

2022 PhD Symposium Book of Abstracts



Welcome to the first annual PhD Symposium for the School of Physical and Chemical Sciences (SPCS). One objective of this Symposium is to bring together all researchers in the new School to explore and celebrate the breadth of research currently being carried out by our student cohorts at all stages of their PhDs. Another objective is to provide a forum for discussion, encourage and facilitate potential interdisciplinary research and promote understanding and tolerance between the differing groups in the school, whilst also helping to make PhD provision more dynamic.

The day will start at 1230 with the Year One poster session and refreshments to open the day. This will involve all of the year one cohort of PhD students as they present posters explaining their projects and the progress they have made since they projects began.

This will be followed at 1300 by short talks to be presented by our final year PhD cohort. These will take place in the People's Palace 1 lecture theatre (PP1) from the Department of Physics and Astronomy. A concurrent parallel session will take place in PP2 from talks from the Department of Chemistry.

Following the talks, we will reconvene in the People's Palace foyer at 1600 for poster presentations from the second year Chemistry cohort, along with further refreshments.

We will conclude the day at ~1645 together with announcements and prize awards for the symposium's best talks and best posters for each section and each of the 3 cohorts. The event will conclude at 1700.

We would like to sincerely thank all of our presenters, participants, judges and attendees who have contributed to this event and hope that everyone leaves with a better understanding of the research scope and people that make up SPCS, while generating new ideas and opportunities to work together and to explore new horizons in the future.

Kostya Trachenko and Gregory Chass (Directors of Graduate Studies)

School of Physical and Chemical Sciences**1st Annual PhD Symposium****Tuesday 17 May, 2022****People's Palace, Queen Mary University of London****SCHEDULE**

- 1230** **Welcome and Opening – PP Foyer**
(Prof. Kostya Trachenko and Dr. Gregory Chass)
- 1235-1325** **Posters – Year 1 Cohort – PP Foyer**
- 1330-1445** **Talks Group 1**
Physics and Astronomy – PP1 (Chair Dr Akram Alomainy)
Chemistry – PP2 (Chair Dr. Gregory Chass)
- 1445-1500** **Break – Tea & Cafe**
- 1500-1600** **Talks Group 2**
Physics and Astronomy – PP1 (Chair TBC)
Chemistry – PP2 (Chair Dr. Gregory Chass)
- 1600-1645** **Posters – Year 2 Cohort Chemistry**
- 1645-1700** **Awards and closing statements**
(Prof. Kostya Trachenko and Dr. Gregory Chass)
- 1700** **End of Symposium**

Name: Chinmaya Bhargava (1)

Group: Centre for Theoretical Physics (CTP)

Project title: Investigating the operator spectrum of Argyres-Douglas theories

Poster title: Using symmetry to solve difficult problems

Strongly coupled quantum field theories are difficult to study. Traditional techniques using a Lagrangian work for QFTs that are weakly coupled, allowing one to use perturbation theory to make predictions. However, QFTs that display extra symmetries - conformal symmetry, and supersymmetry, allow one to utilise special techniques in order to solve subsectors of strongly coupled QFTs. We focus on certain QFTs of this type discovered in the 90s, called Argyres-Douglas theories. These non Lagrangian techniques we use are the Operator Product Expansion, and the Superconformal Index, and they allow us to learn more about these superconformal QFTs.

Name: Kymani Armstrong-Williams (2)

Group: Centre for Theoretical Physics (CTP)

Funding: EPSRC

Project title: Gravity as a Double Copy of Gauge Theory

Poster title: Double Copy: Turning Electricity into Black Holes

An open problem in theoretical physics is to combine all four of the fundamental forces of nature into one single theory. Problematically, gravity has proven difficult to reconcile with the other forces. Recently, relationships between scattering amplitudes (the quantity related to the probability for an interaction to occur between two or more particles) in non-abelian gauge theories and theories of quantum gravity have led to the discovery of a relation known as the double copy. The double copy relates scattering amplitudes in quantum gravity as the square for those in non-abelian gauge theories. This property has been extended to relate solutions in classical electromagnetism with those in general relativity, via a theory known as the classical double copy.

Name: Isabelle Ye (3)

Group: Astronomy Unit,

Project title: Extracting cosmological observables from large-scale structure surveys

Poster title: A first detection of Doppler Magnification

This is the very first attempt to observe a relativistic effect, the Doppler magnification dipole, from the large-scale structure of distant galaxies. Due to the additional velocity that the galaxies gain when they are near a larger cluster of matter, the emission lines from the galaxies will be red-shifted or blue-shifted. It causes a Doppler lensing effect that will magnify or demagnify the image we take of the universe and will greatly dominate over gravitational lensing at low redshift. We can observe this dipole pattern by cross-correlating the galaxy density with the estimated galaxy sizes. Right now, our first task is to characterize how well we can measure the galaxy sizes, as the galaxy density is easy to obtain. The amplitude of this dipole pattern can be a probe of the peculiar velocity field, as well as our understanding of general relativity.

Names: Xiang Li, Nivetha Jeyachandran, Ilaha Hasanova (4)

Group: Chemistry (Cristina Giordano Group)

Funding: CSC, QMUL, State Program for Increasing International Competitiveness of the Higher Education System of the Republic of Azerbaijan in 2019-2023

Project title: Metallic nano-ceramics designed for the production of green energy

Poster title: Metallic nano-ceramics designed for the production of green energy

The increasing demand for energy is worldwide and urgently requires the substitution of fossil fuels with sustainable and renewable energies to prevent devastating consequences to our environment. An important role is played by catalysts that must be stable and favor high yield in the reaction.

Our research is dedicated to the synthesis of nanosized metals and metallic ceramics (namely transition metal nitrides, carbides, oxides and metallics MN/MC/MO/MO) to serve as catalysts for energy related applications. Nanomaterials possess an intriguing combination of properties (e.g. high specific surface area, catalytic, tailored properties via size and shape etc.) which allow us to envisage numerous applications. We investigate into a broad range of applications including electrochemical water splitting, electrocatalytic reduction of CO₂ into added-value chemicals and biomass valorization.

The synthesis is achieved based on a green, cost-friendly, and facile method, called the urea glass route.¹ The route also allows to prepare nanoparticles with different crystallinity from monometallic nanoparticles to more complex bimetallic systems. Regarding electrochemical applications, Mo₂C@C and CuNi@TiO₂ nanoparticles were designed for Hydrogen Evolution Reaction and CO₂ reduction reactions, respectively. For the biomass valorization, Ni and Fe based catalysts were designed for the conversion of biomass model compounds.

References

[1] C. Giordano, C. Erpen, W. Yao, B. Milke and M. Antonietti, Metal Nitride and Metal Carbide Nanoparticles by a Soft Urea Pathway, *Chem. Mater.*, 2009, 21, 5136–5144.

Name: Chris Addis (5)

Group: Particle Physics Research Centre (PPRC)

Funding: Science and Technology Facilities Council (STFC)

Project title: Estimating the galaxy bispectrum in redshift space

Poster title: Estimating the galaxy bispectrum in redshift space

The 3-point correlation function and its Fourier counterpart, the bispectrum, are the lowest order n-point functions which can probe the non-gaussian statistics of the field. Due to the presence of redshift-space distortions the observed galaxy clustering is dependent on the line-of-sight (LOS); therefore the anisotropic bispectrum is usually expressed by expanding it in spherical harmonics about the LOS. These multipoles contain a wealth of cosmological information. The odd moments are sourced predominantly by relativistic effects and therefore the detection would be a smoking gun for a relativistic effects. Therefore with next generation of galaxy surveys around the corner, efficient, robust and accurate estimators of the bispectrum are necessary for detailed analysis which can probe a wide variety of cosmological effects and parameters. Here we explore and test two different Fast Fourier Transform based estimators for all the bispectrum multipoles.

Name: Jing Li (6)

Group: Yao Lu

Funding: China Scholarship Council (CSC)

Project title: Preventing lead leakage for lead halide perovskite solar cells.

Poster title: Preventing lead leakage for lead halide perovskite solar cells.

As an inexhaustible green energy, solar energy has become the focus of research because of the energy crisis worldwide. Perovskite solar cells are one of the most promising new technologies in academia and industry, as a potential alternative to silicon and other commercial solar cells. Despite the remarkable performance progress being made, environmental concerns remain for lead halide perovskite solar cells (PSCs) because of the possible water dissolution of lead ions (Pb^{2+}) into the environment. The large amount of lead in a perovskite solar farm could potentially cause serious damage to the environment and to humans, this is a huge challenge for perovskite technology at present. Here, a holistic interface modification strategy was explored to effectively improve the stability of PSC and prevent lead leakage by embedding Pb-adsorbing layers inside perovskite absorbers to prevent Pb leakage.

Name: Kai Chen (7)

Group: Matteo Palma

Funding: China Scholarship Council (CSC)

Project title: Fabrication of next generation MoS₂-based nanodevice and its application

Poster title: MoS₂ based Nano-heterostructure fabrication (Study of functionalization degree and distance-dependent quenching behaviour)

The aim of this project focuses on developing novel nano-heterostructure to study the charger transfer mechanism between different building blocks and its further application in biosensing or/and optoelectronic device. 2D nanomaterial (MoS₂) will be conjugated with 0D nanomaterial (quantum dot, QD) by employing DNA oligonucleotide as linker. Thanks to the flexibility of DNA oligonucleotide in chemistry, different functionalization strategies and special designs of such heterostructure become possible and reliable. In addition, the functionalization degree of all three strategies and the distance-dependent quenching behaviour can be studied based on the developed nano-heterostructure.

Name: Raphael Picard (8)

Group: Astronomy Unit

Funding: Science and Technology Facilities Council (STFC)

Project title: Constraining early universe models using small scale data

Poster title: Behaviour of scalar and tensor perturbations during inflation

Inflation is a postulated period of accelerated expansion in the very early universe which is consistent with today's observations. Inflation provides a solution for problems that puzzled cosmologists, namely the homogeneity of the CMB whilst also providing a mechanism for structure formation by inflating small inhomogeneities present in the early universe. It also predicts a stochastic background of gravitational waves that should be detectable in the future by interferometers like LISA. In this work I present the behaviour of quantum fluctuations and gravitational waves produced during inflation and derive the corresponding primordial power spectrum.

Name: Katrine Alice Glasscock (9)

Group: Astronomy Unit

Funding: European Research Council

Project title: Mapping diffuse emission for the 21 cm sky using the Hydrogen Epoch of Reionization Array

Poster title: Mapping diffuse emission for the 21 cm sky using the Hydrogen Epoch of Reionization Array

The large scale structure of the universe can be probed using 21-cm tomography. This is done by measuring the 21-cm signal of neutral hydrogen and how it is statistically distributed at different epochs. In order to do so, we need to be able to separate the actual cosmological signal from the contaminating signal we get from foregrounds, which can be orders of magnitudes larger. Modeling these foregrounds is a crucial step towards fully mapping the 21 cm sky. In this study the focus has been to develop a code that implements using spherical harmonics as a basis for the sky as a way of simulating interferometer visibilities. By making the rotations rely purely on linear algebra, the aim is also to bring down the computational costs of the problem. The entire problem is thus set up as a linear system that will later allow us to plug it into a Gibbs sampler (a statistical sampling method) to do a further analysis. The code is developed for the Hydrogen Epoch of Reionization Array (HERA) but will be applicable to other interferometers as well.

