



**RSC INTEREST GROUP
CHEMICAL NANOSCIENCE
AND NANOTECHNOLOGY**

Royal Society of Chemistry

**Chemical Nanosciences and
Nanotechnology Network
Annual Symposium 2022**

**Nanotechnology for Energy,
Environment and Biomedicine**

Burlington House, London, U.K.

17th – 18th January 2022

Welcome to the 2022 RSC Chemical Nanoscience & Nanotechnology Symposium. The annual flagship event consists of plenary speeches, invited talks, contribution presentations, and poster sessions, covering a wide range of topics in Chemical Nanoscience & Nanotechnology.

Nanoscience is at the core of emerging technologies for energy, environmental and health care applications, involving thermal catalysis, photocatalysis, electrocatalysis, solar fuels, batteries, photovoltaics, fuel cells, sensors, biomaterials, and targeted drug delivery. This symposium, organised by the RSC Chemical Nanoscience and Nanotechnology (CNN) Group, covers the recent development in fundamental studies, novel material development and reactor engineering in these areas with the aim to provide a forum for researchers to exchange information, share ideas, and discuss recent advances and the scientific challenges.

Welcome to the Burlington House and hope you all enjoy the in-person symposium after nearly two year isolation!

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Scientific Programme

Monday, 17th January 2022

12:00	Registration	
12:55	Welcome and Introductions Dr Clare Hoskins , <i>University of Strathclyde</i>	
	Session Chair: Prof. Junwang Tang , <i>University College London, UK</i>	
13:00	Plenary Lecture From Lithium Batteries to Perovskite Solar Cells: Exploring Energy Materials at the Nanoscale Prof Saiful Islam , <i>University of Oxford, England, UK</i>	P1
13:45	Protein Corona of nanogels and its impact on the air/water interface Mr Federico Traldi , <i>Queen Mary University of London, England, UK</i>	O1
14:05	P-N junction-based ZnO flexible nanogenerator for biomechanical energy harvesting and self-powered sensing Ms Qinrong He , <i>Queen Mary University of London, England, UK</i>	O2
14:25	Development of NIPAM-based nanogels for brain-targeting drug delivery Ms Roberta Bilardo , <i>Queen Mary University of London, England, UK</i>	O3
14:45	CEM Microwave technology – Dr Matt Burwood	SO1
14:55	Oxford HighQ – Dr Laura Pala and Dr Darren Andrews	SO2
15:05	Afternoon Tea	
	Session Chair: Dr Aaron Lau , <i>University of Strathclyde, UK</i>	
15:30	Plenary Solar-driven Synthesis of Fuels and Chemicals from Biomass and Plastic Waste Using Semiconductor Nanomaterials Prof. Erwin Reisner , <i>University of Cambridge, England, UK</i>	P2
16:15	Invited Lecture A Strategy of Synthesizing High Capacity Silicon-based Anode Using Barley Husks Dr Yimin Chao , <i>University of East Anglia, England, UK</i>	I1
16:40	Redox responsive manganese-based MRI theranostics for cancer therapy Miss Beatriz Brito , <i>University of Hull, England, UK</i>	O4
17:00	Graphene Nanowalls Grown on Copper Substrates Prof Pedro Costa , <i>King Abdullah University of Science and Technology, Saudi Arabia</i>	O5
17:20	Poster Session	
18:00	Close of Sessions	
18:30	Conference Dinner	

Scientific Programme

Tuesday, 18th January 2022

08:45	Coffee & Refreshments	
	Session Chair: Dr Susete Fernandes, NOVA University Lisbon, Portugal	
09:00	Invited Lecture Cucurbit[n]uril mediated aggregation of quantum dots: solution phase assemblies for energy transfer, molecular sensing and surface modification Dr William Peveler, University of Glasgow, Scotland, UK	I2
09:25	Photoelectrocatalytic Disinfection of Water: Evaluation of photoanodes, cathodes, and radicals produced Mr Stuart McMichael, University of Ulster, Northern Ireland, UK	O6
9:45	Gemcitabine-loaded Metal-Organic Frameworks as a treatment for Pancreatic Cancer Ms Rachel Foulkes, University of Glasgow, Scotland, UK	O7
10:05	Cu-doped Mesoporous Silica Nanoparticles as a Platform of Antibacterial Activity Mr Mark Hunter, University of Liverpool, England, UK	O8
10:25	Zeiss Microscopy – Dr Maadhav Kothari, Dr Andrew Elliott and Dr Andy Holwell	SO3
10:35	Morning Tea	
	Session Chair: Dr Paul McNaughter, University of Manchester, UK	
11:00	Plenary Lecture Synthesis and biofunctionalization of Plasmonic and Magnetic Nanoparticles for Biomedical Application Prof. Nguyen Thanh, University College London, England, UK	P3
11:45	pH-responsive Vesicles: A De Novo Nano System for Sustained and Targeted Delivery of Hydrophobic Drug Prof. Naved Malek, Sardar Vallabhbhai National Institute of Technology, India	O9
12:05	Solution-based synthesis of Barium Titanate-Hematite Nanocomposite Thin Films for Enhanced Photocatalytic Activity Dr Joe Briscoe, Queen Mary University of London, England, UK	O10
12:25	Lunch and Posters	
13:35	Poster Prizes and Closing Remarks Dr Yimin Chao, University of East Anglia, and Dr Clare Hoskins, University of Strathclyde	

