to UV photolysis. Encompasses all 18 core photolysis reactions included in the Master Chemical Mechanism, and extends the data to hundreds of calculated photolysis thresholds, from which generalisable structure–activity relationships (SARs) were identified. This framework of SARs will allow atmospheric models to move beyond unmodified 'surrogate' photolysis of carbonyls, and better model these radical forming reactions that are of central importance to atmospheric chemistry. Theoretical protocols for photolysis thresholds and excitation energies were extensively validated to the available spectroscopic and kinetic data for $\pm$ 10 kJ/mol accuracy.

Selected examiner comments

*"I am very satisfied that the candidate has demonstrated an outstanding achievement against all of the examination criteria"*
*"The thesis represents a very significant and very substantial work."*
*"I was impressed by the candidate's careful characterization of the various theoretical methods and as a logical consequence his masterful choices among them."*
*"...strived to provide insight essentially about everything he calculated...All of the conclusions are supported by the data."*
*"...the standard of accuracy is very high and I compliment the candidate on this, particularly given the complexity of the information presented."*
*"The Appendices are a good idea...These short summaries of additional explanation are very helpful, both to the reader and no doubt future researchers."*
*"...shows a thorough understanding and engagement with the literature over a very broad range of themes."*

**B.Sc. (Adv.) Honours Class 1 - 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

## 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 $\alpha$-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

## 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 1$^{st}$ 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

## Group Workshops Organised

**ORCA workshop**: Configuration, simple & block input, "Jacob's ladder", singlepoint energies, geometry opmitisations, frequencies & Hessians, excited-state calculations, RI approximations, auxiliary basis sets, double-hybrid functionals, spectroscopic properties, NMR prediction

**Chemical visualisation masterclass**: VMD, Pymol, Matplotlib, orbital analysis, trajectories

**Group and 'Super-group' organiser**: Organised weekly group meetings, and monthly four group 'super-group' meetings, sourcing speakers (including external academics), coordinating schedules

## Conference Presentations

**PhysChem Webinar** (*2 minute thesis*) Online
*RACI Physical Chemistry Webinar* *Sep. 2020*

**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*

**RACI Phys.Chem. Division Conference** (*poster*) UWA - Perth
*Principle Phys.Chem. meeting on spectroscopy, computational chemistry, & surfaces* *Feb. 2019*

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

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

**RACI Centennary Congress** (*poster*) MCEC - Melbourne
*Congress for 100th anniversary of the Royal Australian Chemical Institute* *Jul. 2017*

**RACI Phys.Chem. Student Conference** (*talk*) RSL - Katoomba
*Student run conference for physical chemistry graduate students to present work* *Sep. 2016*

**Molecular Modelling 2015** (*poster*) UNSW - Sydney
*Organised by the Association of Molecular Modellers of Australasia (AMMA)* *Dec. 2015*

**Molecular Modelling 2014** (*poster*) Lamington National Park - Queensland
*Theme: "From biomolecules to materials"* *Jul. 2014*

## Teaching Experience

**Postgraduate Teaching Fellow & Tutor**
*School of of Chemistry UNSW* *2016–2018, 2019–2020*
Tutor feedback form average **4.6/5**
1st year tutorials, mentoring, 3rd year physical chemistry resource development, exam marking, outreach

**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

**Lab Demonstrator**
*School of Chemistry UNSW* *2014–2015, 2019–2020*
CHEM3011 course **satisfaction rose from 65% to 94%**
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

## Computer Skills

**Quantum Chemistry**: ORCA, G16, DALTON
**Molecular Dynamics**: Amber, VMD
**Programming**: Python, Bash, C, Fortran
**Analysis**: Excel, Python, Pandas
**Documents**: LaTeX, Overleaf, Word, LibreOffice
**Figures**: Matplotlib, Chemdraw, GNU IMP

## 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)