Name: Molly McVea (10)

Group: Dr Szilagyi / Dr Nielsen / Dr Fenwick

Funding: EPSRC

Project title: Thermoelectric Metal-Organic Frameworks: Design, Synthesis and Assessment

Poster Title: Thermoelectric Metal-Organic Frameworks: Design, Synthesis and Assessment

Thermoelectric materials offer the potential to aid in the current energy crisis, by being able to recycle waste heat into useful electrical energy. Metal-Organic Frameworks (MOFs) are a promising material in this field due to their ability to harness the benefits of both traditional inorganic and organic materials. Their long-range order offers pathways for electrical conductivity, while their highly porous structure helps to scatter phonons, yielding low thermal conductivities; both desirable for thermoelectric applications. 2D planar MOFs, based around the same family of linkers (HXTP and HXB), have been shown to be the most successful to date, with high conductivities due to their graphene-like structures. However, whilst MOFs exhibiting thermoelectric behaviour have been successful, their Power Conversion Efficiency is still not high enough to compete with current commercial thermoelectric materials. This is due to a current lack in understanding of the electronic transport mechanisms and band structures in MOFs, preventing systematic design of new MOFs for thermoelectric materials. This project will focus on a systematic assessment of range of MOFs. Varying the MOF metal centre, ligand heteroatom, and the shape and size of the ligand - with the aim to develop a better understanding of the origins of thermoelectric behaviours in MOFs. This insight will allow for strategic design linkers for novel MOFs, with improved thermoelectric properties, aiming to challenge current thermoelectric materials.

Name: Pritha Paul (11)

Group: Large Scale Structure Cosmology

Funding: Queen Mary University of London

Project title: Wide – Relativistic Corrections to the Bispectrum

Poster title: Wide - Angle Power Spectrum with Doppler Corrections

I will be presenting a brief description of the power spectrum and the 2-point correlation function. I have also added the wide-angle corrections to the power spectrum which would be including the red-shift space distortions and the relativistic doppler corrections. Multi-tracers with different galaxies and galaxy biases such as the magnification and the evolution bias have also been taken into account. The power spectrum, which is the Fourier transform of the 2-point correlation function, has been expanded to give corrections to the plane parallel approximation for each of the multipoles of the power spectrum. The expansion has been done in inverse powers of the mean distance to the galaxies.

Name: Gabriela Rath (12)

Group: Resmini Research Lab

Funding: E. C. Marie Curie Actions through grant Marie Skłodowska-Curie (Grant agreement n° 956977)

Project title: Understanding the relationship between chemical structure of polymeric gels and their interfacial behaviour with membranes using neutron scattering.

Poster title: Development of new micro-polymers for intranasal drug delivery

Neurological diseases are a considerable social and economic burden in the world, being the leading cause of disability and the second cause of mortality in Europe [1]. However, the treatment of such diseases remains a challenge due to the presence of a physiological barrier called the Blood-Brain Barrier (BBB), which restricts the delivery of drugs to the brain. Other alternatives have been studied to avoid the passage of drugs through BBB, beyond which the intranasal administration stands out as it is non-invasive and easy to perform by the patient [2]. Besides, the use of engineered nanostructured drug delivery systems (DDS) – such as polymeric nanogels – can enhance the treatment efficiency, as it can improve accumulation and penetration in the target site. Nanogels are highly versatile DDS, as their properties can be tailored by adding functional monomers and changing the synthesis method [3]. Therefore, this project aims at developing nanogels for neurological treatment via intranasal administration. Different synthetic conditions (e.g., temperature and solvent nature) were employed to produce covalently linked N-isopropylacrylamide (NIPAM) nanogels by high-dilution radical polymerization (HDRP). Nanogel's properties were investigated by Nuclear Magnetic Resonance (NMR), Dynamic Light Scattering (DLS), and UV-vis spectroscopy. We showed that the synthetic conditions have a dramatic effect on the nanogel's properties, especially on its hydrodynamic size and thermoresponsive behaviour. Further studies will investigate the best formulation for intranasal administration.

References

[1] Feigin, V. L. et al. *The Lancet Neurology* 19, 255–265 (2020).

[2] Sosnik, A., das Neves, J. & Sarmiento, B. *Progress in Polymer Science* 39, 2030–2075 (2014).

[3] Vdovchenko, A., Pearce, A. K., Freeley, M., O'Reilly, R. K. & Resmini, M. *Polym. Chem.* 12, 6854–6864 (2021).

Name: Lucy Haddad (13)

Group: CCMP, (Supervisor: Andrei Sapelkin);

Funding: Diamond Light Source/Queen Mary University of London

Project title: Pair correlations and treatment of disorder in Magic Size Clusters;

Poster Title: EXAFS: Background Subtraction, Interpolation Method & Models of Disorder

Finding the atomic level structure of ultra-small nanoparticles is a problem due to their lack of periodicity and large surface-to-volume ratio [1]. EXAFS is a spectroscopy method that is sensitive to short-range order, correlation of atomic motion and anharmonicity. However, it has limits in its use to study local dynamics and even with local structure there are issues that arise. In treatment in experimental data before analysis, background removal is employed however methods currently used give no errors in this removal and it is very easy to overfit or underfit a background, making the data inaccurate. For analysing challenging samples, such as ultra-small nanoparticles, it is crucial that we have as much information about the sample as possible in the data. In this poster I present an application of recent work [2] on using Bayesian statistics on curve fitting to background subtraction for EXAFS spectra, which should be a fast way of obtaining errors from background subtraction of the spectra and should also ensure it is sufficiently removed. I also briefly introduce how errors can arise from modelling disorder in these spectra due to Einstein and Debye models of atomic MSDs and how the recent Interpolation Method [3] allows us to model disorder more accurately.

[1] Y. Liu, L. Tan, G. Cibir, D. Gianolio, S. Han, K. Yu, M. T. Dove, and A. V. Sapelkin, Analysis of the atomic structure of CdS magic-size clusters by x-ray absorption spectroscopy, *Nanoscale* 12, 19325 (2020),

[2] D. J. Dunstan, J. Crowne, and A. J. Drew, Easy computation of the bayes factor to fully quantify Occam's razor 10.48550/ARXIV.2007.09702 (2020),

[3] E. V. Yakovlev, M. Chaudhuri, N. P. Kryuchkov, P. V. Ovcharov, A. V. Sapelkin, and S. O. Yurchenko, Experimental validation of interpolation method for pair correlations in model crystals, *The Journal of Chemical Physics* 151, 114502 (2019).

Name: Lei Chen (13)

Group: Alan Drew's group

Funding: China Scholarship Council (CSC)

Project title: Reduction of Carbon Dioxide Catalyzed by metal-porphyrin complexes

Poster title: Metal-Organic Framework (MOF) material and its application in catalysing CO₂ electroreduction.

Since the industrial revolution, human activities have led to a large number of carbon dioxide emissions, which become the main reason for the greenhouse effect. Reducing CO₂ by electrocatalysis to useful products, such as methanol, ethylene and ethanol, become a promising way to solve this problem. however, the low efficiency and selectivity of CO₂ electroreduction hamper its practical application and there still needs a proper catalyst to improve reaction performance. MOF, benefiting from its controllable reticular structure and element components, become one of the potential candidates of CO₂ electroreduction. We aim to synthesis a MOF material to achieve high CO₂ electroreduction efficiency with a low cost and clarify the mechanism of CO₂ reduction on the MOF surface.

Name: Tingting Zheng (14)

Group: Matteo Palma Group

Funding: China Scholarship Council (CSC)

Project title: DNA Origami Nanoarrays for Dissection of Multivalent Cancer Cell Signalling

Poster title: DNA Origami Nanoarrays for Dissection of Multivalent Cancer Cell Signalling

Integrins play a critical role in cancer, which are transmembrane proteins that promoted the contact of cells or the extracellular matrix (ECM) to regulate cells' behaviours. Around one-third of all solid tumours upregulate epithelial-specific integrin $\alpha\beta6$, which has been related to a worse overall survival rate in several malignancies. As $\alpha\beta6$ enhances receptor tyrosine kinases (RTKs) dependent breast cancer migration, invasion, and carcinogenesis, including HER2-dependent and EGFR-promoted breast cancers, it is important to find the spatiotemporal control of these integrin/RTK dependent biological activities at the molecular level. The purpose of this project is to develop biomimetic nanoarrays with a versatile and designable surface using DNA origami and nanolithography techniques. By design, DNA origami can be assembled into desirable shapes to simulate the spatial position between cell receptors and the ligands, as well as the interaction between different ligands for dissection of multivalent cancer cell signalling. Substrates can be patterned via scanning probe thermal lithography, which will lead to the selective fabrication of biomolecular nanoarrays and achieve ECM mimicking biochips with nanoscale spatial resolution, single-molecule control, and multivalence.

Name: Tancredi Schettini Gherardini (15)

Group: Centre for Theoretical Physics (CTP)

Funding: Science and Technology Facilities Council (STFC)

Project title: SU(2)-like Instantons in Exceptional Field Theory

Poster Title: Twisted Instantons

Field Theory is the basic tool at our disposal to describe the intimate nature of the universe. Supergravity is an example of a field theory, and a very promising one. It aims at improving and extending Einstein's theory of General Relativity. It was recently shown that the theory of Supergravity can be written in many equivalent ways, with each of them displaying explicitly a specific property of the theory. One of these reformulations of Supergravity, which goes under the name of E₇ Exceptional Field Theory, has been fully constructed, and the study of its solutions is an active field of research. This project aims at presenting a very specific solution, which is inspired by a famous phenomenon known as "instanton". An instanton is a "particle" that appears from nowhere at a given point in spacetime and suddenly disappears. "Are there instantons in E₇ Exceptional Field Theory?" is the question behind this project...

Name: Shen Zhang (16)

Group: Stellios Arseniyadis Group

Funding: China Scholarship Council (CSC)

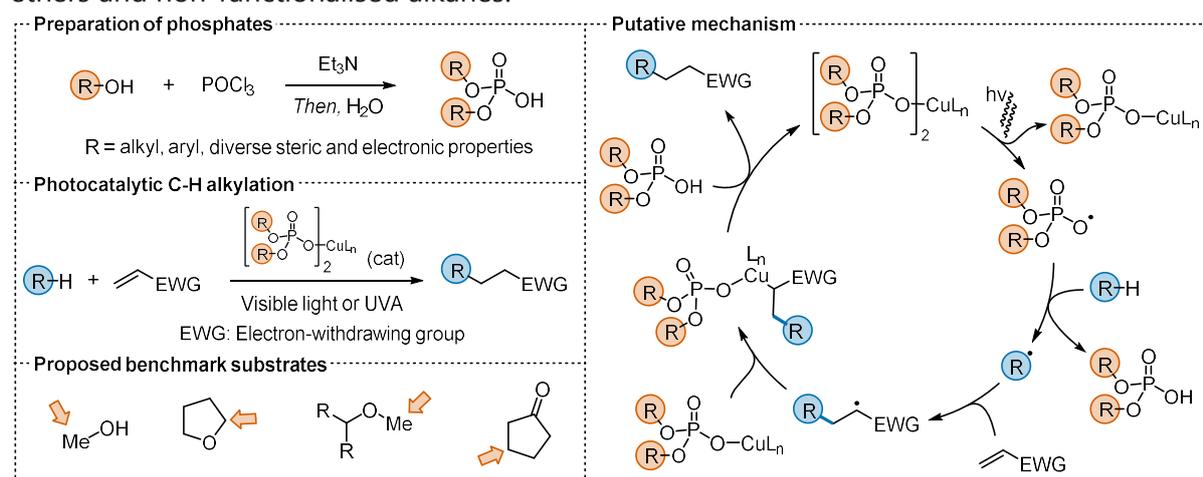
Project title: Tuneable Cu(II) hydrogen atom transfer catalysts for photocatalytic sp³ C-H functionalisation

Poster title: Photocatalytic methods for selective C-H functionalisation of aliphatic compounds

C-H functionalisation methodologies offer great potential for the fast construction and derivatisation of organic compounds, allowing for more direct synthetic routes. While the functionalisation of sp and sp² C-H bonds has been extensively developed, mainly using transition metal organometallic catalysis, sp³ C-H bonds remain more challenging. Recently, photocatalytic methods based on light-promoted hydrogen atom transfer (HAT) have emerged as a promising strategy. Remarkably, compounds as simple as CuCl₂ have been shown as effective catalysts promoting the functionalisation of electron-rich C-H bonds through light-promoted release of Cl radicals.³ Although efficient under mild conditions, the usefulness of this approach is limited by poor regio- and stereoselectivity and few opportunities for optimisation given that the active species involved in the HAT event is just a Cl radical.