Plenary and Invited Speakers

From Lithium Batteries to Perovskite Solar Cells: Exploring Energy Materials at the Nanoscale

SAIFUL ISLAM

Department of Materials, University of Oxford

Further breakthroughs in lithium-ion batteries and perovskite solar cells require advances in new compositions and underpinning materials science. Indeed, a greater fundamental understanding and insights into these energy-related materials require atomic-scale characterization of their structural, defect and transport behaviour. In this context, combined modelling-experimental work is now a powerful approach for investigating these properties at the nanoscale. This presentation will describe such studies [1,2] in two principal areas: (i) ion conduction mechanisms and redox chemistry in Li-rich electrodes and solid electrolytes for Li-ion batteries; and (ii) ion transport and mixed A-cation effects in hybrid iodide perovskites for solar cells.

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Solar-driven Synthesis of Fuels and Chemicals from Biomass and Plastic Waste Using Semiconductor Nanomaterials

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Abstract

Artificial photosynthesis is a sustainable process that utilises solar energy to drive endothermic multi-electron chemical reactions for the production of fuels. This process often relies on expensive materials and device architectures as well as the dependence on the thermodynamically and kinetically water oxidation reaction, which challenges the development of ultimately economical devices.

This presentation will give an overview about our recent progress in developing semiconductor nanoparticle systems to perform efficient full redox cycle solar catalysis using inexpensive components. Our approach bypasses the need for water oxidation as it employs the sustainable oxidation of waste biomass and plastics. This process is known as photoreforming and co-produces clean H₂ fuel and organic chemicals. Thus, the bottleneck in classical artificial photosynthesis can be avoided while mitigating waste streams and expanding the chemical reaction space to improve the economics of this process. The principles and design considerations for the solar-driven photo-reforming process will be compared to traditional artificial photosynthetic systems and benefits and disadvantages discussed.

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Synthesis and biofunctionalization of Plasmonic and Magnetic Nanoparticles for Biomedical Application

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Abstract

The development of new chemical methods for the next generation of nanoparticles with very high magnetic moment, fine tuning Au nanorods and novel hybrid and multifunctional nanostructure is presented.

Detailed mechanistic studies of their formation by sophisticated and advanced analysis of the nanostructure allows tuning of the physical properties at the nanoscale; these can subsequently be exploited for diagnosis and treatment of various diseases. The studies are conducted to provide insight for future material design approaches. It will also help to identify the critical process parameters that can be manipulated in order to obtain the suitable physical properties for the intended applications.

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A Strategy of Synthesizing High Capacity Silicon-based Anode Using Barley

Husks

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Abstract

Energy sector decarbonisation requires enormous growth of renewable energy sources and storage to facilitate the variable output of renewables and transport electrification. Over the past decade lithium-ion batteries (LIBs) have dominated in commercial electric vehicles (EVs) and stationary power sector applications. With increasing demand for quick charge-discharge of LIBs, high-power density is extremely desirable in the design of electrode materials for the LIBs. Silica is considered to be a promising material in terms of its relatively high theoretical capacity and low discharge potential. However, several intrinsic drawbacks still need to be overcome, such as poor electrical conductivity, large volume change during charge-discharge process and the sluggish electrochemical kinetics.

The novel approach is to combine a carbonaceous material with silica in order to improve the electrical conductivity and to alleviate the volume change. Properly selected biomass should be an excellent natural combination of silica and carbon source.

The SiO₂ exists in barley husks (BH-SiO₂) in the form of uniform nanoscale structure and are coated by organic carbon component. The porous structures of BH-SiO₂ are formed during the natural growth process of barley that allows BHs to be processed into a promising SiO₂-based anode material.

Keywords: *Lithium-ion batteries; anode; silica; high capacity; barley husks*

Cucurbit[n]uril mediated aggregation of quantum dots: solution phase assemblies for energy transfer, molecular sensing and surface modification

KATIE J MCGUIRE (1), TUNG CHUN LEE (2), **WILLIAM J PEVELER** (1)

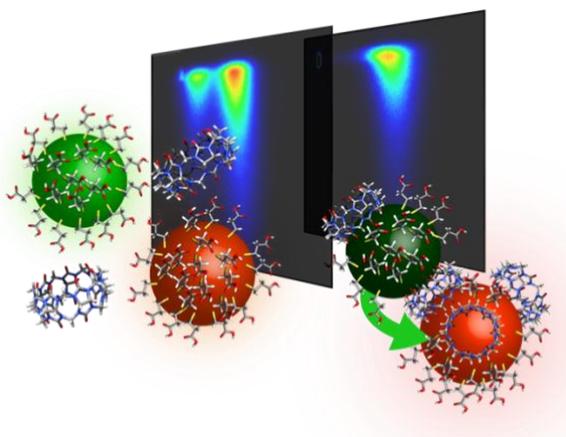
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ABSTRACT

The control of nanoparticle self-assembly to form bulk materials has important applications in energy systems, optical devices, and sensors. Key to these applications is the ability to form stable aggregates with controlled interparticle gap size, ordering and surface chemistry. Aggregation of semiconducting quantum dots (QDs) has been explored extensively in the solid phase for the formation of thin films,[1] but solution phase aggregates with small interparticle distances and a high degree of bulk and surface control have been less widely demonstrated.[2]

