# ICS Final Year PhD Talks 2025

*25th July 2025*

*Postgraduate Centre, PGG.01*

11:00 Welcome

11:05: Introduction, Prof. Scott Dalgarno

11:10: Session 1 Chair: Dr Justyna McKinlay

11:10: Luca Craciunescu “*Utilising Computational Chemistry to Explore Photochemical Processes*”

11:40 Kacper Krakowiak “*Finding Sustainable Replacements for Peat in Scotch Whisky*”

12:10 Fred Powell “*In Search of Enzyme Activation: A Computational Approach to Allosteric Drug Discovery*”

12:40: Lunch, PGR Centre Foyer

13:45 Presenters’ Photo, PGR Foyer

14:00 Session 2 Chair: Dr Liam Donnelly

14:00: Zara Standring “*Thermomechanical recycling of PET based textiles*”

14:30: Leonardo Amicosante “*Green-Light Photocatalysis: Borylated Benzo[c][1,2,5]thiadiazole (BTZ) Enables Continuous Flow Phosphorylation of Quinoline Derivatives*”

15:00: Domantas Laurinavicias “*Applications of Cold Plasma for Polymer Gasification and Recycling*”

15:30 Close and Prizes

# Utilising Computational Chemistry to Explore Photochemical Processes

Luca Craciunescu[a], Martin J. Paterson[a]

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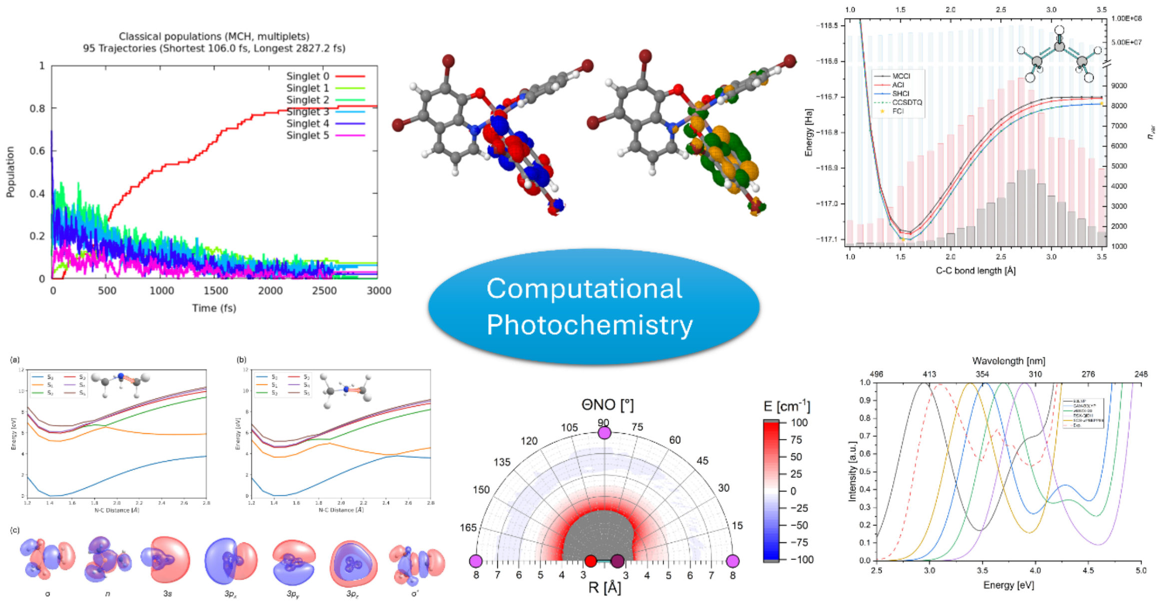
Over the past few decades, computational chemistry has made significant progress. Today, a wide range of software packages and computational tools are available to address nearly any chemical problem. These tools are invaluable both for providing electronic-level insights that complement experimental findings and for offering predictive power to guide future experiments.
In the Paterson group, our primary focus is on the interactions between light and molecules—specifically, photophysical processes and the properties of various molecular systems. This talk will present an overview of several such projects. We begin with high-accuracy explorations of potential energy surfaces involving small systems of three to five atoms, supporting studies of excited-state gas-phase collisions[1,2]. We then move on to the photochemistry and dynamics of small organic molecules, and finally examine the mechanisms of action of light-activated transition metal complexes with medicinal applications, which involve systems comprising several hundred atoms[3]. The talk will also briefly touch on our work in developing and benchmarking electronic structure methods—particularly, the use of selected configuration interaction approaches to achieve accurate, affordable, and black-box multi-reference treatments[4].