We hypothesise that the same type of catalytic behaviour can be achieved with other Cu(II) salts involving organic ligands, and that structural fine-tuning of the ligands will enable the development of highly regio- and stereoselective photocatalytic C-H functionalisation reactions. To start this investigation, we have chosen organic phosphate ligands, there are easily synthesised from alcohols, with a wide range of structures to explore.^{4,5}

The principal aim of this project is to synthesise a library of Cu(II) phosphate-based catalysts for photocatalytic C-H functionalisation, and evaluate them in the direct alkylation of alcohols, ethers and non-functionalised alkanes.



References:

- (1) Godula, K.; Sames, D. C-H Bond Functionalization in Complex Organic Synthesis. *Science* (1979) **206**, 312 (5770), 67–72. <https://doi.org/10.1126/SCIENCE.1114731>.
- (2) He, J.; Wasa, M.; Chan, K. S. L.; Shao, Q.; Yu, J.-Q. Palladium-Catalyzed Transformations of Alkyl C-H Bonds. **2016**. <https://doi.org/10.1021/acs.chemrev.6b00622>.
- (3) Abderrazak, Y.; Bhattacharyya, A.; Reiser, O. Visible-Light-Induced Homolysis of Earth-Abundant Metal-Substrate Complexes: A Complementary Activation Strategy in Photoredox Catalysis. *Angewandte Chemie - International Edition*. John Wiley and Sons Inc September 20, 2021, pp 21100–21115. <https://doi.org/10.1002/anie.202100270>.
- (4) Morton, C. M.; Zhu, Q.; Ripberger, H.; Troian-Gautier, L.; Toa, Z. S. D.; Knowles, R. R.; Alexanian, E. J. C-H Alkylation via Multisite-Proton-Coupled Electron Transfer of an Aliphatic C-H Bond. *J Am Chem Soc* **2019**, *141* (33), 13253–13260. <https://doi.org/10.1021/jacs.9b06834>.
- (5) Margrey, K. A.; Czaplinski, W. L.; Nicewicz, D. A.; Alexanian, E. J. A General Strategy for Aliphatic C-H Functionalization Enabled by Organic Photoredox Catalysis. *J Am Chem Soc* **2018**, *140* (12), 4213–4217. <https://doi.org/10.1021/jacs.8b00592>.

Name: Davide Mazzali (17)

Group: Resmini Research Lab

Funding: Marie Skłodowska-Curie grant ^{agreement No 956977}

Project title: Development of new polymeric nanogels as drug delivery systems

Poster title: Development of novel chitosan-grafted nanogels for intranasal drug delivery of biological molecules

Around 11 million people in the UK live with a neurological condition¹. The Blood brain barrier (BBB) complicates treatments harshly, reducing the number of drugs that can effectively reach the brain. Nanogels are polymeric nanoparticles with good cargo properties and the ability to form stable colloidal solution in water²; they have shown to cross blood brain barrier in animal models and according to the starting synthetic materials they can obtain stimuli-responsive properties to changes in the external conditions, such as pH and temperature³. Their application in intranasal drug delivery of biological drugs could be a breakthrough for therapy of hard-to-treat conditions.

In this work N-isopropylacrylamide and acrylamide based cross-linked nanogels were synthesised using high dilution radical polymerisation; correlation between formulation and real chemical structure was assessed using Neutron Magnetic Resonance together with chemical yields. Nanogels were then furtherly characterised using UV-Vis spectroscopy and dynamic light scattering.

¹ neuro facts, <<https://www.brainresearchuk.org.uk/info/neuro-facts>> (2022).

² Kousalová, J. & Etrych, T. Polymeric Nanogels as Drug Delivery Systems. *Physiological Research*, S305-S317, doi:10.33549/physiolres.933979 (2018).

³ Judah, H. L., Liu, P., Zarbakhsh, A. & Resmini, M. Influence of Buffers, Ionic Strength, and pH on the Volume Phase Transition Behavior of Acrylamide-Based Nanogels. *Polymers* 12, 2590, doi:10.3390/polym12112590 (2020).

Name: Stefano Zazzera (18)

Group: Astronomy Unit

Project title: Cross-correlations with Gravitational Waves

Poster title: Cross-correlating Gravitational Waves and Galaxies

Gravitational waves are produced by compact objects which usually reside inside galaxies, and therefore can be used as tracers of the large-scale structure of our universe. In this work, we investigate the cross-correlation between galaxies and gravitational waves sources to ultimately understand the distance-redshift relation, as both tracers can inherently provide a measurement of the object's luminosity distance. We produce a modified version of the publicly accessible code CAMB to compute such cross-correlation implementing relativistic effects in luminosity distance space. Additionally, we present models for the magnification and evolution biases present in the cross-correlation formalism using different types of binary black hole populations.

Name: Weiyang Hong (19)

Group: Matteo Palma Group

Funding: Chinese Scholarship Council

Project title: Specific chirality single-wall carbon nanotube systems and applications

Poster title: Peptide-functionalized specific chirality single-walled carbon nanotubes as tumour targeting platform

Single-walled carbon nanotubes (SWCNTs) are versatile 1D nanostructures with use in a variety of fields, from potential cargo delivery and optical system for in-vitro and in-vivo investigations to transducers in biosensing electrical devices, and nano-electrodes for single-molecule investigations

In this project, we investigate methodologies to selectively functionalised SWCNTs that we pre-sort in terms of their chirality, hence dimensions and opto-electronic properties. In particular, we started designing them as tumour-targeting therapeutic vectors. We based our strategy on SWCNTs selectively sorted and functionalized to target integrins $\alpha\beta6$ which has been found highly expressed in lung, colorectal, lip, and oral cancer cells. Due to the high-affinity peptide A20FMDV2 for integrin $\alpha\beta6$, we used A20FMDV2 as a target molecule immobilization of SWCNTs wrapped by specific DNA sequences; fluorescent molecules will be attached to each of the SWCNT-A20FMDV2 hybrids in order to observe their trajectory after intercellular distribution.

Overall, the initial aim of the project is to explore the possibility of forming a drug delivery platform from A20FMDV2 and SWCNT. We will then explore the same strategy for the design of SWCNT hybrids as nanoelectrodes for molecular electronics applications and as transducers in biosensing devices, in line with ongoing and published work in the Palma group.

Name: Kevin Vockerodt (20)

Group: Particle Physics Research Centre (PPRC)

Funding: Science and Technology Facilities Council

Project title: Measurement of the muon antineutrino charged-current interactions without mesons in the final state, in the NOvA near detector

Poster title: Investigating Antineutrino Interactions in the NOvA Near Detector

NOvA is an experiment based at Fermilab in the US, with the aim of measuring neutrino and antineutrino oscillations to better understand electroweak interactions and the origin of the universe. To measure neutrino oscillations, we need to learn and understand how neutrinos and antineutrinos interact with matter. Antineutrino interaction cross sections are currently poorly constrained, and processes such as meson exchange currents are not well understood in the antineutrino sector. This study is to develop a measurement of muon antineutrino interactions which do not contain mesons (e.g., pions or kaons) in the final state, in the NOvA near detector. The sample is dominated by quasi-elastic and meson exchange current processes, and the selection will be developed in order for the cross section to be extracted as a function of the kinematics of the outgoing particles. This can then be compared to current theoretical models, providing vital data to the neutrino community and helping to disentangle effects in past antineutrino oscillation measurements.

Name: Mi Zhang (21)

Group: Christopher R. Jones Group with Petra Szilágyi

Funding: China Scholarship Council (CSC)

Project title: Design and assessment of solid-state alkali metal-ion conductor 1D channelled framework materials

Poster title: 1-D Channelled Silicate Organic Framework as Solid-State Electrolyte

Metal-ion batteries (MIBs) are deemed to be the potential candidates for next-generation secondary batteries. However, the formation of dendrites and flammable organic solvents rise severe safety hazards. In order to address this issue, solid electrolytes (SEs) are widely used to substitute liquid organic electrolytes (LOEs), also acting as a separator to create an all-solid-state battery (ASSB). With several popular features such as insularity, structural rigidity and high internal surface area, covalent organic frameworks (COFs) are considered promising materials for SEs. In addition, the ordered and easy-tuned ion conductive pathways endow an effective ion shuttle.

In this project, the novel silicate organic framework with propyl side groups (Pr-SOF) was prepared with SiO₆²⁻ centre nodes, constructing two-dimensional (2D) planes. Layers were stacked by strong electrostatic forces between them to enable the formation of 1 D channels, providing fast ion passways. The successful formation of Pr-SOF with rigid crystallinity was proven by solid-state NMR, FTIR, XPS and the PXRD pattern. The high surface area of 1069.44 m² g⁻¹ and great heat tolerance (400 °C) enable it to be a powerful host to accommodate a large number of lithium ions for fast transportation. Under SEM spectroscopy, obtained Pr-SOF shows the morphology of wrinkled assemblies established by platelets. Those results support the great potential of this 1-D channelled material applied as SE and the ion conductivity will be measured in future works.

Name: Sid Baines (22)

Group: Particle Physics Research Centre (PPRC)

Funding: Science and Technology Facilities Council

Project title: Search for a heavy Higgs boson at the ATLAS experiment at the LHC

Poster title: Search for a heavy charged Higgs boson via $H^+ \rightarrow W^+ h \rightarrow lvbb/qqbb$ boosted decay

This poster introduces a search for a heavy charged Higgs boson decaying into a W boson and Standard Model Higgs at the ATLAS detector, focusing on the boosted decay channel. The analysis uses data corresponding to 139 fb⁻¹ of pp collisions at $\sqrt{s} = 13\text{TeV}$, recorded during run 2 of the LHC in 2015-2018. The search will consider the production of a charged Higgs boson in association with a top and bottom quark: $pp \rightarrow tbH^+ \rightarrow tbWh$. This poster will discuss the theory behind a heavy charged Higgs, the ATLAS detector, signal selection and relevant backgrounds, and pre-fit data/simulation comparison.

Name: Sarah Alsharif (23)

Group: Centre for Condensed Matter Physics

Funding: Saudi Scholarship Council

Project title: A Study on Organic/Inorganic Hybrid Photodetectors

Poster title: A Study on Organic/Inorganic Hybrid Photodetectors

This report shows the work done during the first year toward the Ph.D. in Condensed Matter Physics. The aim is to increase the photogenerated efficiency of organic/inorganic hybrid photodetectors. This work includes studies on drop-casting different thicknesses, 5 - 66 μm , of P3HT; the effect of changing the concentration and volume of the material. Bruker DektakXT profilometer was used to measure the thickness despite the coffee rings and gels/aggregation due to the high regioregularity of P3HT. It opened a window to form organic/ inorganic composites using P3HT: TiO₂ with several ratios. Drop casting the films were examined at 1500C, 600C, 400C, and room temperature. Microscopic magnifications were checked to figure out the defects facing such composites. The hybrid layer was suffering from cracks, pinholes, clumps, and low adhesion, particularly for the 1500C films.

Device fabrications were performed using 10% P3HT: 90% TiO₂ active layers and I-V characteristics were measured, from -40 to 40 V, using Keithley 4200-SCS Semiconductor Characterization System under N₂, vacuum, and air. Our results show a negative differential conductivity response in the reverse bias for these devices. Charge transport was investigated in 50% P3HT: 50% PCB, an organic blend semiconductor device by the transient time of flight (ToF) using a green laser of 20 Hz for both pulse and DC field. The average electron and hole mobilities were $\mu_e = 9 \times 10^{-5}$ and $\mu_h = 9 \times 10^{-5} \text{ cm}^2 \text{ V}^{-1} \text{ s}^{-1}$. However, the space charge of electrons was one-third of the space charge of holes. This is an indication that the electrons are filling a deep trap level, which agrees with a previous measurement taken for the same device.