I present here the synthesis of small (c.100 nm), solution-phase, colloidal QD aggregates with precision inter-dot spacing, mediated by surface bound cucurbit[n]uril.[3] The mechanism and kinetics of this approach are discussed with reference to luminescence, light-scattering and NMR spectroscopy, and demonstrate control of the inter-QD energy transfer by creating an energy cascade between QDs of multiple different colours, with utility as a sensor for nitroaromatic species hosted within the cucurbit[n]uril guest on the QD surface.[3]



The discovery of QDs interfacing with cucurbituril offers potential for on-QD host-guest chemistry for labelling and sensing applications, as has been previously seen with gold nanoparticles,[4] and I present our recent research in this direction. The interfacing of QDs with other nanoparticles that are known to bind CB well, such as gold or ferrite nanoparticles, should lead to the creation of multimodal plasmonic or magnetic aggregates with applications in biomedicine and photonics.[5]

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Oral Presentations

Protein Corona of nanogels and its impact on the air/water interface

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Abstract

In the last decades, nanomaterials have emerged as attracting platforms for drug delivery and imaging.¹ Despite the great potential of nanoparticles in nanomedicine, their application in clinical settings is hindered by the limited knowledge of their interaction with bio-interfaces. When dispersed in biological media, nanomaterials may be coated with proteins in solution and form a “protein corona”. Extensive research has demonstrated that the formation of protein corona can deeply affect the behaviour of nanoparticles in biological systems.^{2,3} However, the limited knowledge of how the properties of nanomaterials drive the formation of the corona poses a serious obstacle to their rational design. New methods to characterise the nanoparticle corona in its biologically relevant environment are hence required to bridge this knowledge gap.

In this work we developed a novel approach towards the characterisation of protein corona of polymeric nanogels based on dynamic surface tensiometry. Nanogels’ characteristics, such as low toxic profile and high colloidal stability make them ideal candidates for drug delivery applications. A series of acrylamide-based nanogels were synthesised via high dilution radical polymerization. To investigate the effect of electrostatic forces on the affinity of nanogels for proteins, negative or positive charged co-monomers were incorporated in the polymer matrix. Evaluation of protein corona formation was carried out using dynamic light scattering, circular dichroism and surface tensiometry. The latter provides an attractive novel tool for the characterisation of protein corona of nanogels.

We showed that dynamic surface tension could be used as a sensitive technique for the *in situ* detection of protein corona. Moreover, impact of protein corona formation on the properties of nanogels at the air/water interface was investigated. These data advance the understanding of the impact of protein corona on the physico-chemical properties of nanoparticles and enable a more effective rational design of nanomaterials for drug delivery application.

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P-N junction-based ZnO flexible nanogenerator for biomechanical energy harvesting and self-powered sensing

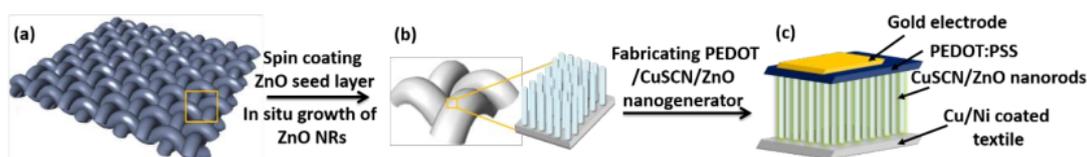
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Abstract

Mechanical energy is considered as one of the most promising resources because it is abundant and accessible in various environments such as body movements, vibration, flowing air and muscle stretching. In addition, with increasing development of portable/wearable electronic devices such as smart watches, health or activities monitors, it is particularly desirable to research a flexible energy harvester that can capture multiple forms of mechanical energy with enhanced energy conversion efficiency, which holds great promise in personal smart devices.

Herein, p-n junction-based ZnO flexible nanogenerator has been designed to combine the advantage of ZnO piezoelectricity and textile or fibre flexibility. ZnO nanorods were synthesized on flexible substrates such as copper-nickel and silver coated textile, and carbon fibres. PEDOT:PSS and CuSCN are used to reduce the external and internal screening effect by forming a P-N junction and surface passivation to enhance the performance.¹⁻² The textile-based nanogenerator can generate increasing output voltage from 0.2 V to 1.81 V as the shaking frequency increases from 19 Hz to 26 Hz with high stability and durability under 26000 cycles test by shaking at 26 Hz. The output voltage from the device can activate an LCD screen display by shaking at its resonant frequency.³ In addition, carbon-fibre based nanogenerator exhibits the ability of self-powered acceleration sensing, which shows increasing output voltage from 1.4 V to 7.6 V when the acceleration ranges from 0.1 to 0.4 m/s². Both of the above flexible nanogenerators are able to harvest energy from different biomechanical forces such as impacting force, flicking and gentle finger tapping and pressing. Our results can be utilized for future flexible self-powering nanogenerator design to harvest a larger amount of electricity from the environment.



Scheme 1. Fabrication process of PEDOT:PSS/CuSCN/ZnO textile nanogenerator. (a) Cu/Ni coated textile, (b) enlarged section of textile with grown ZnO nanorods, (c) schematic of nanogenerator.

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Development of NIPAM-based nanogels for brain-targeting drug delivery

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Abstract

The access of drugs to the brain is highly restricted by the presence of the blood brain barrier (BBB). To address this issue, the use of nanoparticles as drug delivery systems has been broadly investigated, and – among these – polymeric covalently cross-linked nanogels have been considered very promising candidates¹. Nanogels have physico-chemical properties which can be finely tailored by using specific functional monomers and are characterised by high drug uploading capability thanks to the formation of stable colloidal solutions while retaining a high volume-to-surface ratio². Moreover, relatively easy incorporation of fluorescent labels allows their tracking *in vitro* and *in vivo* to ensure that the targeted area is reached.

In this study, neutral and negatively charged nanogels, having N-isopropylacrylamide (NIPAM) as backbone monomer and containing a fluorescent label, were synthesised and investigated. Covalently linked to the polymeric matrix to prevent its leakage, the fluorophore was successfully incorporated as confirmed by studying the nanogels' optical properties. The effects on the nanoparticle size due to the introduction of the fluorescent monomer were evaluated by dynamic light scattering, revealing negligible differences between the fluorescent nanogels and their non-fluorescent counterparts. UV-Vis spectroscopy analysis showed that the thermoresponsive behaviour of these nanogels was instead more affected by the presence of the dye. *In vitro* assessment of the most promising nanogel formulations on a human BBB model revealed that these nanoparticles were biosafe up to 0.1 mg mL⁻¹ and able to permeate the BBB. Besides, both their biocompatibility and their biodistribution were investigated *in vivo*, in zebrafish larvae. Excluded any toxic effects, successful tracking of these fluorescent nanoparticles indicated that these could be used within this animal model and allowed to evaluate different administration routes.

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Redox responsive manganese-based MRI theranostics for cancer therapy

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Abstract

Smart theranostics are dynamic platforms that integrate multiple functions, including at least imaging, therapy and responsiveness, in a single agent.¹ Different smart theranostic systems have been devised in the search for improved diagnostic and therapy efficiency, particularly in oncology, where these agents can respond to changes in the pH, redox environment, or enzymes.^{1,2}

Using facile ultrasonication chemistry,³ we investigated a series of Mn_xO_y -Pt(IV) nanoparticles regarding their performance as redox-responsive MR contrast agents. Relaxometry studies revealed signal enhancements as high as 136-fold for nanoparticles with lower Pt/Mn ratios after treatment with a reducing agent, in agreement with the MRI contrast enhancement observed in phantom images acquired at clinical fields of 3 T (Figure 1B). Cell cytotoxicity of the nanoparticles was assessed in a lung carcinoma (A549) cell line. Results in 2D cultured cells show that the toxicity for the MnO_2 -Pt(IV) nanosystem ($IC_{50} = 100.0 \mu M$) is considerably higher toxicity than that of a Pt(IV) prodrug ($IC_{50} = 420.5 \mu M$). This highlights a dual therapeutic effect where the released Mn(II) species play a role by potentially leading to the activation of ferroptosis in addition to apoptosis (by cisplatin).

These nanosystems are then capable of inducing a T_1 switch as the drug is released in cancer cell lines, making them promising theranostic agents.

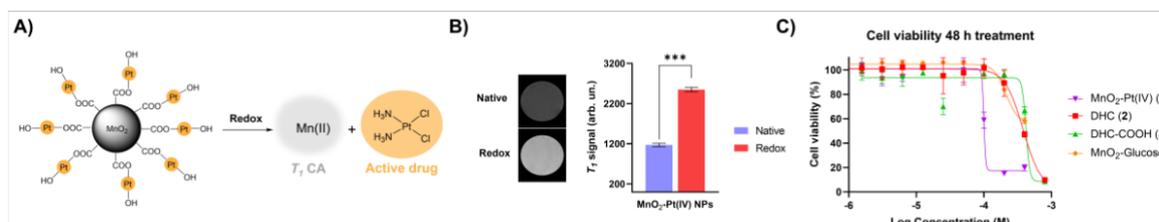


Figure 1 - A) Schematic representation of the reduction MnO_2 nanoparticles. B) T_1 -weighted MRI phantom images for MnO_2 -Pt(IV) nanoparticles and corresponding signal shift with addition of AA (10 mM), $[Mn] = 0.2$ mM, $***p < 0.0001$. C) Cell viability of A549 cells after 48 h of treatments ($n=3$). Concentration refers to Pt concentration for all treatments except for MnO_2 -Glucose, in which the Mn concentration is presented.

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Graphene Nanowalls Grown on Copper Substrates

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Abstract

A graphene nanowall (GNW) can be described as a nanoscaled graphitic sheet that is oriented vertically on a substrate. Existing techniques to grow GNWs are mostly based on plasma-enhanced chemical vapour deposition (PECVD) and the use of different substrate materials (Cu, Ni, C, etc.) shaped as foils or filaments [1].

Here, we report the growth of patterned GNW films, using PECVD and perforated planar substrates. Controlling the pattern of the substrate results in a carbon film replica that contains arrays of customised cavities. Although patterned GNW films have been reported [2], the present process significantly simplifies the production as it does not rely on costly clean room procedures.

In the example we will describe, a cm²-scaled Cu mesh (50 μm thick), containing an array of square-shaped micrometre cavities, was employed (**Figure 1a**). Working with a DC plasma (150 W), a uniform mat of GNWs grew on the top of the Cu threads. As shown in **Figure 1b**, the height of the walls was quite regular and attained 300 nm. To understand the structure and composition of the GNWs, further characterisation included atomic force microscopy, Raman spectroscopy and X-ray photoelectron spectroscopy.

The same process was used in a cm²-scaled Cu foil (50 μm thick). In contrast to the mesh, the GNWs grew mostly at the edges of the metal sheet (also with ca. 300 nm height). Away from the edges, carbon deposition was noticed but this was much less structured and non-uniform.

The different outcome is understood as a consequence of the changes in the plasma environment. In the perforated substrates, there is a higher density of metallic edges which tend to concentrate electric fields. These are known to be instrumental in promoting and directing the growth of the walls.

Thus, perforated metal foil substrates enhance the growth of GNWs in PECVD and offer the possibility of new film morphologies that are less expensive and simpler to fabricate than the current methods based in clean room processes.

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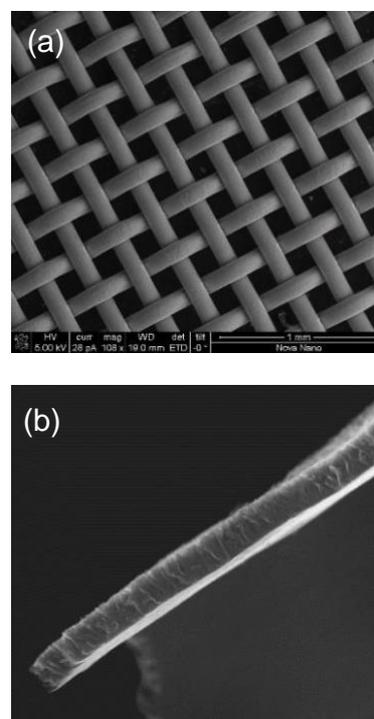


Figure 1. Scanning electron microscopy images showing (a) the morphology of the Cu mesh used and (b) the side-view of a GNWs film.

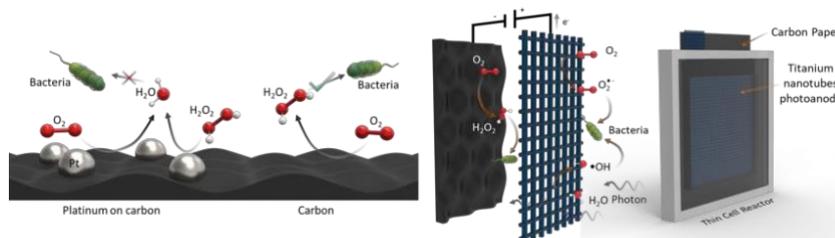
Photoelectrocatalytic Disinfection of Water: Evaluation of photoanodes, cathodes, and radicals produced

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Abstract



For photoelectrocatalytic (PEC) water treatment and disinfection a considerable amount of research has focused on improving the photoanode efficiency; however, the generation of reactive oxygen species (ROS) at the cathode is desirable for disinfection. In this work, a TiO₂ nanotube (TiNT) array was used as the photoanode and different cathode materials were investigated (platinum, carbon felt, carbon paper and carbon paper modified with Pt nanoparticles (PtNP)) based on the onset potential for the oxygen reduction reaction (ORR), current density and peroxide generation. For the PtNP the onset potential for the ORR was shifted more positive than for platinum and higher current density was observed; however, with Pt or PtNP carbon no significant production of H₂O₂ was observed. The non-modified carbon paper had the highest Faradaic efficiency for the generation of H₂O₂ (15.5%). The highest rate of *E. coli* inactivation was achieved with the non-modified carbon electrode (2.51 log reduction) compared to Pt (0.79 log reduction) in a small scale reactor. This demonstrates the importance of cathode material selection to ensure that ROS generation is maximised. The TiNT photoanode was shown to generate hydroxyl radicals and superoxide radical anion by the reduction of O₂ by conduction band electrons. A customised thin cell PEC reactor with a TiNT photoanode and carbon cathode achieved a 5.0 log reduction of *E. coli* in 20 min using real surface water under 45.6 Wm⁻² UV.

Acknowledgements: Department for Economy (DfE) Northern Ireland for funding Stuart McMichael, the Global Challenges Research Fund (GCRF) UK Research and Innovation for funding SAFEWATER (Grant Reference EP/P032427/1) and European Union's Horizon 2020 research and innovation programme under grant agreement No 820718 (PANIWATER)

Gemcitabine-loaded Metal-Organic Frameworks as a treatment for Pancreatic Cancer

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Abstract

Pancreatic cancer (PC) is associated with poor survival rates, with as many deaths as there are cases based on global estimates (GLOBOCAN).¹ Gemcitabine (Gem) is an anticancer drug commonly used in treating patients with pancreatic cancer, however resistance has decreased its use clinically.^{2,3} Metal-organic frameworks (MOFs) are crystalline, porous materials, composed of secondary building units and organic linkers.⁴ The structures of these materials allow, potentially, for drugs to be loaded into their framework or attached via the terminal points on the organic linkers that make up the frameworks. Here, MOFs have been used as a drug delivery system for PC as an attempt to avoid this resistance.

The zirconium MOFs UiO-66 (Universitetet i Oslo) and MOF-808 were loaded with Gem (Gem@MOF) over 24 hours, with the loading determined by HPLC.

Subsequent characterisations were completed post-loading to ensure that the Gem@MOF remained unchanged, where powder X-ray diffraction and scanning electron microscopy showed that the crystallinity and morphology was retained. Further techniques were used to determine whether Gem was successfully loaded, where nuclear magnetic resonance and gas adsorption appear to evidence successful loading either on the surface of the MOF or within the pores. Finally, in vitro testing was completed over 24, 48 and 72 hours in three PC cell lines (BxPC-3, MiaPaCa-2, and PANC-1) using the free drug, MOF, and Gem@MOF to determine whether the Gem@MOF provided a cytotoxic effect and whether this was comparable or superior to that of the free drug.

Acknowledgements (optional): EPSRC

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Cu-doped Mesoporous Silica Nanoparticles as a Platform of Antibacterial Activity

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Abstract

Bacteria may persist in challenging environmental conditions through the establishment of a biofilm.¹ In large-scale water distribution systems, such as those in hospitals, this can be problematic as formation of biofilm has been associated with the spread of disease and poor health outcomes.² In such systems, nanostructured surfaces offer potential as an effective method of preventing biofilm formation through broad spectrum antimicrobial activity, and low toxicity.

At present, effective methods of water disinfection involve chlorination, ozonation, or UV irradiation.² Whilst effective, these methods often require a large amount of energy. Recent advances in metallic nanomaterials, such as those based on copper, have shown significant promise both for their biocidal activity and as a relatively energy efficient mode of disinfection or control. Integrating Cu into a nanocomposite structure may mitigate associated problems with metallic nanoparticle aggregation, and increase longevity of ion release.³ The aim of this research project is the incorporation of Cu into mesoporous silica nanoparticles (MSNs) in a facile, one-pot synthesis.

Cu-doped MSNs were prepared in a one-step synthetic method using a modified-Stöber protocol.⁴ MSNs were characterised by FTIR, DLS, UV-vis, SEM, SEM-EDX, TEM, and BET analysis. Several synthetic parameters were systemically varied to investigate the effect on nanoparticle characteristics, such as morphology, particle size, and porosity. MSNs doped with 5 to 20 mol% of Cu were analysed for their antimicrobial efficacy against gram positive (*Enterococcus faecalis*) and gram negative (*Pseudomonas aeruginosa*) bacteria at 4- and 24-hour time points in copiotrophic and oligotrophic media. Increasing concentrations of doped Cu demonstrate an increasing antimicrobial effect up to 10 mol%.

In conclusion, we have developed and optimised Cu-doped MSNs which have shown broad spectrum activity against gram positive and gram negative bacteria. Produced materials show promise for future biofilm remediation in water distribution systems.

Acknowledgements: This work was financially supported by the Low Carbon Eco-Innovatory and Feedwater Ltd.

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pH-responsive Vesicles: A *De Novo* Nano System for Sustained and Targeted Delivery of Hydrophobic Drug

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Abstract

Self-assembling of the new age surfactants, ionic liquid based surfactants (ILBSs) leads to diverse morphological structures including worm-like micelles, vesicles and molecular gels to name a few. Among these, vesicles because of their high surface-to-volume ratio hold advantage over others and found applications in variety of fields, such as drug delivery, the food industry, and cosmetic formulations. In the present work, we report a study on the self-assembling of a new type of ILBS, Choline Oleate ([Cho][OI]) in dilute aqueous solutions with and without addition of Glutamic acid (GA). [Cho][OI] was studied for its biocompatibility and biodegradability as well as surface behaviour. GA induced morphological transition from spherical micelles to unilamellar vesicles was confirmed through various state of the art analytical techniques including small angle neutron scattering and fluorescence resonance energy transfer (FRET). The formation and size of the unilamellar vesicles depends directly on the pH of the solution. The designed vesicles were then explored for sustained and targeted release of model fat soluble hydrophobic drug, Sudan-III. The proposed study would pave the way for the preparation of biocompatible and stimuli responsive vesicles as drug carrier for targeted drug delivery of highly hydrophobic drugs.

Acknowledgements: NM acknowledges the financial assistance of UGC-DAE for the Collaborative Research Scheme (UDCSR/MUM/AO/CRS-M-276/2017).

Solution-based synthesis of Barium Titanate-Hematite Nanocomposite Thin Films for Enhanced Photocatalytic Activity

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Novel photo-electrocatalysts (PEC), such as Fe₂O₃, BiVO₄, CuWO₄, have recently gained great attention aiming to achieve unassisted water splitting to produce solar fuels. Even if they possess narrow bandgaps in the range of 2-2.5 eV, they suffer from high level of surface recombination and low carrier mobility¹. Ferroelectric polarization has emerged as new strategy in photocatalysis to induce opposite band bending at material surfaces facilitating charge migration towards different sites and promoting selective redox reactions².

Herein, we combine ferroelectric BaTiO₃ with the photocatalyst Fe₂O₃ in parallel at the nanoscale to improve the photocatalytic performance (Figure 1).

Porous BaTiO₃ (pBTO) thin films are synthesized by soft template-assisted sol-gel method. Using different concentrations of organic template, the porosity of pBTO is controlled to obtain suitable thin films for photocatalyst integration. The overall porosity and surface area of the pBTO thin films is determined by SEM analysis and ellipsometry.

The ferroelectric phase of pBTO is confirmed by XRD analysis and Raman spectroscopy. The switching of spontaneous polarization of pBTO by an electric field is verified by Piezoresponse Force Microscopy (PFM). The alignment of polar dipoles to the ferroelectric surface (P_{up} or P_{down}) is evaluated by testing the PEC performance of pBTO after electrochemical (EC) poling at ±8V, which show that the photoanode performance is improved for P_{down}.

Lastly, the pBTO/Fe₂O₃ thin film shows an enhancement of the photocurrent density compared to either the bare Fe₂O₃ (by ~2 times) and pBTO thin films (by ~20 times), which could be correlated to the upward band bending induced by the ferroelectric polarization of pBTO. The PEC response in pBTO/Fe₂O₃ is accordingly regulated by EC poling without significantly affecting the Fe₂O₃ layer (as confirmed by XPS). This research work shows a facile and low-cost approach for the development of novel ferroelectric/photocatalyst photoanodes with switchable control of their PEC performance, which possess a great potential for photoelectrochemical applications.

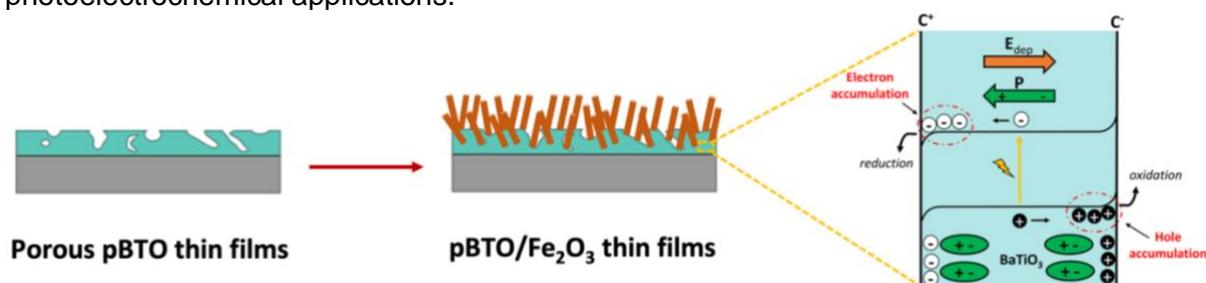


Figure 1 Schematic on the combination of pBTO thin film with the Fe₂O₃ photocatalyst, where the ferroelectric polarization of pBTO promotes the improvement of the photoanode PEC performance.

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Poster Presentations

List of Poster Presentations

Poster Number	Title and Presenting Author
P1	Safety optimisation of a hybrid nanoparticle based on thermo-responsive delivery system for pancreatic cancer treatment Rachel Onchuru
P2	Mechanochemically Synthesized CsPbBr ₃ Perovskite Nanocrystals Ankit Goyal
P3	Preparation of Novel Magnetofluids Wangchao Yuan
P4	Engineering upconversion nanoparticles for non-invasive trans-tissue measurement of blood oxygen <i>in vivo</i> Lewis E. MacKenzie
P5	Highly emissive lanthanide-doped gadolinium oxysulfide nanocrystals Ian P. Machado
P6	Hydrophilic C flakes as electrode materials for aqueous Al batteries Pedro M. F. J. Costa
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P8	"Inverse vulcanisation" sulphur polymers and titanosilicate photocatalysts for water purification Joseph C. Bear
P9	Novel Lipid Based Nanoparticles for the Stimulation of Plant-Fungal Mycorrhizal Symbioses. Iain Lawson
P10	Silver nanoparticle-polypyrrole nanocomposite treated linen textiles for personal thermal management Ashleigh Naysmith
P11	Effect of BaTiO ₃ polarisation on photocurrent generation and charge carrier dynamics in ferroelectric photoanodes for photoelectrochemical water splitting Chloe Forrester
P12	Peptoid Nanosheets targeting Breast Cancer Asma Mukhtar
P13	Creating High-Capacity Anode Materials from Barley Husks for Energy Storage Chenghao Yue
P14	Developing and Understanding Nanoscale Design Features in Nanostructured MRI Contrast Agents Connor J. R. Wells

