M^4 Symposium – 11 November 2022

Storey Hall Auditorium, RMIT, 336-348 Swanston St, Melbourne

Welcome / Opening Remarks

8.30am – 8.50am Registration
8.50am – 9.00am Dr Nicholas Smith – Welcoming participants & opening the meeting

Keynote Lecture 1: *chaired by Dr Andrew Christofferson*
9.00am – 9.50am **Dr Lars Goerigk (University of Melbourne)** – Tackling valence excitation energies with time-dependent DFT: tips, warnings and latest developments

Keynote Lecture 2: *chaired by Dr Tu Le*
9.50am – 10.40am **Dr Drew Berry (WEHI) –** The molecular engines of Metabolism

Tea Break

10.40am – 11.00am Served in the foyer

Morning Session: Materials *chaired by Dr. Fangfang Chen*
11.00am – 11.30am **Prof Katya Pas (Monash University)** – Fully ab initio multi-scale calculations enabled by GPU technology
11.30am – 12.00am **A/Prof Zhe Liu (University of Melbourne)** – Solvation-involved nanoionics: using high-performance computing for new physics and developing multiscale models for engineering design
12.00pm – 12.30pm **Prof Michelle Spencer (RMIT)** – DFT Modelling of Materials for Battery and Electronic Device Applications

Lunch

12.30pm – 1.15pm Served in the foyer

Afternoon Session: Biomolecular *chaired by Em. Prof. Brian Smith*
1.15pm – 1.45pm **Prof Tiffany Walsh (Deakin University)** – TBC
1.45pm – 2.15pm **Dr Jia Truong (RMIT)** – Computer aided drug design and molecular diagnosis
2.15pm – 2.45pm **Dr Patrick Charchar** – Origins of the pH-Responsive Photoluminescence of Peptide-Functionalized Au Nanoclusters

Afternoon Tea

2.45pm – 3.05pm Served in the foyer

HDR Student Session *chaired by Mr Alexander Hill*

3.05pm – 3.25pm **Rashad Kariuki** – Behaviour of citrate-capped ultrasmall gold nanoparticles on a supported lipid bilayer interface at atomic resolution

3.25pm – 3.45pm **Kenee Custodio** – Identifying structure/property relationships in flame-retardant bio-based resins via molecular dynamics simulations

3.45pm – 4.05pm **Xue Yan** – Lithium ion intercalation induced dynamic evolution of moiré superlattices in graphene on SiC (0001)

4.05pm – 4.25pm **Zahra Zahir** – Robust DFT-based strategies for predicting valence tautomeric complexes

4.25pm – 4.45pm **Anindya Ganguly** – The composition and structure of soot precursors formed by acetylene pyrolysis – Insights from reactive molecular dynamics

Closing Remarks

4.45pm – 4.50pm Dr Nicholas Smith – Closing of the meeting

Poster Session

4.50pm – 6.00pm In the foyer

5:45pm Poster Awards

2022 Organizing Committee

Dr Nicholas Smith	La Trobe University
Dr Andrew Christofferson	RMIT University
Dr Tu Le	RMIT University
Dr Fangfang Chen	Deakin University
Dr David Chalmers	Monash University
Mr Alexander Hill	Swinburne University

Posters

1. **Ashakiran Maibam (RMIT University)**
   Modelling single site catalyst anchored 2D materials for sustainable ammonia production

2. **Alexander Lamb (RMIT University)**
   Aminopropyl grafted silica catalysts for tributyrin transesterification: a molecular dynamics study

3. **Rashad Kariuki (RMIT University)**
   Behavior of citrate-capped ultrasmall gold nanoparticles on a supported lipid bilayer interface at atomic resolution

4. **Sallam Alagawani (Swinburne University)**
   Halogen impact on 4-anilinoquinazoline ERFR-TKIs using IR and NMR spectroscopy

5. **Islam Alagwani (Swinburne University)**
   Evaluation of SARS-CoV-2 Main Protease Inhibitor, ml188, Using Molecular Dynamics and Density Functional Methods

6. **Kenee Kaiser Custodio (Deakin University)**
   Identifying structure/property relationships in flame-retardant bio-based resins *via* molecular dynamics simulations

7. **Garima Dobhal (Deakin University)**
   Development of a force field to model recovery of neodymium from ionic liquids

8. **Shehani Perera (Deakin University)**
   Structure and properties of stone wool glasses and interfaces from molecular dynamics simulations

9. **Xue Yan (University of Melbourne)**
   Lithium ion intercalation induced dynamic evolution of moiré superlattices in graphene on SiC (0001)

10. **Zahra Zahir (University of Melbourne)**
    Robust DFT-based strategies for predicting valence tautomeric complexes

11. **Amy Hancock (University of Melbourne)**
    Do modern TD-DFT methods rise to the challenge of noncovalent excited-state binding?

12. **Dominique Wappett (University of Melbourne)**
    Benchmarking Density Functional Theory for reactions catalysed by metalloenzymes

13. **Diego Chaparro (University of Melbourne)**
    Effect of Al doping and on the formation and growth of flame-made titania nanoparticles

14. **Diego Chaparro (University of Melbourne)**
    Unrevealing Nanosilver leaching by Reactive Molecular Dynamics

15. **Anindya Ganguly (University of Melbourne)**
    The composition and structure of soot precursors formed by acetylene pyrolysis – Insights from reactive molecular dynamics

16. **Sherif Tawfik (Deakin University)**
    Improved lithium diffusion in anion-substituted Li_7TaO_6

17. **Dale Lonsdale (University of Melbourne)**
    A Thorough Investigation of the One-Electron Self-Interaction Error in Model Systems

18. **Karen Bayros (RMIT University)**
    The effect of pinholes on Josephson transport in AlO_x tunnel junctions

19. **Kevin Tran (RMIT University)**
    Restoring the piezoelectric properties of two-dimensional zinc oxide by surface modifications

20. **Felix Schmalz (University of Melbourne)**
    Automated analysis of accelerated reactive molecular dynamics with ChemTraYzer

21. **Annelisa Rigoni (RMIT University)**
    Perfluorocarbons as Electrolyte Additives: Enhancing Li-air Battery Performance

22. **Jiaou Song (University of Melbourne)**
    Homogeneous Nucleation of Nitrogen at Cryogenic Conditions by Atomistic Simulations

23. **Patrick D. Taylor (RMIT University)**
    Tuning the band alignment of van der waals heterostructures with ferroelectric materials

24. **José María Castillo Robles (ICN2, RMIT University)**
    Effect of the electrode potential on the adsorption mechanism of 2-mercaptobenzimidazole (MBI) on Cu (111) surface

25. **Arash Fakharnezhad (University of Melbourne)**
    Evaluation of soot nucleation rate by reactive Molecular Dynamics simulations