In addition to the experimental work, simulation was done using COMSOL Multiphysics 6. A 2D photodiode model was reached with 1 μm out of plane thickness. This model can be used to study the photoresponse of our organic/ inorganic hybrid photodetectors. Finally, we plan to use more inorganic materials to form different P3HT/BN and P3HT/ B₄C hybrid materials in addition to P3HT/TiO₂. Zitasizer will be used to measure the particle size to reach composite homogenization and the optimum optical performance. Also, adding hole and electron blocking layers is considered to prevent short circuits.

Name: Aled Horner (24)

Group: Particle Physics Research Centre (PPRC)

Funding: AWE and NuSec

Project title: Evaluating the suitability of Organic Semiconductor Detectors for Nuclear Security

Poster Title: Evaluating the suitability of Organic Semiconductor Detectors for Nuclear Security

This poster explores the concepts of organic semiconductor devices for radiation detection. This includes an explanation of the formation and the physical concepts employed for the detection of alpha particles and neutrons. A description of a novel material's recent detection capabilities is given for alpha particles from an Am-241 source in the physics department. Future prospects of the project are discussed, highlighting the formation of a portable array of detectors allowing for detection and triangulation of radioactive sources for nuclear security.

Name: Marco Anselmi (25)

Group: Dr Devis Di Tommaso

Funding: Queen Mary University Alumni Research PGR

Project title: Machine Learning Guided Discovery of Catalysts for CO₂ Conversion

Poster Title: Machine Learning Guided Discovery of Catalysts for CO₂ Conversion

The rising level of CO₂ in Earth's atmosphere is the single most important environmental challenge that our society must face. One of the most attractive solutions to reduce climate change emissions is the chemical conversion of CO₂ into added-value chemicals (carbon monoxide, formic acid, ethylene, and others). The main challenge lies in the inertness of CO₂, making catalysts requisite to decrease the energy required to convert CO₂ to hydrocarbons. The aim of this PhD project is to develop machine-learning protocols to help expedite the design and selection of catalysts for CO₂ conversion. These protocols will include the creation of molecular representations readable by machine-learning models, and the training of machine-learning models for the prediction of properties of catalysts.

Chemistry Talks:**Name:** William Neal**Group:** Nielsen Group**Funding:** EPSRC**Project title:** Nanoscale bioelectronics for point-of-care diagnostics and wearable devices**Presentation Title:** Aptamer functionalisation of semiconducting polymer thin-films for applications in bioelectronics

William G. Neala, Christian B. Nielsen, Matteo Palma

aSchool of Physical and Chemical Sciences, Queen Mary University of London

Point-of-care (POC) devices are a class of powerful technology indispensable towards progressing the future of personalised healthcare¹. Progress targeting the improvement of secondary preventative strategies, by detecting a disease in its early stages of development². Multipurpose, portable and easy-to-use sensing devices will increase the accessibility of diagnostics, resulting in earlier detection and treatment of disease. Integration into wearable technology would enable constant health monitoring effectively minimising diagnostic times³. Developing upon initial work published within our group, we propose to incorporate favourable solution processable organic semiconducting polymers into a similar device structure⁴. A field-effect transistor functionalised with receptors, will allow for selective and amplified detection of analytes⁵. Functionalisation of the polymer thin-film utilises a blended approach with the cross-linking agent glutaraldehyde (GA)⁶. Bio-detecting aptamers will enable highly selective and chemically resistant sensing properties⁷. Presented is a review of the foundational work carried out towards fabricating a platform for biosensing. Device architecture and polymer thin-film functionalisation strategies will be discussed, and how once further optimised, combined to fabricate a sensor for detection of target biomarkers.

1 C. Dincer, R. Bruch, A. Kling, P. S. Dittrich and G. A. Urban, *Trends Biotechnol.*, 2017, **35**, 728–742.

2 S. T. Keene, D. Fogarty, R. Cooke, C. D. Casadevall, A. Salleo and O. Parlak, *Adv. Healthc. Mater.*, 2019, **8**, 1901321.

3 Y. H. Lee, M. Jang, M. Y. Lee, O. Y. Kweon and J. H. Oh, *Chem*, 2017, **3**, 724–763.

4 X. Xu, P. Clément, J. Eklöf-Österberg, N. Kelley-Loughnane, K. Moth-Poulsen, J. L. Chávez and M. Palma, *Nano Lett.*, 2018, **18**, 4130–4135.

5 E. Macchia, R. A. Picca, K. Manoli, C. Di Franco, D. Blasi, L. Sarcina, N. Ditaranto, N. Cioffi, R. Österbacka, G. Scamarcio, F. Torricelli and L. Torsi, *Mater. Horizons*, 2020, **7**, 999–1013.

6 C. Sun, M. V. Vinayak, S. Cheng and W. Hu, *Anal. Chem.*, 2021, **93**, 11305–11311.

7 N. Saraf, E. R. Woods, M. Peppler and S. Seal, *Biosens. Bioelectron.*, 2018, **117**, 40–46.

Name: Jinlei Zhang

Group: Stellios Arseniyadis Group

Funding: China Scholarship Council (CSC)

Project title: Innovative DNA-based asymmetric catalysis

Presentation Title: Advances in radical difluoromethylation chemistry under photoredox catalysis

Jinlei Zhang,^a Elias Selmi-Higashi,^a Xacobe C. Cambeiro,^b and Stellios Arseniyadis^a

^aQueen Mary University of London, Department of Chemistry, Mile End Road, E1 4NS, London, UK

^bUniversity of Greenwich, School of Science, Central Ave, Gillingham, Chatham, ME4 4TB, UK

Abstract The incorporation of fluorine atoms in drugs has been shown to often improve their metabolic stability, enhance their lipophilicity, and increase their membrane permeability and bioavailability.¹ In recent years, the difluoromethyl group has attracted much attention due to its special chemical properties. Both CHF₂ and CF₃ have strong lipophilicity and electron-withdrawing properties, and the hydrogen atoms in CHF₂ can also participate in hydrogen bonding as a hydrogen bond donor, which can more effectively enhance the physiological activity of organic molecules.² Therefore, difluoromethylation has become an effective means to modify biological activities and has been paid increased attention in the design of new drugs and pesticides. Nonetheless, unlike the fluorination and trifluoro-methylation reactions which have been widely explored over the years, examples of efficient and reliable difluoromethylations are sparser.

We report here an efficient and highly straightforward access to difluoromethylated ketones through a visible light-mediated difluoromethylation of readily available enol silanes, which is practical, scalable, and provides the corresponding CHF₂ ketones in good to excellent yields.

(a) Purser, S.; Moore, P. R.; Swallow, S.; Gouverneur, V. *Chem. Soc. Rev.* **2008**, *37*, 320–330. (b) Cametti, M.; Crousse, B.; Metrangolo, P.; Milani, R.;

Resnati, G. *Chem. Soc. Rev.* **2012**, *41*, 31–42. (c) Wang, J.; Sánchez-Roselló, M.; Luis Aceña, J.; del Pozo, C.; Sorochinsky, A. E.; Fustero, S.; Soloshonok, V.A.; Liu, H. *Chem. Rev.* **2013**, *114*, 2432–2506. (d) Gillis, E. P.; Eastman, K. J.; Hill, M. D.; Donnelly, D. J.; Meanwell, N. A. *J. Med. Chem.* **2015**, *58*, 8315–8359. (e) Zafrani, Y.; Yeffet, D.; Sod-Moriah, G.; Berliner, A.; Amir, D.; Marciano, D.; Gershonov, E.; Saphier, S. *J. Med. Chem.* **2017**, *60*, 797–804. (f) Meanwell, N. A. *J. Med. Chem.* **2018**, *61*, 5822–5880.

(a) Kirsch, P. *Modern Fluoroorganic Chemistry: Synthesis, Reactivity, Applications*, Wiley-VCH, Weinheim (Germany), **2013**. (b) Besset, T.; Poisson, T.;

Pannecoucke, X. *Eur. J. Org. Chem.* **2015**, 2765–2789.

Name: Ye Cao

Group: Sheriff Group

Funding: China Scholarship Council (CSC)

Project title: Manganese catalysed reduction of dioxygen to hydrogen peroxide for the degradation of Bisphenols: Kinetics study, degradation pathways, mechanisms and influencing factors.

Presentation Title: The application of in situ generated hydrogen peroxide in corrosion inhibition, disinfection and pollutants degradation

An in situ advanced oxidation process is proposed here to address the water pollution caused by azo dye discharge, which involves the formation of $[\text{MnII}(\text{T})_2]^{6-}$ (where $\text{T} = 1,2$ -dihydroxybenzene-3,5-disulfonate, disodium salt (Tiron)) as the catalyst for the in situ generation of H_2O_2 , and manganese(II) ions (Mn^{2+}) and bicarbonate as the co-catalysts for the oxidative degradation of Calmagite (CAL, 2-hydroxy-1-(2-hydroxy-5methylphenylazo)-4-naphthalenesulfonic acid), which is a typical azo dye, at room temperature. A one-eighth-lives method was applied to investigate the degradation kinetics. The results quantitatively showed the effect of pH, buffer type and Mn^{2+} concentrations on the degradation of CAL. These parameters were also evidence of the degradation mechanisms that high-valent manganese species: Mn(IV)=O , was found to be the main reactive species, while percarbonate (HCO_4^-) and hydroxyl radicals ($\cdot\text{OH}$) were the subsidiary reactive species for CAL degradation. Using HPLC/ESI-MS, the degradation intermediates of CAL were identified as 1-amino-2-naphthol-4-sulfonate ion, 1-amino-2-naphthol-4-sulfinic ion, 1-amino-2-naphthol, and 1-nitroso-2-naphthol.

In addition, we confirmed this formulation can be used as an anti-corrosion and anti-bacteria formulation due to the consumption of O_2 and the in situ generation of H_2O_2 . In the future, we are considering synthesizing other materials such as bis(3,5-ditertbutyl-1,2-benzoquinone mono-oximato)CuII to take the place of $[\text{MnII}(\text{T})_2]^{6-}$ for the degradation of more emerging contaminants like bisphenol AF (BPAF). The preliminary investigations have been completed and any promising results will be presented at the conference.

Name: Zara Farooq

Group: Howell Group

Project title: Targeting the G protein-coupled protein receptor, CB2, towards the development of novel anticancer therapeutics.

Presentation Title: Targeting the G protein-coupled receptor, CB2, towards the development of novel anticancer therapeutics.

G protein-coupled receptors (GPCRs) are the largest class of membrane proteins consisting of ~800 members with ~30% of currently marketed drugs targeting them. The cannabinoid receptors, CB1 and CB2 are two GPCRs involved in many important physiological processes. Emerging evidence has demonstrated that CB2 is involved in a number of diseases, including neurodegenerative disorders and various cancers, which make it an attractive pharmacological target. Classically, a protein active site or orthosteric binding site where the endogenous ligand binds to, is used as a target for the design of most small molecule drugs. This can become a problem when it comes to biologically similar proteins, such as the cannabinoid receptors as evolutionarily, their orthosteric binding sites are similar. An alternative option is to target sites that are unique to the receptor that still impact receptor function, termed allosteric sites. These sites are distinct between similar receptors like CB1 and CB2. Targeting allosteric sites is akin to picking the lock of these hidden grooves within the CB2 protein and is a crucial step towards selectivity and specificity for drug design and development. With the recent establishment of the human cannabinoid receptor 2 X-ray crystal structure, this has aided the prospective discovery of a CB2 allosteric site using computational software. In vitro signalling assays using known allosteric modulators and CB2 agonists have been used to verify the in-silico data. This potential identification provides promising outcomes for the development of selective and specific CB2 ligands for anticancer therapeutics.

