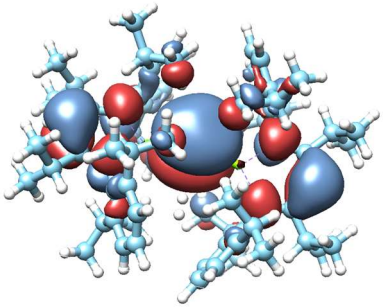
Royal Society of Chemistry

Theoretical Chemistry Group Graduate Student Meeting

RSC INTEREST GROUP
THEORETICAL CHEMISTRY



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University of Warwick
September 13th, 2024

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Overview

2024 Royal Society of Chemistry (RSC) Theoretical Chemistry Group (TCG) Graduate Student Meeting will take place on Friday, 13th September 2024 at the University of Warwick. All lectures along with the poster session will take place on the Main Campus in the **Faculty of Arts Building**. The lectures will take place in **Lecture Theatre 2** and the poster session will be in the **Rehearsal Room**. Refreshments will be served in the **Multi-Purpose Engagement Space** just outside the lecture theatre. The outline programme and posters are summarised below.

Programme

Agenda	Start	Finish
Arrivals / Logistics / Introductions	13:30	13:45
'*Tuning Zeolite Catalysts using Organic Additives*' **Matt Robinson, University of Cardiff**	13:45	14:05
'*Excited State Dynamics of Azanaphthalenes*' **Lauren Bertram, University of Oxford**	14:05	14:25
'*Exploring and Predicting Sigma-hole Interactions in the Cambridge Structural Database*' **Harry Nash, University of Sheffield**	14:25	14:45
'*Transferable Insights: Predicting Molecular Crystal Structures from Prior Convex Hull Landscapes of Similar Systems*' **Jennie Martin, University of Southampton**	14:45	15:05
'Drinks' / Poster Session	15:05	16:00
'*Numerical Tensor Methods for Few Particles Quantum Systems*' **Kammegne Brice, University of Sussex**	16:00	16:20
'*Stereochemistry of the Insertion of Diphenylacetylene in a magnesium(I) Dimer*' **Rochelle Ferns, University of St Andrews**	16:20	16:40
'*Direct Wavepacket Dynamics for Photodissociation and Towards Explicit Solvation*' **Leon Cigrang, University College London**	16:40	17:00
'*Spectral Map: Extracting Collective Variables for Enhanced Sampling Methods*' **Tuğçe Gökdemir, University of Torun, Poland**	17:00	17:20
Prizes & closing remarks	17:20	17:30

Posters

P1	**Gregor Lauter, University of Birmingham** '*Covalent Organic Frameworks for Drug Delivery*'
P2	**Mario Antonio Ongkiko, University of Birmingham** '*Agostic Interactions in the Machine-learning Accelerated Structure Prediction of Mercury Imidazolate MOFs'*
P3	**Marvellous Arabambi, University of Bristol** '*Protein Dynamics and the Temperature Adaptation of Enzyme Catalysis: Simulations of Wild Type and Mutants MalL'*
P4	**Vera Brieskorn, University of Bristol** '*Time-dependent Study of Light-induced Hapticity Changes in a Ruthenium Sandwich Complex'*
P5	**Papu Kalita, University of Bristol** '*L1 Metallo- β -Lactamase Antimicrobial Resistance Enzyme: A Computational Reaction Mechanism Study'*
P6	**Sara Rodriguez, Catalan Institute of Nanoscience and Nanotechnology, Spain** '*Electrolyte Dynamics with Potential-induced Charges on Electrodes: Implementation and Usage as a Starting Point for DFT Calculations'*
P7	**Hassan Kotey, University of Development Studies, Tamale, Ghana** '*In-silico and in-vitro Investigation of Antiviral Compounds Molecular Mechanisms for Potentially Inhibiting Dengue Virus NS2B-NS3 Protease'*
P8	**Chi Cheng Hong, University of Edinburgh** '*Insight into the Correlated Disorder of Fumarate-Based MIL-53 Frameworks: A Computational Study of Free-energy Landscapes'*
P9	**Asma Feriel Khoualdi, Newcastle University** '*De Novo Design of GALK1 Inhibitors in a Flexible Binding Pocket*'
P10	**Annina Lieberherr, University of Oxford** '*Vibrational Strong Coupling in Liquid Water from Cavity Molecular Dynamics*'
P11	**James Merrick, University of Oxford** '*Investigating the Nonadiabatic Dynamics of 1,2-dithiane*'
P12	**Shoubhik Maiti, University of Oxford** '*Automating Transition State Search in Metal Catalysed Reactions*'
P13	**Mamaru Alem, University of Pretoria, South Africa** '*Modeling Charge Transfer States in Phycobilisomes*'
P14	**Nasiru Aminu Rano, University of Sheffield** '*Understanding the Effect of sp^3 Carbon on the Properties of Graphene Quantum Dots for Energy Application*'
P15	**Sophie Bennett, University of Southampton** '*Guiding the Discovery of Non-linear Optical Materials with Crystal Structure Prediction*'
P16	**Jay Johal, University of Southampton** '*Exploring Chemical Space using Evolutionary Algorithms and Crystal Structure Prediction*'

P17	**Humahuti Dihingia, Nicolaus Copernicus University, Torun, Poland** '*Non-orthogonal Pauli-blockade: Towards Accurate Description of Induction in Intermolecular Interaction*'
P18	**Lauren Cook, University College London** '*Simulating Nonadiabatic Dynamics using the Meyer-Miller-Stock-Thoss Hamiltonian: A Comparison of Algorithms*'
P19	**Olivia Bennett, University College London** '*Quantum Dynamic Simulations of Luciferin Derivatives*'
P20	**Andras Petho, University College London** '*Investigating Conductive Properties of a Single-heme Cytochrome*'
P21	**Alexandre Ferreira, University College London** '*Understanding Conformational Free Energy Surfaces through Enhanced Sampling Molecular Dynamics and Unsupervised Clustering Methods*'
P22	**James Green, University College London** '*Theoretical Approaches for Accelerated spectral prediction and rapid screening of chromophores*'
P23	**Jaymee Coonjobeeharry, University College London** 'Mixed-quantum-classical or Fully-quantized Dynamics? A Unified Code to Compare Methods'
P24	*Withdrawn*
P25	**Zhuoyang Ti, University of Warwick** '*Effective Harmonic Potential Study of Mg Interstitials Using Neural Network*'
P26	**Henry Snowden, University of Warwick** '*Non-equilibrium electrons generated from the extended two-temperature model to drive chemical dynamics at surfaces*'
P27	**Alexander Spears, University of Warwick** '*Molecular Dynamics Investigation of the Role of Lattice Heating in Laser-driven Hydrogen Evolution at Copper Surfaces*'
P28	**XueXun Lu, University of Warwick** '*Nonadiabatic Energy Loss During Hydrogen Scattering on Semiconductors*'
P29	**Henjian Jia, University of Warwick** '*Predicting the Blood Brain Barrier Permeability of Druglike Molecules*'
P30	**Thanawitch Chatbipho, University of Warwick** '*Exploring Cluster Surface Adsorption: A Proof-of-Concept Investigation of Phase Space Volume Using Nested Sampling*'
P31	**Daniel Abbott, University of York** '*Using Computational Chemistry to Predict Industrially Important Reactions*'
P32	**Oscar van Vuren, Cardiff University** '*Developing Standardised Modelling Workflows for QM/MM Simulations of Metal Oxides*'