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NEWSLETTER - 15 MARCH 2023

Greetings from the Physical Chemistry Division of the RACI, our first webinar last week got off to a flying start with Dr Laura McKemmish and Dr Philip Jiale Feng bridging astrochemistry down to triplet states! Over the next month we have two more exciting webinar series across Machine Learning, Radical Ions, Hydrogen Fuel Cells, and even DNA! Read below to find out more.

2023 RACI Physical Chemistry Division Lectureship Nominations Extended to Midnight Friday 23 June

The Division of Physical Chemistry has separated the 2022 and 2023 lectureships and subsequently is extending the call for nominations for the 2023 RACI Physical Chemistry Division Lectureship. We are seeking applications from early to mid-career researchers who display research excellence, independence, creativity, impact and vision in any area of physical chemistry, including theoretical/computational chemistry. The deadline extension ensures effective communication to all Division members, gives everyone a breather after ARC DP submissions, and recognizes that March is a busy time for teaching.

Applicants will be assessed by explicitly considering five equally weighted criteria:

- research excellence: demonstrated by, for example, research output, impact (as evidenced by, for example, citations, invitations to present or submit articles, or similar), funding & award successes
- independence: clear evidence of research leadership demonstrated by, for example, establishing new ideas, directions & collaborations separate from previous advisors, mentorship of students
- creativity: clear evidence of imaginative, novel & useful ideas addressing important problems and/or important gaps in the literature
- impact: impact of their research papers & ideas, and research-related service activities (e.g. conference organisation, RACI involvement, workshops, support of students outside their group etc) on any relevant community
- vision: clear & strong idea of their research portfolio, strengths & future directions.

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Note, that we define research broadly in this award as novel contributions to knowledge; within the scope of physical and theoretical/ computational chemistry, contributions to technological innovation and implementation, educational innovation (not routine delivery of courses) or similar can form part of the nominee's case.

The Lectureship application documentation has been updated, which more explicitly specifies the assessment process including procedures to manage perceived and real conflicts of interest.

As part of this award, the Physical Chemistry Division of the RACI has established a funded Lectureship to allow the awardee to travel around Australia and present the results of their research work. In the 2023 lectureship (giving lectures in 2023-24), lectures may be delivered in person and/or virtually.

Nominations must be submitted to the Division by **midnight on Friday 23 June 2023.** Electronic submissions only will be accepted and should be sent to email: **Physical.div@raci.org.au**. For all enquiries, please contact the Division Secretary, Dr Laura McKemmish, or Chair, Prof David Wilson.

WEBINAR SERIES - The Physical Chemistry Division Webinars Fortnightly Wednesdays 12:00noon AEDT – Free to attend

1. Wednesday 22nd of March: 12:00noon – 1:00pm AEDT
Prof. David Winkler - **Problems and Promises of AI/ML for Applied Molecular Sciences**
Mr Oisin Shiels - **Kinetics of Distonic Radical Ions: Predicting and Controlling the Influence of Internal Electric Fields**

2. Wednesday 5th of April: 12:00noon – 1:00pm AEDT
Dr Quentin Meyer - **How to Make Hydrogen Fuel Cells Cheaper and More Efficient**
Dr Kimberley Callaghan - **A Simple(r) Approach to Making DNA: Entropy**

Zoom Link:
https://unimelb.zoom.us/j/85813477461?pwd=U2RzNU1scmlpaWtNa3pzMXNpeUY4UT09
Password: 271211
Calendar Invite (Webinar Series - March to May): iCal

We are also calling for volunteers to chair these Webinar sessions, if you're interested please send an email through to Physical.div@raci.org.au.

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Physical Chemistry Division

Job Openings

Prof. Ben Powell (University of Queensland) has a postdoctoral researcher position open in his group to work on the theory of spin crossover materials. Find out more or apply here: https://www.seek.com.au/job/61855463

Have something to advertise to the RACI Phys Chem Division?

Upcoming job opportunities, Ph.D. scholarships, some research you're particularly proud of, or a conference you're organising – anything Phys Chem related please send us an email on: Physical.div@raci.org.au and we will look to incorporate into future newsletters

Webinar Abstracts for the Wednesday 22nd of March 2023

Prof. David Winkler: La Trobe Institute for Molecular Science, Monash Institute of Pharmaceutical Sciences, School of Pharmacy, University of Nottingham

Problems and Promises of AI/ML for Applied Molecular Sciences

Artificial intelligence and particularly, its subset of machine learning has created a large paradigm shift in the way science and most other areas of human endeavour are performed. The past few years have seen the amazing developments in prediction of protein structure from sequence (AlphaFold and its ilk) and more general machine intelligence (ChatGPT). In the molecular and biological sciences, the use of ML to solve complex problems has increased exponentially.

This seminar will draw on three decades of research into the application of ML to chemical and biological problems. Work initially was to understand the main factors influencing the quality, robustness, and applicability of ML models. This involved understanding the effects of data set size, quality and diversity and the relevance of descriptors/features (mathematical entities encoding properties of molecules or materials). We also tackled problems of sparse feature selection, model overfitting and overtraining, and choice of ML algorithm. We also studied the best way to quantify predictivity of models using test sets, and have more recently tackled the complex problems of model interpretation and feature importance, still thorny issues, inversion of models using generative methods, and the first steps towards fully autonomous (no human in the loop) molecular design systems.

The seminar will provide several recent examples of the use of ML to design new molecules and materials, their application to micro-topographies and well as chemistry, and the application of evolutionary methods to explore larger regions of chemical, materials, and topographical spaces to find useful solutions.

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Oisin Shiels: The University of Wollongong

Kinetics of Distonic Radical Ions: Predicting and Controlling the Influence of Internal Electric Fields

Oisin is a third year PhD candidate studying under the supervision of Prof. Adam Trevitt at the University of Wollongong. His research project, titled 'understanding the effect of charge on the reactivity and fate of gas-phase radicals', attempts to uncover the key factors controlling ion-molecule reactions by exploiting both experimental mass spectrometry techniques and theoretical calculations.

In this presentation a modelling framework for ion-molecule reactions is investigated targeting the reactions of eighteen distonic ions featuring phenyl-type sigma radicals. The statistical reaction-rate model, utilising Rice-Ramsperger-Kassel-Marcus (RRKM) theory master equation, was developed for each reaction to predict the second-order rate coefficient, indicating that it is the key (barrierless) entrance transition state that controls the kinetics. Expanding on this work, protonation site specific reactions of two quinazolinium distonic radical cation isomers are also investigated using a combination of ion mobility filtering and quadrupole ion-trap mass spectrometry techniques. These reactions have the advantage of modifying the orientation of the internal electric field without altering the rest of the reacting molecule, therefore probing solely for the changing electrostatic effect. Ion-molecule reactions of these mobility-selected isomers reveal that reaction rates double when the proton approaches the radical site due to through-space (electrostatic) effects. Importantly, various popular quantum chemistry methods were found to be insufficient to predict these experimental differences with only the double-hybrid method providing adequate results.

Physical Chemistry Division Committee: