Dr Keiran Rowell | Curriculum Vitæ

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Research Interests

Topics

Electronic structure calculations, Photochemistry, Atmospheric chemistry, Carbonyl reactions, Structure–activity relationships, Gas-phase reactions, Code development, Spectroscopic 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*), Molecular dynamics (*Amber*), Reaction kinetics (*RRKM, MultiWell*)

Education

PhD - Computational Carbonyl 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.) - Chemistry - Honours Class 1 - Angyal Prize
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 α-bond Cleavage of Tropospheically Important Carbonyls", *The Journal of Physical Chemistry A*, **(2019)**, 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

4. — Juan, C.Z.T; Syme, A-M.; **Rowell, K.**; *et al.*, "Computational Infrared Spectroscopy of 956 Phosphorus-bearing Molecules", *Frontiers in Astronomy and Space Science* [accepted]

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

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 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 experiencee

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 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)

Academic

- Prof. Scott Kable (Supervisor - HoS Chem UNSW)
- Prof. Meredith Jordan (Co-supervisor - USYD)
- Dr Laura McKemmish (Lecturer - UNSW)

Tutoring Employment

- Dr Alex Argyros (Head of Science - Matrix)
- Dr Kim Lapere (Teaching Fellow Coordinator)
- Dr Peter Jurd (Head of Junior Science - Matrix)