Name: Wangchao Yuan

Group: Giordano Group

Funding: China Scholarship Council (CSC)

Project title: Preparation of Novel Ferrofluids

Presentation Title: Study on the structure vs activity of designed non-precious metal electrocatalysts for CO₂ conversion

Wangchao Yuan, Tingke Rao, Nivetha Jeyachandran, Azeem Ghulam Nabi, Devis Di Tommaso and Cristina Giordano.

The rising level of carbon dioxide (CO₂), mainly a consequence of human activities, is leading to devastating consequences to our environment and has raised concerns in public opinion. To face this issue, governments are working to reduce CO₂ emissions, whilst the scientific community is focusing on implementing the electro-chemical conversion of CO₂ (CO₂RR) as a source of added value chemicals. Due to the high stability of the CO₂ molecule, to make its conversion practical, the process requires a suitable electrocatalyst. With the aim to understand the mechanism toward specific CO₂RR products and thus increase selectivity, in this study, we have explored copper-based nanoparticles (Cu NPs) as one of the most promising catalysts for CO₂ conversion¹ and investigated the reactivity as a function of selected experimental parameters. The Cu NPs, prepared via an unconventional sol-gel process^{2,3}, were shown to be pure, homogeneous in size and morphology, and showed a total FE above 90% toward CO₂RRs. The higher FE toward the production of C₂H₄ (up to 33% at an applied potential of -1.0 V) is one of the highest FE reported so far for Cu, without using expensive support or co-catalysts. The final products were characterized using X-ray diffraction (XRD), scanning electron microscopy (SEM) and elemental mapping (EDX).

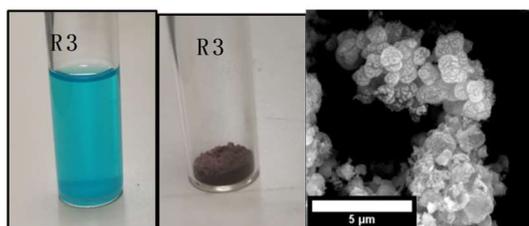


Figure 1. a) Cu-Urea complex in solution, b) corresponding products after heat treatment and c) SEM of Cu particles.

1. A. A. Peterson, F. Abild-Pedersen, F. Studt, J. Rossmeisl and J. K. Nørskov, *Energy & Environmental Science*, 2010, 3.
2. C. Giordano, C. Erpen, W. Yao, B. Milke and M. Antonietti, *Chem. Mater.*, 2009, 21, 5136-5144.
3. T. Rao, W. Yuan, N. Jeyachandran, A. G. Nabi, D. Di Tommaso and C. Giordano, *ChemRxiv*, 2021.

Name: Amir Sidat

Group: Crespo-Otero group

Funding: EPSRC

Project title: Mechanistic models for phosphorescent organic crystals

Presentation Title: Ultralong organic phosphorescence and thermally activated delayed fluorescence in phenone-carbazole derivatives

Carbazole derivatives have been identified as compounds that display ultralong organic phosphorescence (UOP) and thermally activated delayed fluorescence (TADF). Optoelectronic materials with these properties have applications in organic light emitting diodes (OLEDs), anti-counterfeiting and bioimaging technologies.[1] 24-, 34- and 35CPhCz are isomeric phenone-carbazole derivatives, each with a different arene substitution pattern.[2] This simple change results in a significant shift in emissive properties, as 24CPhCz displays UOP, 34CPhCz displays UOP and TADF while 35CPhCz displays TADF. This work aims to understand the factors behind the change in emission across these systems using a computational approach. Elucidating the mechanism allows for the proposal of design principles that modulate the type of emission, its lifetime, and the quantum efficiency.

To understand the differences between each crystal, we analyse the dimer conformations, calculate the exciton coupling and describe the types of intermolecular interactions present. We use a cluster model with time-dependent density-functional theory to capture the effect of these interactions, obtaining excited state potential energy surfaces and the rate constants for intersystem crossing (ISC) and reverse ISC (rISC). We find that the ISC process mainly populates the second triplet state and that the rISC rates are lower in the systems that display UOP. This implies that UOP in these systems is dependent on sustaining a large population of the triplet states, while TADF requires a large enough rISC rate to repopulate the singlet states. We also simulate the presence of isomeric impurities, and propose a mechanism that explains how the lifetime and efficiency of emission can both be increased via the formation of charge-transfer states.[3]

References:

1. S. Cai, H. Shi, D. Tian, H. Ma, Z. Cheng, Q. Wu, M. Gu, L. Huang, Z. An, Q. Peng and W. Huang, *Advanced Functional Materials*, 2018, 28, 1705045.
2. N. Gan, X. Wang, H. Ma, A. Lv, H. Wang, Q. Wang, M. Gu, S. Cai, Y. Zhang, L. Fu, M. Zhang, C. Dong, W. Yao, H. Shi, Z. An and W. Huang, *Angewandte Chemie International Edition*, 2019, 58, 14140-14145.
3. C. Chen, Z. Chi, K. Chong, A. Batsanov, Z. Yang, Z. Mao, Z. Yang and B. Liu, *Nature Materials*, 2020, 20, 175-180.

Name ; Roman Halsaka

Group: Nielsen Group

Funding: Queen Mary University of London

Project title: New Organic Materials for Bioelectronic Applications

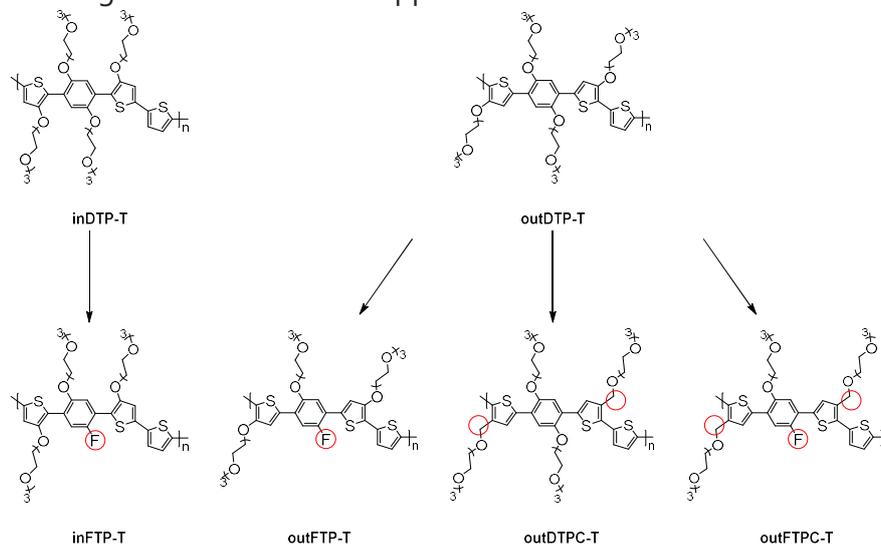
Presentation Title: The Influence of a Backbone Substitution on the Oxidation Potential of Organic Mixed Ionic and Electronic Conductors

The field of organic bioelectronics has experienced a dramatic development in recent years and during its existence has shown a number of applications such as metabolite sensing, drug delivery, fabrication of neuromorphic devices, and many more.

The organic electrochemical transistor (OECT), which combines both a sensor and a signal amplifier in its structure, is an ideal tool for the interface between biological and artificial systems. Currently, the OECT research is dominated by commercial PEDOT:PSS, which, however, has a number of disadvantages, such as operation in depletion mode, the difficulty of its chemical modification, and very high acidity. Therefore, it is necessary to focus development on other materials as well to remedy these unwanted properties.

Both ionic and electrical conductivity are required for OECTs to function properly. It is therefore beneficial to functionalize the OECT active materials with hydrophilic moieties (such as glycol chains) to ensure ionic conductivity, but it is also important to pay attention to the type of conjugated backbone substituents, as these are directly responsible for the HOMO and LUMO energy levels and influence to a large extent the electrical conductivity.

Based on our previous work with OECT materials, four novel p-type glycolated polymers were synthesized and electrochemically characterized in this study. The structure of the given materials is based on the material inDTP-T, which reached high values of transconductance (963 μ S), but its oxidation in an aqueous environment occurred after applying a very small potential (0.14 V) to the gate electrode, which can have a negative effect on its long-term stability. To overcome this problem two approaches were tested. First, the replacement of one glycol side-chain with a fluorine atom and, second, the use of a methylene linker between the glycol side-chain and the conjugated backbone. While the first method achieved a change in oxidation potential of only tens of millivolts, the second method allows a change in oxidation potential in the order of hundreds of millivolts. By combining both methods, a finer tuning can be achieved, which can lead to the possibility of synthesizing polymers with precisely defined properties according to the needs of the application.



Name: Fariha Aktera

Group: Fornili Group

Funding: EPSRC

Project title: Targeting cardiac myosin: a structure-based approach to design conformation-selective modulators

Presentation Title: In silico design of cardiac myotropes for the treatment of cardiovascular diseases

Fariha Aktera, Julien Ochalab,c and Arianna Fornilia

a. School of Physical and Chemical Sciences, Queen Mary University of London, Mile End Rd, Bethnal Green, London E1 4NS.

b. Centre for Human & Applied Physiological Sciences, King's College London, Great Maze Pond, London SE1 9RT

c. Department of Biomedical Sciences, University of Copenhagen, Blegdamsvej 3B, København N, DK-2200

Heart disease is one of the leading causes of mortality worldwide, despite medical advancements. Recent research has indicated that new promising treatments can be developed by designing drugs that can directly bind the key cardiac motor protein myosin II and modulate its contractile activity in diseases such as hypertrophic and dilated cardiomyopathy¹. Myosin can adopt different conformations during its functional cycle. Compounds that can selectively stabilise these conformations are expected to have different effects on myocardial contractility². This research aims to rationally design new conformation-selective compounds of human β -cardiac myosin.

Various conformation-selective ligands were identified using virtual screening, molecular docking, and molecular dynamics (MD) simulations. Hydrogen bond and contact map analyses showed that selectivity towards a specific conformation was related to a higher number of protein-ligand interactions. MD simulations confirmed a stabler binding to the expected state for each ligand. Moreover, new possible target conformations were identified with enhanced-sampling MD simulations (steered MD and umbrella sampling) of the recovery stroke transition. Pocket tracking analyses revealed that the binding site is very dynamic with significant changes in physicochemical properties such as size and polarity. These findings will be used to guide the design of drugs that can selectively stabilise intermediate states in the myosin recovery stroke.

The best candidates will be tested in vitro on single cardiac myosin molecules to measure their effect on myosin force, velocity, and power and determine the type of activity (activation or inhibition) of each ligand³.

1 S. J. Lehman, C. Crocini and L. A. Leinwand, *Nat Rev Cardiol*, 2022, <https://doi.org/10.1038/s41569-022-00682-0>.

2 S. Hashem, W. G. Davies and A. Fornili, *J. Chem. Inf. Model.*, 2020, **60**, 6438–6446.

3 J. Ochala, M. Li, M. Ohlsson, A. Oldfors and L. Larsson, *The Journal of Physiology*, 2008, **586**, 2993–3004.

Name: Thomas Keenan

Group: Stellios Arseniyadis Group

Funding: Queen Mary, University of London/ Laboratoires Servier

Project title: Advances in Asymmetric Palladium catalysis

Presentation Title Novel, bench-stable chiral pre-catalysts for improved Palladium-catalysed asymmetric alkylations.

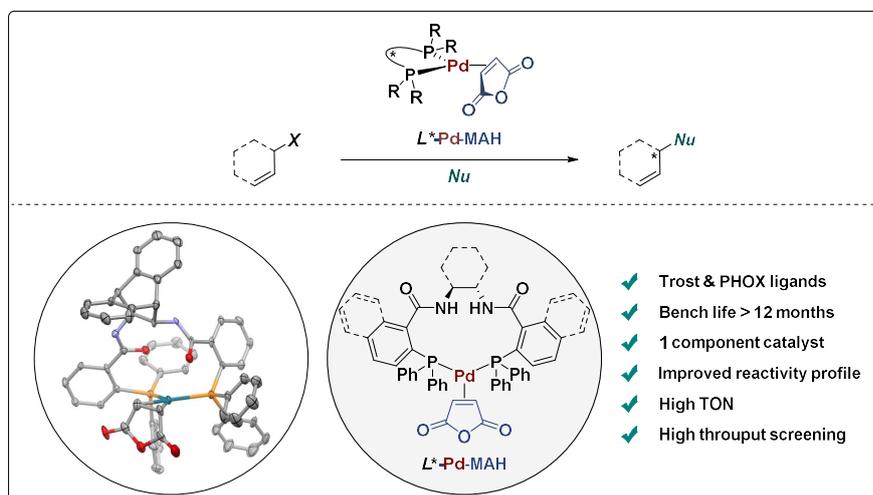
Thomas Keenan,¹ Jingun Huang,² Alexandre Jean,³ David Leitch,² Stellios Arseniyadis¹

¹Department of Chemistry, Queen Mary University of London, London E1 4NS, U.K

²Department of Chemistry, University of Victoria, Victoria, BC V8P 5C2, Canada

³Industrial Research Centre, Oril Industrie, 76210 Bolbec, France

Palladium catalysis is at the heart of organic synthesis, from making drugs, to agrochemicals, to fragrances, it has re-invented how we construct complex molecules.^{1,2} Furthermore, the revolution of asymmetric Pd catalysis is of profound importance, giving us the ability to make single enantiomers while reducing synthetic effort, cost, and waste.³ Although significant, the area is not without its strife; unstable Pd sources and catalysts are the source of many headaches when undergoing complex syntheses, moreover the environmental toll from the preparation of such catalysts is substantial.⁴ As there are limited alternatives to Pd catalysis, it is imperative that when employing the metal, we use it efficiently and effectively. To that end, we report the preparation of novel chiral Pd complexes and the evaluation of their catalytic activity in various asymmetric alkylations. The catalysts have shown significantly greater practicality, activity, and efficacy than the current best standards. This greater reactivity profile has implications for uncovering new methodologies as well as improving large scale processes. We believe that developing such catalysts will set a mind change and unquestionably place Pd-AAA in the process chemists' toolbox.



Department of Physics and Astronomy Talks

Name: Ali Barlas

Group: Astronomy Unit

Funding: Science and Technology Facilities Council (STFC)

Project title: Dynamics and evolution of natural satellites concerning formational irregularities

Presentation title: The mystery of Iapetus

The Solar System is home to curious objects, from moons that could hold the keys to life to ring systems that may have been the birthplace of moons. Amongst these celestial bodies, one moon has perplexed scientists since the 1600's - Iapetus, the third largest moon of Saturn. The Cassini mission in 2007 gave us an in-depth look at the features of Iapetus through images and revealed many interesting geophysical properties that to this day are disputed.

Sometimes called the Yin Yang moon, Iapetus has two hemispheres with a completely different colour as well as a flattened shape that resembles a walnut. Most interestingly, a large continuous ridge covers most of the equator of Iapetus. It has interesting dynamical properties too, such as being tidally locked to Saturn despite its distance being too large for tidal locking to make sense!

My research looks at the dynamics of Iapetus and aims to apply our knowledge about the Earth's Moon, using N-body simulations and semi-analytic expressions, looking at similarities and trying to come up with answers for features such as the ridge.

Name: Lewis Sword

Group: Centre for Theoretical Physics (CTP)

Funding: Science and Technology Facilities Council (STFC)

Project title: Holographic Superconductors

Presentation title: Holographic Superconductors

A superconductor is a material that experiences zero electrical resistance and expels magnetic fields, when driven below a critical temperature. With the introduction of the AdS/CFT correspondence, the gravitational dual to a superconductor has now been discovered. This talk aims to understand what this dual description is, by delving into its construction and exploring its various features. Key concepts like the condensate and critical temperature will be covered, as well as the general methodology in building such a "holographic superconductor". Finally, some of the interesting interior and exterior phenomena that emerge from the numerical solutions, will be discussed.

Name: Joe Davies

Group: Particle Physics Research Centre (PPRC)

Funding: Queen Mary, University of London/DiscNet CDT

Project title: The Search for Dark Matter at the ATLAS Detector using Machine Learning

Presentation title:

Name: Bernet Meijer

Group: Centre for Compressed Matter Physics

Funding: Queen Mary, University of London/ISIS Neutron and Muon Source (STFC)

Project title: Routes to barocaloric materials: importance of rotational dynamics in ammonium sulfate

Presentation Title: Routes to barocaloric materials: importance of rotational dynamics in ammonium sulfate

Solid-state cooling using barocaloric materials is a promising avenue for eco-friendly, inexpensive and efficient cooling. However, in order to design barocaloric compounds it is essential to understand the mechanisms behind this group's large pressure-driven entropy change.

To this end, we studied the rotational dynamics in the giant inverse barocaloric ammonium sulfate. Using a newly developed low background, high-pressure gas cell, quasi-elastic neutron scattering experiments under pressure have afforded detailed insight into the origin of the barocaloric effect. In the low-entropy phase, jump-rotations of the ammonium cations increase with pressure. This is the result of pressure destabilising the structure and driving the material to the high entropy phase, where rotations are maximally activated. We argue that this mechanism is the result of competing hydrogen bond networks between the two phases; this feature can be a guide in the search for new caloric materials.

Name: Tong Qui

Group: Particle Physics Research Centre (PPRC)

Funding: China Scholarship Council (CSC)

Project title: search for a heavy pseudo scalar Higgs boson decaying into a Z boson and a light Higgs boson with the ATLAS detector

Presentation title: Search for a new particle using data collected by the ATLAS detector at the Large Hadron Collider

The talk presents a search for a new heavy particle decaying into a Z boson and a Higgs boson, with the Z boson decaying into two leptons and the Higgs boson decaying into two b quarks. The search uses data collected by the ATLAS detector at the Large Hadron Collider during 2015 - 2018.

The search is motivated by two beyond-the-Standard-Model theories: the Two-Higgs-Doublet Model and the Heavy Vector Triplet Model. The Two-Higgs-Doublet Model predicts the existence of five Higgs-like bosons: two charged (H^\pm), two CP-even (h, H) and one CP-odd (A). The Heavy Vector Triplet Model predicts the existence of two heavy vector bosons: Z' and W' . The search examines the reconstructed invariant mass of Zh candidates in a mass range of 220 GeV to 5 TeV. The result of the analysis is consistent with the Standard Model prediction. Upper limits are set on the production cross section of A and Z' .

Name: Gergely Kantor

Group: Centre for Theoretical Physics (CTP)

Project title: Exact and Numerical Techniques in (Super)Conformal Field Theories

Presentation title: Machine Learning Techniques in Theoretical Physics

In this talk we will aim to give a small taste of some novel machine learning techniques and their applications to theoretical physics. In recent years, the topic of machine learning has become a highly sought-after technique in industry as well as in some areas of experimental physics. For these areas, the abundance of data makes it natural to apply machine learning methods. In contrast, what happens in areas of theory, where data is not so readily available? The answer lies with a contemporary branch of machine learning, known as reinforcement learning. This type of learning generates its own data and can solve problems in very diverse settings. For our case, the setting will be to solve for the parameters of certain highly restricted theories in two-dimensional physics. We will ask the algorithm to minimise a set of non-trivial simultaneous equations, by tuning the parameters in up to 100-dimensional parameter spaces. We will find that reinforcement learning can find the theory that we are looking for, and we will argue that its applications in theoretical physics would very well complement existing numerical and analytic techniques.

Name: Evangelin Hutamaningtyas

Group: Centre for Condensed Matter Physics

Funding: Queen Mary, University of London

Project title: SANS Investigations of N₂ and CO₂ Adsorption in Soft Templating Porous Carbon

Presentation Title: SANS Investigations of N₂ and CO₂ Adsorption in Soft Templating Porous Carbon

Nanostructured porous carbons are widely used in a wide range of applications including catalysis, water treatment, energy storage, and gas sorption. Porous carbons have microporosity that holds an important role in the gas adsorption of light molecules. Porous carbon can be synthesized by treating cellulose, starch, or other sugar molecules in a pressure vessel at a high temperature, 230°C

in an aqueous solution and additional carbonization heating. Depending on the temperature used during the carbonization, the porosity and interlayer spacing are varied. Combining hydrothermal carbonization with templating agents and/or activation can open the pore structure and enhance textural properties. From the previous work, it was found that glucose-based carbon with an additional template has a very promising performance. The physical activation with applying CO₂ gas flow during heat treatment adds to the high CO₂ uptake. In this work, small-angle neutron scattering (SANS) was used to study the behaviour of N₂ and CO₂ absorption at high pressure from 20 to 40 bar, in the micropores of soft-templating porous carbon.

Name: Licheng Zhang

Group: Centre for Condensed Matter Physics

Funding: China Scholarship Council (CSC)

Project title: Excitons and electron spin relaxation in semiconductors probed with muon spin rotation/resonance/relaxation

Presentation title: Universal method to extract average electron spin relaxation in organic semiconductors from muonium ALC resonances

Muon spin spectroscopy and in particular the avoid level crossing (ALC) technique is a sensitive probe of electron spin relaxation (eSR) in organic semiconductors. In complex ALC spectra, eSR can be challenging to extract, as it requires the modelling of overlapping ALCs, where covariance between parameters can result in significant uncertainties. Here we demonstrate a general method to extract eSR rate, which is independent on the number of ALCs resonances present, whether they overlap or not, and what the muonium hyperfine (isotropic and anisotropic) parameters are. This can then be used as guidance for undertaking experiments.

Name: Zaid Dhorat

Group: Centre for Condensed Matter Physics

Funding body: Queen Mary University of London

Project title: Nanopores

Presentation title: Nanopores: Size matters

Nanopore sensors have been an incredibly disruptive technology on the DNA sequencing industry. Nanopore sensors allow for ultra-dilute and rapid real time detection of single molecules and sequencing of DNA. With medicine advancing on personalised health care the use of these sensors as low cost, low skill, in situ sensors is a potentially revolutionary development. While biological nanopores are capable of sequencing they are difficult to integrate into conventional electronic systems, meanwhile their solid-state counterparts are currently unable to sequence DNA but are easily integrated into electronic set ups. As a result of this, developing solid-state nanopores to be capable of replicating the behaviour of biological pores would be a boon to the technology, as it would allow for the use of the cost effective and scalable techniques of the semiconductor fabrication industry.

Solid-state nanopores can be fabricated in thin (less than 20nm) dielectric membranes using Controlled Breakdown enabling the production of nm diameter pores in electrically conductive solutions. This technique allows for pores with dimensions comparable to their biological counterparts, and while these are routinely produced in labs around the globe they perform woefully at sequencing. While much of the work done with nanopores has been focused on DNA sequencing there remains an interest in using them to develop a myriad of techniques, for example, ultra-high density molecular data storage, single molecule detection, and scanning electrochemical microscopy to name a few. Solid-state nanopores face a performance issue as sensors; this is likely due to the poorly understood nature of pore fabrication and the underlying physics that govern the behaviour of the pores. A major short coming is an accurate description of how surfaces charges that from the nanochannels walls interact with ions in the solution and any translocating objects as a result. Here I will present an overview of making nanopores with controlled breakdown and present data showing these pores are not always cylindrical as is commonly assumed in literature.

Year Two Posters Abstracts

Name: Simiao Yu (1)

Group: Christian Nielsen Group

Funding: China Scholarship Council (CSC)

Project title: New materials for bioelectronic applications

Poster title: n-Type small molecules for bioelectronic applications

A series of n-type small molecules based on naphthalene diimide (NDI) and perylene diimide (PDI) building blocks were designed and synthesised. When functionalised with different ion-transporting groups to the imide nitrogen positions, ions and electrons could be conducted in aqueous environment, which made them promising materials for organic electrochemical transistors and biosensor

Name: Peng Ren (2)

Group: Isaac Abrahams Group

Funding: China Scholarship Council (CSC)

Project title: New Li⁺ Ion Conducting Solid Electrolytes for All Solid-State Batteries

Poster title: Composite Materials as Electrolytes for All Solid-State Li-ion Batteries

All solid-state batteries are being considered as for convention Li-ion batteries, that typically contain flammable electrolytes. However, the development of such batteries is limited by the lack of Li⁺-ion conducting solid electrolytes with high conductivity at room temperature. Lithium lanthanum titanium oxide (LLTO) shows promising bulk conductivity, but its grain boundary conductivity is low, leading to low total conductivity. Additionally, the contact between the LLTO electrolyte and the electrodes is generally not intimate, leading to large interfacial resistance. Composite LLTO-glass materials have been proposed as a possible way to improve the grain boundary conductivity of the electrolyte and reduce the interfacial resistance. In this study LLTO-lithium borophosphate (LLTO-LBPO) composites were prepared by adding LBPO glass to LLTO ceramics, aiming to form an amorphous lithium-rich layer at the grain boundary. X-ray diffraction, scanning electron microscopy and electrochemical impedance spectroscopy were used to characterize their composition, microstructure and ionic conductivity. The results show that the total ionic conductivity can be enhanced using this approach, achieve a conductivity of 4.13×10^{-4} S/cm at 24 °C. Further composition optimization is likely to improve on this.

Name: Qi Li (3)

Group: Chris Jones Group

Funding: CSC (China Scholarship Council)

Project title: The Role of Fe in Conjunction with N-doping on Oxygen Electrocatalysis

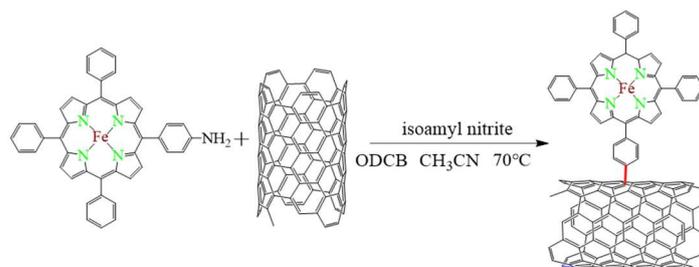
Poster title: Investigating the role of Fe-Pyrrolic N4 configuration in the Oxygen Reduction Reaction via covalently bond porphyrin-functionalized carbon nanotubes

Q. Li^{1,2}, Y. Xu^{1,2}, A. Pedersen², M. Zhang¹, H. Luo², C. R. Jones^{1*}, M.-M. Titirici^{2*}

1. School of Physical and Chemical Sciences, Queen Mary University of London, Mile End Road, London E1 4NS.

2. Department of Chemical Engineering, South Kensington Campus, Imperial College London, SW7 2AZ.

Atomically dispersed iron-nitrogen-carbon catalysts are promising, low-cost, and high-performance electrocatalysts for the oxygen reduction reaction (ORR) in fuel cells. However, for most Fe-N materials generated under pyrolysis at a high temperature (always more than 500°C), it is very difficult to predict the precise outcome of the Fe-N environments. This results in most analysis of the Fe-N environment post-manufacture. In addition, it is very difficult to accurately reproduce the same outcome between two pyrolytic processes. So, the different Fe-N configurations in pyrolytic materials make it confusing to know the best chemical and coordination environment for Fe, as well as obtaining a clearer understanding of their ORR mechanisms.



Scheme 1 Synthetic strategy of FeTPP-CNTs

We look to make bespoke functionalization to produce desired Fe-N environment in a precise manner, therefore allowing the role and activity of each environment to be studied. Herein, carbon nanotubes (CNTs) were covalently functionalized with iron-complexed porphyrin rings (iron 5-(4-aminophenyl)-10,15,20-(triphenyl)porphyrin (FeTPP)) via aryl diazonium methodology which has previously been used to covalently functionalize CNTs and Graphene substrates with different arene components under 100°C.[1,2] With the advantages of high conductive and large surface area, low defect CNTs were chosen as the carbon substrate for TPP in this work. Porphyrin is composed of four pyrrole subunits, connected by methylene bridges, which can efficiently bind an iron atom at the center to form the Fe-Pyrrolic N4 configurations. This exact and controlled configuration of FeTPP-functionalized CNTs can then be clearly studied in the ORR process and lead to a better understanding of the mechanism. Two different samples of TPP-functionalized CNTs have been prepared in this work, one containing Fe-bound porphyrins and one sample without Fe. According to our investigations, it was determined that the TPP-CNTs operated via a 2 electron pathway and with similar ORR performance to pristine CNT, while FeTPP-CNTs material achieved a 4 electron pathway and exhibited a better limiting current density, due to its Fe-Pyrrolic N4 configurations. This research hopes to establish a new way to understand the role of Fe-N configurations in ORR and shed the light on designing and developing high-performance Fe-N-C catalysts.

References:

[1] Z. Guo, F. Du, D. Ren, Y. Chen, J. Zheng, Z. Liu and J. Tian, *J. Mater. Chem.*, 2006, 16, 3021-3030

[2] D. Dasler, R. A. Schäfer, M. B. Minameyer, J. F. Hitznerberger, F. Hauke, T. Drewello, and A. Hirsch, *J. Am. Chem. Soc.*, 2017, 139, 11760–11765

Names: Xiang Li, Nivetha Jeyachandran, Ilaa Hasanova (4)

Group: Christina Giordano group

Funding: CSC, QMUL, State Program for increasing international competitiveness of the higher education system of the republic of Azerbaijan in 2019-2023

Project title: Metallic nano-ceramics designed for the production of green energy

Poster title: Metallic nano-ceramics designed for the production of green energy

The increasing demand for energy is worldwide and urgently requires the substitution of fossil fuels with sustainable and renewable energies to prevent devastating consequences to our environment. An important role is played by catalysts that must be stable and favor high yield in the reaction.

Our research is dedicated to the synthesis of nanosized metals and metallic ceramics (namely transition metal nitrides, carbides, oxides and metallics MN/MC/MO/MO) to serve as catalysts for energy related applications. Nanomaterials possess an intriguing combination of properties (e.g. high specific surface area, catalytic, tailored properties via size and shape etc.) which allow us to envisage numerous applications. We investigate into a broad range of applications including electrochemical water splitting, electrocatalytic reduction of CO₂ into added-value chemicals and biomass valorization.

The synthesis is achieved based on a green, cost-friendly, and facile method, called the urea glass route.¹ The route also allows to prepare nanoparticles with different crystallinity from monometallic nanoparticles to more complex bimetallic systems. Regarding electrochemical applications, Mo₂C@C and CuNi@TiO₂ nanoparticles were designed for Hydrogen Evolution Reaction and CO₂ reduction reactions, respectively. For the biomass valorization, Ni and Fe based catalysts were designed for the conversion of biomass model compounds.

References

[1] C. Giordano, C. Erpen, W. Yao, B. Milke and M. Antonietti, Metal Nitride and Metal Carbide Nanoparticles by a Soft Urea Pathway, *Chem. Mater.*, 2009, **21**, 5136–5144.

Name: Haseeb Ur Rehman Shah (5)

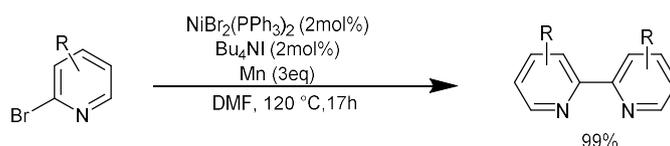
Group: Dr. Christopher Raymond Jones

Funding: Higher Education Commission of Pakistan (HEC)

Project Title: Synthesis of 2,2'-Bipyridines using Nickel Catalysis

Poster Title: Synthesis of 2,2'-Bipyridines using Nickel Catalysis

Bipyridines are ligands coordinates to metals form complexes that are useful in medicinal chemistry. Already used methods use loads of catalysts, long reaction time and large number of reagents. In this project, to overcome these issues, a new method is developed to synthesize these ligands.



Abstract: schematic representations of this study.

Name: Xuankai Huang (6)

Group: Isaac Abrahams Group

Funding: China Scholarship Council (CSC)

Project title: New Materials for Next Generation Battery System

Poster title: High conductivity in Na⁺-ion conducting solid electrolytes for Na-ion batteries

The replacement of the presently used liquid electrolytes by non-flammable solid electrolytes is an important avenue to create safer batteries. The sodium superionic conductor (NASICON), one of the most promising solid electrolyte candidates, displays high bulk ionic conductivity and good stability toward other NASICON -based electrodes and is a potential solid electrolyte for solid-state Na-ion batteries. However, the practical use of NASICON has been impeded by low ion mobility at room temperature (RT) and poor interfacial connectivity. Here, the improvement of both bulk and grain boundary conductivity has been achieved simultaneously via La and Zn co-doping. The highest total conductivity of $4.68 \times 10^{-3} \text{ S cm}^{-1}$ at room temperature was obtained for Na_{3.3}Zr_{1.8}La_{0.1}Zn_{0.1}Si₂PO₁₂, which is amongst the highest values recorded for a NASICON system. Furthermore, the system shows good air stability and could represent a suitable material for application in the field Na-ion batteries

Name: Amina Khatoon (7)

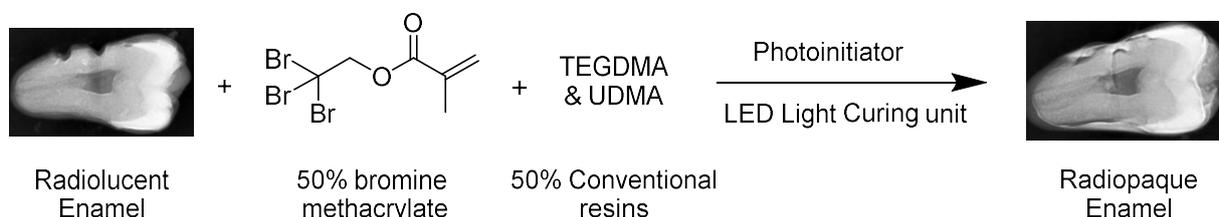
Group: Stellios Arseniyadis Group

Funding: Higher Education Commission of Pakistan (HEC)

Project title: Development of novel polybrominated monomers for radiopaque dental restorative resins

Poster title: Preparation of novel polybrominated monomer for use as early enamel carious lesions

In dentistry, detection of early enamel lesions is a major concern. So, the infiltrant used for enamel carious lesions should have a radiopacity equal to or greater than enamel. Conventional dental resins are generally radiolucent. Addition of heavy atoms such as halogens, generally bromine, make them radiopaque without affecting their properties like viscosity and phase separation. The objective of the project is to develop, characterise, and ultimately incorporate suitable polyhalogenated (polybrominated) monomers into resin infiltrant with different ratios to attain the desired radiopacity, viscosity and curing time.



Name: Christian Osborne (8)

Group: Stoichko Dimitrov Group

Funding: Queen Mary, University of London

Project title: Novel optical spectroscopy analysis of printable semiconductors

Poster title: Extending exciton diffusion in Organic Semiconductors via water passivating dopants

The performance of organic solar cells remains significantly lower than inorganic and perovskite devices, largely due to the fundamental difference in how charges are generated within the photoactive layer. Organic semiconductors are excitonic in nature, by which an exciton must diffuse to an interface and separate into free charges. These materials commonly possess diffusion lengths of a few nanometres and thus require a specific device structure to obtain high power conversion efficiencies. In recent years, it has been suggested that trap states introduced from water molecules present in the thin film can impede both exciton diffusion within the photoactive layer and charge transport in devices. In this work, we use a doping strategy focusing on passivating water with small molecular additives to remove trap states and assess the effect this has on diffusion using transient absorption spectroscopy. We found that a greater than two-fold increase to the exciton diffusion length was achieved upon introducing the molecule 11,11-dicyano-9-anthraquino-10-methane (DCAQ) as a dopant into the thin film of the benchmark semiconducting polymer PM6. This extension is significant, as it could improve exciton dissociation, resulting in higher device photocurrent. Additionally, it could allow for greater flexibility of device structures, increasing viability for large-area printed devices.

Name: Jing Ming (9)

Group: Issac Abrahams Group

Funding: China Council Scholarship (CSC)

Project title: Ceria based solid electrolytes for solid oxide fuel cells

Poster title: A Review of Defect Structure and Conductivity in Ceria Based Solid Electrolytes for IT-SOFCs

Solid oxide fuel cells (SOFCs) have increasingly gained attention due to their high efficiency and flexible fuel options. SOFCs consist of a cathode, anode, and a solid oxygen ion (O_2^-) conducting electrolyte. They have efficiencies in the range of 45 to 65% via the transportation of oxide ions, which meets the requirements of the large power sector. However, the widespread application of SOFCs is hampered by their high operating temperatures (over 800 °C) because of the fast performance degradation at lower temperatures. Lower operating temperatures lead to polarization losses, resulting in a broadened gap between the attained and theoretical efficiency. To overcome this issue, electrolytes of high conductivity and low leakage current at intermediate temperatures (IT) are needed to minimize the polarization losses. Doped ceria-based solid electrolytes are gaining much attention for intermediate temperature solid oxide fuel cells (IT-SOFCs) due to their high oxide ion conductivity in this temperature range (600-800 °C) and their compatibility with electrode materials.

Many different parameters influence the conductivity of CeO_2 and have been analysed by comparing various aliovalent dopants. Recent computational and experimental studies indicate an ideal ionic radius for rare earth and alkaline dopants in ceria. The other parameters such as the energy of vacancy formation, migration and association also influence the conductivity. These parameters set a fundamental basis for effective dopant and co-dopant selections for advanced performances.

The doped ceria electrolytes are currently unable to achieve their theoretical maximum ionic conductivity. Much of this is due to local structural changes not immediately evident in the average structure derived from conventional diffraction experiments. A clearer picture of local structure can be obtained from analysis of total neutron scattering, which is the aim of the present work. In this way, a deep understanding of the defect chemistry can be obtained including defect trapping, blocking and vacancy-vacancy repulsions, which have significant influence over the conductivity in these important electrolytes.

Name: Pauline de Bigault de Cazanove (10)

Group: Marina Resmini Group

Funding: Queen Mary University of London

Project title: Bioplastic: Understanding the chemistry and its environmental impact

Poster title: Bioplastic: Understanding the chemistry and its environmental impact

The impact, behaviour, and fate of plastic polymers in the environment is the subject of global concern and debate, therefore leading to an accelerated search for viable alternatives. The novelty of the market has attracted the development of many products termed bioplastics with varied, yet confusing statements such as biodegradable, compostable, or oxo-degradable. It refers to the conditions in which the product will further degrade and do not always conform with the preconceived idea of biodegradability. The degradation rate of a given product is related to the processing conditions and expected decomposition media, often performed in standardised mediums. It is believed that the process is induced by environmental factors that act in combination to fragment the polymeric material into shorter units which allow further biotic degradation by microorganisms. Understanding the fate of bioplastics in the environment is critical, and yet unknown, as the biopolymers and their breakdown products may impact on biota, microbial communities, and more broadly on global biogeochemical cycles.

One aspect of the project focuses on the study of the degradation profile of unaged and artificially aged polymers. A combination of UV irradiation and thermal exposure is used to obtain reproducible data consistent with natural weathering of plastic. Fourier Transform Infrared Spectroscopy allows the measurement of the carbonyl index which monitors the formation of carbonyl species induced by these processes. Another aspect of the project involves the in-vitro evaluation of the biodegradability of different plastic samples by quantifying the amount of CO₂ produced by bacterial activity using gas chromatography.

Preliminary results demonstrate that the combination of photo-degradation and thermal-degradation gives an excellent protocol for artificial weathering and is promising to help predicting what would happen in the environment. The measurement of the carbonyl index provides evidence of further biodegradability by microorganisms. The different species of bacteria show distinct strategies of biodegradation according to the polymer type in the media.

Pauline de Bigault de Cazanove, Ruth Roseb, Perry Higgsc, Marina Resminia

a. School of Physical and Chemical Sciences, Queen Mary University of London, E1 4NS

b. School of Biological and Behavioural Sciences, Queen Mary University of London, E1 4NS

c. Symphony Environmental Technologies, 6 Elstree Gate, Elstree Way, Borehamwood, Herts, WD6 1JD

Name: Yaojia Long (11)

Group: Yao Lu Group

Funding: China Council Scholarship (CSC)

Project title: High efficiency photothermal systems with the assistance of superwetting materials

Poster title: High efficiency photothermal systems with the assistance of superwetting materials

Seawater desalination and wastewater purification are mainstream strategies to overcome the shortage of fresh water, which is currently a pressing worldwide challenge. Photothermal materials and adsorbents are the main components of solar-driven seawater desalination and wastewater purification, respectively. Herein, improved from generation to generation, five generations in total have been fabricated from polydimethylsiloxane (PDMS) by a sugar silk templated method, which can achieve the aim of obtaining a simple and integrated photothermal water evaporation system to produce clean water and solve the salt accumulation problem. The designed device not only enables sufficient water evaporation through the hydrogel, but also offers a high light-to-heat conversion efficiency originating from the added graphite powder. Furthermore, the efficiency and durability of the fabricated device need to be measured for adapting in convenient recycling program and practical applications.

Name: Qi Zhao (12)

Group: Devis Di Tommaso; Group

Funding: China Scholarship Council (CSC)

Project title: Heterogeneous Catalysis with Earth-Abundant Metal Oxides

Poster Title: Mechanistic insights into the of graphene mesosponge via catalytic methane decomposition on metal oxides

Graphene mesosponge (GMS) is a new class of mesoporous materials with high electric conductivity, elastic and flexible nature, unprecedentedly high electrochemical stability due to their three-dimensionally continuous and seamless nanostructure. GMS is synthesised via chemical vapour deposition (CVD) of CH₄ onto a template of metal oxides such as MgO and Al₂O₃, which catalyses methane conversion at high temperatures. Here, we report a computational investigation of the early stage of CH₄ activation toward the porous nanocarbon formation on different metal oxides.

Name: Anant Khanna (13)

Group: Rachel Crespo-Otero Group

Funding: Leverhulme Trust

Project title: TOWARDS THE RATIONAL DESIGN OF HIGHLY EMISSIVE MATERIALS

Poster Title: Analysis of structures and properties for design of OLED materials

Phosphorescent organic light-emitting diodes (PhOLEDs) have attracted attention because of their prospective use in display monitors and lighting applications and their higher energy efficiencies. However, designing blue PhOLEDs with longer operational lifetimes remains to be a challenge. In this work, we use a database of PhOLEDs¹ to analyse the structures and theoretical properties of 191 hosts and 11 guests to gather property-structure and property-property relationships. Donor (D), acceptor (A) and linker (L) moieties of the hosts were identified, with carbazole (Cz), pyridine (Py) and benzene (Bz) as the most commonly occurring D, A and L, respectively. We also analysed the alignment of the energy levels of the hosts and guests to find combinations of dopant-host with reduced charge trapping. We believe these results contribute to a better understanding of how we can design PhOLED devices with the most promising host and dopant combinations.

[1] Chan et al, Organic Electronics, 63, 257-266, (2018)"

Name: Yaquan Wang (14)

Group: Yao Lu Group

Funding: China Council Scholarship (CSC)

Project title: Highly stretchable cellulose-based hydrogel for green electronic devices

Poster title: Double-network ionic conductive hydrogels for strain sensor

Stretchable, flexible, and wearable hydrogels are developed as strain sensors for human motion monitoring due to their capabilities to convert external stimulus into electric signals. However, traditional hydrogels have the problems of water dehydration at room temperature, and lower strain range. In addition, they inevitably lose elasticity and ionic conductivity at sub-zero temperature due to water freezing. In order to overcome these challenges, double-network hydrogels were constructed to enhance mechanical performances, reduce water loss and improve anti-freezing properties using cellulose and poly(vinyl alcohol). Furthermore, the as-prepared hydrogels were used to demonstrate their potential of strain sensors.

Name: Linchao Sun (15)

Group: Yao Lu Group

Funding: China Council Scholarship (CSC)

Project title: Intelligent biomimetic actuating materials

Poster Title: Recyclable moisture-driven biomimetic actuator based on carbon/sodium alginate (SA)/polyvinyl alcohol (PVA) composite film

The moisture-responsive actuators that convert external energy into kinetics energy and move spontaneously and continuously have been intensively investigated as energy-harvesting devices. Here, we propose a sustainable methodology to prepare the soft actuator using environmentally friendly raw materials and fabrication process. The raw materials including the carbon-based materials, sodium alginate and polyvinyl alcohol are utilized to prepare the sustainable actuating (SusAct) composite films through the direct water evaporation method. It was demonstrated that programmable motion and mimicking biological behavior could be achieved by tuning the geometry of the membrane. The composite film and appropriate geometry featured strong figures of merit and capabilities with 250° maximum bending angle under 85% RH. Moreover, the applications including walkers, smart switch, flexible excavators and hand-shaped actuator were further achieved by modulating the shape of film actuator. Thus, the composite films make it applicable to potentially promising applications due to inherent adaptive integration and low-cost manufacturability.

Name: Xu Leng (16)

Group: Dr. Yao Lu

Funding: China Scholarship Council (CSC) S

Project title: Durable bioinspired materials for antibiofouling applications

Poster Title: Bioinspired antifouling surfaces with autocrine aqueous lubricant property based on freeze-dried sodium alginate/polyvinyl alcohol matrices embedded with polyethylene oxide

Biofouling is a severe problem for many applied technical surfaces ranging from ships and piers to water inlets and medicine. Fishes can always maintain clean body surfaces when they are exposed to contamination. Inspired by the fish skin, an antifouling material with autocrine hydrated lubricant property was designed. The porous freeze-dried sodium alginate (SA) hydrogel functioned as the skin tissue to release embedded polyethylene oxide (PEO) as mucus. To control the release of PEO, polyvinyl alcohol (PVA) was introduced to fabricate SA/PVA blend matrices. The average pore size, porosity, release rate of PEO, compressive modulus, oil resistance, and antibiofouling performance of the prepared antifouling matrix were investigated. Results showed that by the addition of PVA greatly decreased the pore size of blend matrix and thus slowed the release of PEO. Besides, SA/PVA showed enhanced compression resistance compared to pure SA/matrix. Due to the autocrine PEO layer on the surface, the SA/PVA blend matrix with PEO embedded showed stimulus-response and self-healing features which were beneficial to repelling oil adhesion and preventing settlement of microorganisms. This design for fabricating the bio-inspired antifouling material has a broaden application potential in coatings, oil-water separation, seawater desalination and other fields.

Name: Christos Matsingos (17)

Group: Fornili Group

Funding: BBSRC-LIDo

Project title: The activation mechanism of GPR68: a computational study

Poster Title: The activation mechanism of GPR68: a computational study

GPR68 is an orphan G protein coupled receptor (GPCR) that is part of a family of proton sensing GPCRs. The members of this family are unique in that they are activated not by a ligand directly but rather by changes in extracellular pH. GPR68 is involved in various physiological processes and has been found in a variety of tissues. Interestingly, recent evidence implicates low and high levels of GPR68 with the progression of neoplastic pathologies^{1,2}. The receptor, however, remains pharmacologically dark and little is known about its activation mechanism. Our work adopts an *in silico* approach to study the activation mechanism of the receptor. Molecular Dynamics simulations of the receptor in different protonation states were used to determine the amino acids that are most likely to be affected by changes in pH and how these changes lead to receptor activation. We have determined a possible sequence of protonation events on the extracellular and transmembrane region of the receptor that are associated with changes in microswitches indicative of activation. These insights into the mechanism of proton sensing and the structure of GPR68 serve to guide drug discovery research in designing specific modulators of GPR68 as possible drugs for the treatment of cancer.