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# Finding Sustainable Replacements for Peat in Scotch Whisky

## *Kacper Krakowiak*

Many Scotch Whiskies have a characteristic, smoky flavour imparted into the spirit through burning of peat, particularly those originating from the island of Islay. Peat is a limited resource, due to many years of excavation for fuel and compost. As the availability of peat diminishes, the whisky industry will find it more difficult to source it, affecting the ability to produce smoked whiskies. A possible solution to this issue may be finding a more sustainable replacement for peat, which will provide a similar sensory experience.

In order to identify suitable replacement candidates, a combination of analytical methods have been employed, such as NMR spectroscopy, GC-MS and pyrolysis to study peat and various lignocellulosic materials, including spent coffee grounds and different types of wood. Importantly, these methods were used to analyse the thermal degradation products, which reflect what flavour compounds can be found in the smoke.

Obtained results show that despite differences in composition between the materials, smoke produced by them contains similar compounds, including congeners which have been previously linked to smoky characteristics such as guaiacol, cresols or furfural. Analysis of new make spirits produced using malt smoked with peat and alternative materials have also showed promising similarities in their chemical profiles.

# In Search of Enzyme Activation: A Computational Approach to Allosteric Drug Discovery

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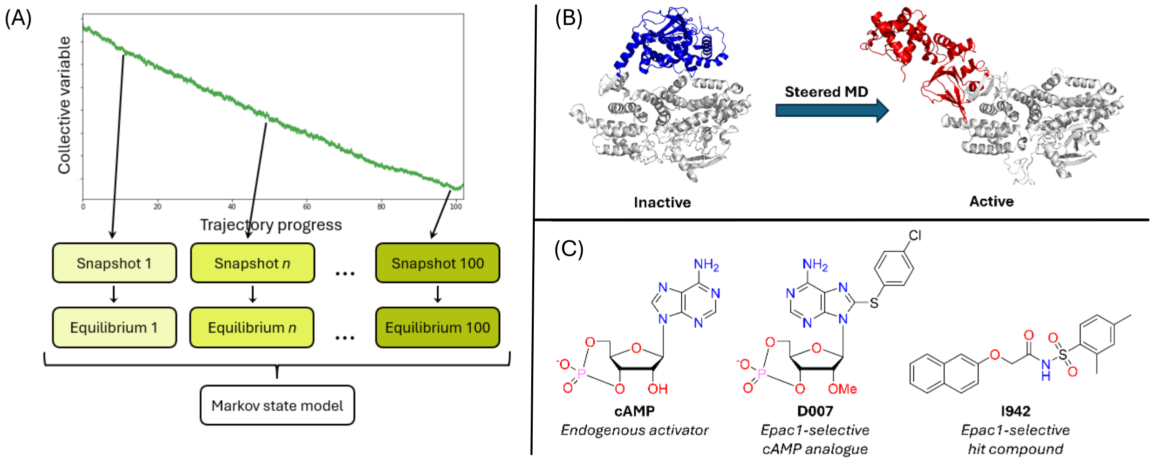

Enzyme activation is an underutilised mode of therapeutic intervention. This is due to its inherent complexity over enzyme inhibition and the lack of standardised methods for discovering enzyme activators. Activation relies on exploiting delicate allosteric networks, which can be effectively probed using molecular modelling techniques.[1] We have developed a computational workflow using steered molecular dynamics (sMD) and Markov state modelling (MSM) to predict the allosteric potential of drug candidates (see *Fig. A*).[2] We first apply sMD to explore the conformational dynamics of the target system, accessing a greater volume of conformational space than can be achieved under routine MD timescales. We then evenly sample the conformational space using multiple short, equilibrium MD trajectories, before pooling the trajectory data and constructing MSMs. This affords us insight into the metastable states of the target protein and predicts how the conformational ensemble will shift upon binding of an allosteric ligand.

We have applied our workflow to the cell-signalling enzyme Epac1.[3] Epac1 activation can counter the vascular inflammation associated with most cardiopulmonary diseases, including idiopathic pulmonary fibrosis (IPF). IPF is a devastating condition which currently lacks an effective treatment and has an 80% mortality rate within 5 years of diagnosis. Roughly 6000 people are diagnosed with IPF per year in the UK.[4]

sMD was used to simulate the large-scale domain rearrangement Epac1 undergoes during activation (see *Fig. B*). We then constructed MSMs, which captured the activation of wild-type Epac1 by cAMP and D007 and reflected the “partial” activation achieved by hit compound I942 (see *Fig. C*).[5] To further validate our sMD/MSM workflow, we investigated the Epac1$^{L273W}$ mutant, which is insensitive to activation by cAMP. Finally, we sought to investigate the mechanism behind the weak activation by I942, applying artificial restraints to mimic missing interactions engaged by cAMP. Our results have since guided the design of novel I942 analogues, yielding highly selective and potent Epac1 activators (undergoing IP protection).

## References:

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## Thermomechanical recycling of PET based textiles

**Zara Standring**

The textile industry faces major sustainability issues due to the very large volume of waste produced. 84-92 million tonnes of pre and post-consumer textile waste is collected globally per year of which 66-75% ends up in landfill. In fact, of the 10% of textiles that are recycled globally less than 1% are recycled back into new textiles, leading to a growing global textile waste problem and pressure on virgin resources. One of the most common textile fibres is poly(ethylene terephthalate) (PET). PET may be chemically or thermo-mechanically recycled. Although ‘recycled polyester’ clothing is available, to date, this is almost exclusively obtained from recycled plastic bottle waste. Textile-to-textile PET recycling is a much more complex process that is yet to be developed on a large scale.

Starting from different PET textile waste samples supplied by Project Plan B, sequential thermo-mechanical reprocessing has been performed to determine if the changes in properties are similar to those seen for PET plastic bottles. Analytical techniques including FTIR, DSC, TGA, viscosity measurements and carboxylic index have been used to assess the quality of these samples. The importance of keeping the feedstock dry before extrusion has been shown not only by the large decreases in viscosity of the processed material, but also by problems during processing. Machine learning is being used to predict the changes in PET viscosity that occur during extrusion and to determine the amount of virgin material needed to reach optimum physical properties. This will help to determine if it is environmentally beneficial recycling certain textile waste feedstocks.

Attempts to increase the quality of the PET using solid state polymerisation (SSP) and chain extenders have also been made, with the aim of reducing the reliance on virgin materials. It was hypothesised that due to the lower viscosities needed for fibre grade PET, shorter residence times and lower amounts of chain extenders would be sufficient to improve the properties to a useable standard. However, during experimentation, these increases were not as significant as expected. This was thought to be due to the high level of contamination in waste textile samples hindering polycondensation and chain extension. This led to a study of the literature to determine what type of contaminants could be responsible for the findings. The vast variety and possibly large levels of contaminants make it difficult to correlate the experimental observations with any specific set of contaminants.

Key words: Polyester, thermo-mechanical recycling, fibre-to-fibre, textile-to-textile

# Green-Light Photocatalysis: Borylated Benzo[c][1,2,5]thiadiazole (BTZ) Enables Continuous Flow Phosphorylation of Quinoline Derivatives

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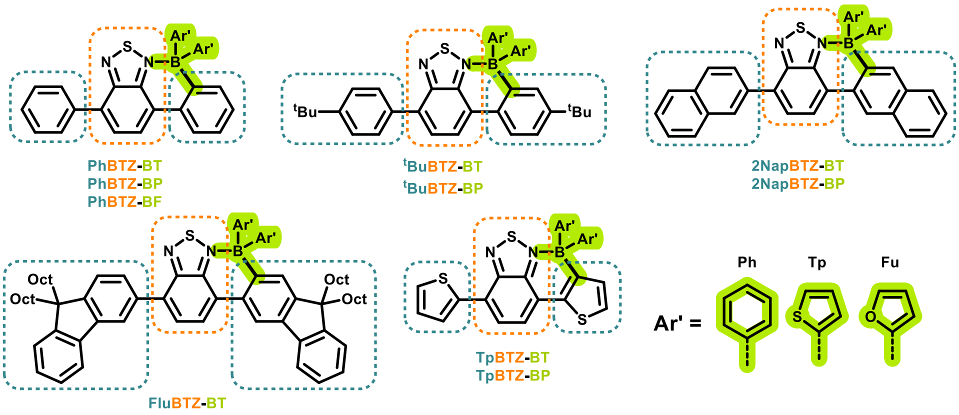
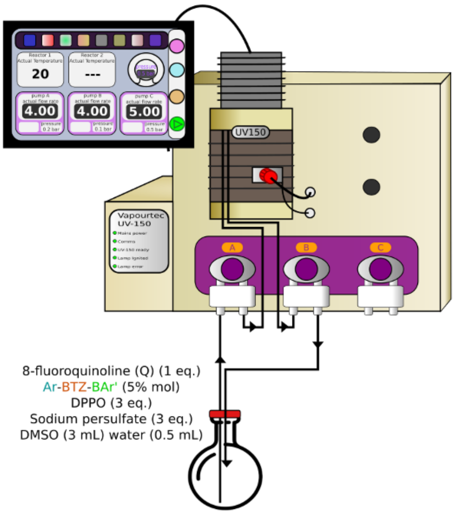
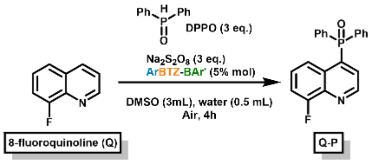
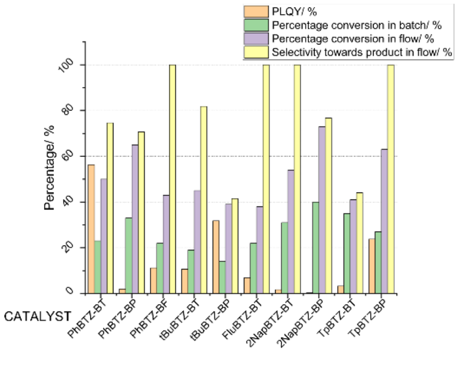
The widespread historical exploitation of non-renewable chemical feedstocks has driven increased focus towards solar light-harvesting technologies such as photocatalysts (PCs).[1] While efficient Ir and Ru-based PCs rely on expensive, scarce and toxic transition metals, all-organic PCs, such as those based on structures like the Benzo[c][2,1,3]thiadiazole (BTZ) heterocycle, are gaining popularity for their affordability and tunable optoelectronic properties. However, these organic PCs currently face limitations with lower efficiency and near-UV light absorbance.[2]
Herein, we introduce a targeted library of PCs that we have developed *via* selective *ortho*-borylation and ring fusion of Donor-Acceptor BTZ building-blocks,[3] achieving significant bathochromic shifts that extend the PCs' light absorption to lower-energy green wavelengths. These new PCs were tailored for contemporary photoredox catalysis reactions, such as the photocatalytic phosphorylation of quinoline derivatives, achieving up to 40% conversion in batch reactions and 73% in continuous flow set-ups within just 4 hours.[5]

To further demonstrate the versatility of these PCs, we also conducted a second reaction involving the Minisci C-C bond formation[4] in a flow setup, incorporating in-line UV-Vis monitoring for non-destructive tracking of reaction progress. The ability to initiate automated sequential reactions without purifying the initial step enables seamless process progression, reducing the need for human intervention and providing an efficient, low-cost approach for synthesizing valuable pharmaceutical intermediates and products.[6]









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# Applications of Cold Plasma for Polymer Gasification and Recycling

*Domantas Laurinavicius*

The ongoing increases in plastic use has exacerbated waste mismanagement, leading to low rates of recycling and high rates of incineration and landfilling. Recycling existing plastic waste through mechanical methods, i.e., re-extrusion, requires clean feeds of well-separated plastics. The cost associated with this process is high, and the lower quality products do not incentivise its use.

Chemical recycling (thermal gasification), however, is not sensitive to the chemical makeup or level of degradation of the plastic waste, allowing for the production of valuable feedstocks. Traditional chemical recycling suffers from high temperatures and pressures - an area that can be optimised. Thus, plasma-assisted gasification is a promising field for conversion of plastic waste to gas products.

A selection of materials (high-density polyethylene (HDPE), polypropylene (PP), polyethylene terephthalate (PET), polystyrene (PS), polyvinyl chloride (PVC), polytetrafluoroethylene (PTFE), nitrile-butadiene rubber (NBR)) treated with a variety of plasma gas sources (O2, CO2, Air, N2, 20:80 H2/N2) were investigated using gravimetry, attenuated total reflectance infrared spectroscopy, X-ray photoelectron spectroscopy, and time-of-flight secondary ion mass spectrometry.

Low-surface area HDPE treated with O2 plasma at 200 W reached a maximum of ~6.3% mass loss after 4 hours, and a high surface area PP film lost ~98% mass after 9 hours. While O2 plasma showed the greatest rates of mass loss, air, containing only ~20% O2, showed mass loss rates 43-75% that of pure O2. NBR samples treated with water-saturated air plasma showed limited mass loss, but increases in tensile strength and strain, as well as a modest decrease in the Young's modulus were seen.

Overall, plasma is a viable tool in the management of polymeric wastes and has potential for growth, especially with greater powers and higher surface-area wastes.