- P15 Graphene flowers Grown on Carbon Nanowalls Deposited on Ni/Cu Alloys
Mohammed Bahabri
- P16 Amorphous nanoparticles for the electrocatalytic reduction of CO₂ into added-value chemicals
Nivetha Jeyachadran
- P17 Concentration-dependent optical properties of Indium Phosphide Quantum Dots
Hélio M. Gil
- P18 Guest Mediated prevention of Quantum Dot Aggregation by Surface Bound Cucurbit[7]uril
Katie McGuire
- P19 Development and Optimization of Dual Drug loaded Nanolipidic Carriers for Effective Management of Diabetic Foot Ulcer using Box-Behnken Design
Parina Kumari
- P20 Development of multifunctional mesoporous silica nanoparticles for treatment and diagnosis of hepatocellular carcinoma
Marwa M. I. Rizk
- P21 Amphiphilic Self Assembly of Fatty-Alcohol in Silica-Salt Hydrogels. Implications for Abiogenesis
Seham Alanazi
- P22 Synthesis of magnetic biochar composites for enhanced soil toxic metal pollution adsorption
Mahsa Sanaei
- P23 Development of highly fluorescent Carbon Dots from abundant non-commercial weeds for environmental remediation
Pooja Chauhan
- P24 Photocatalytic decolourization of a new water-insoluble organic dye based on phenothiazine by ZnO and TiO₂ nanoparticles
Fatimah A. M. Al-Zahrani
- P25 Morphology control of silk fibroin nanoprecipitation under bulk and microfluidic mixing regimes
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- P26 Templated Growth of Nanoparticles to Indicate the Reductive Potential of Whisky
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- P27 Protocol for the Rapid Detection of Salmonella by using Antibody Functionalized Immuno-magnetic Iron Oxide Nanoparticles
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- P28 Investigation into the use of microfluidics in the manufacture of metallic gold coated iron oxide hybrid nanoparticles
Adeolu Oluwasanmi

- P29 Spherical polymer nanoparticles and nanocomposites, their biofunctionalization and proposed applications
Narmin Suvarli
- P30 Organogels as versatile biomaterials for skin-delivery
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- P31 Green synthesis, textural and magnetic properties of water dispersible gold coated superparamagnetic iron oxide nanoparticles
Bamidele M. Amos-Tautua
- P32 Fabrication of nanosilver imbued polymer wafers
Ernest Man
- P33 Metallic Ceramics: the New Generation of (Elettro-)Catalysts for Sustainable Energy Production
Jing Ming

Safety optimisation of a hybrid nanoparticle based on thermo-responsive delivery system for pancreatic cancer treatment

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Abstract

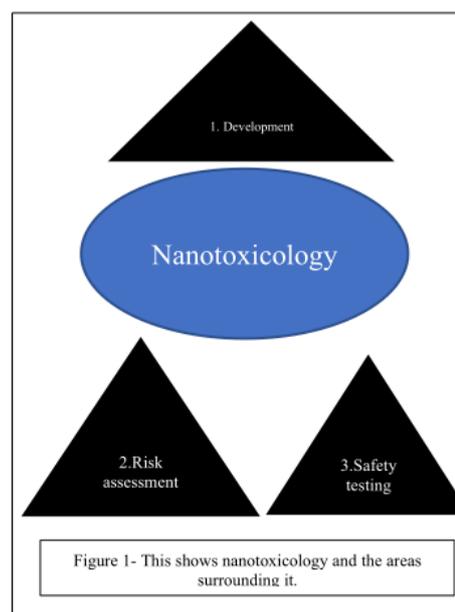
Pancreatic cancer is the 4th most aggressive cancer in the western world. In the United States, it is the third leading cause of cancer-related deaths. The overall 5-year rate of survival for this type of cancer is 9%; very low in comparison to other cancers¹. The lack of symptoms results in a delayed diagnosis and therefore, a delay in treatment of the cancer. Current therapies for pancreatic cancer include fluorouracil, gemcitabine and nab-paclitaxel. Nanotechnology offers the benefit of enhancing drug delivery to the targeted tissue because of increased drug permeability. This also reduces side effects and sustains drug release over a long period of time².

Despite all the positive impact that comes along with nanotechnology, there are some risks associated with it. As with most technological revolutions, there are hardly never issues and side effects. Infact, materials behave differently in the nanoscale than they do in the macroscopic world. Among the concerns there are with nanoparticles include toxicity, selectivity, permeability of cell membranes and penetration of the brain via the nose and olfactory nerve³.

The aim of this project is to synthesize a gold-iron oxide hybrid nanoparticle, loaded onto a drug and safely optimize it by running toxicology testing for the use in pancreatic cancer treatment and possibly diagnosis of the same as well. This will have a positive impact on the prognosis of the disease and will enable cure for the cancer patients. Currently, the hybrid nanoparticles (50-100nm) have been synthesized and characterization analysis performed using TEM, Zeta potential, UV-Vis spectroscopy and SQUID analysis. Zeta potential charge, for example, gives an insight into the interactions with the cell wall in the body and can aid in determining probable toxicity of the nanoparticles. Further work is ongoing to determine the *in vitro* and *in vivo* acceptability of the particles.

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Quantum Confinement Triggered Blue-Green Emission from Mechanochemically Synthesized CsPbBr₃ Perovskite Nanocrystals

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Abstract

Cesium lead halide perovskites are family of bright, visible light emitting materials with near unity photoluminescence quantum yield (PLQY) in nanocrystals (NCs). This family of light emitters offers spectral tuneability in the entire visible range. Reports on strong quantum confinement in these materials are scarce and should show size-dependent PL tuneability. Often, visible light emission tuneability is achieved by mixing different halides, which leads to phase separation and to instability. Herein, we report alternative facile, green, and scalable high energy mechanochemical synthesis of size-tuneable, quantum confined cesium lead bromide (CsPbBr₃) NCs. Scanning electron microscopy and atomic force microscopy (AFM) confirms the presence of NCs of sizes ~3-7 nm. We performed micro-PL spectroscopy correlated with AFM to see size-tuneability of the PL spectra. The PL QY of ~85 % even after 100 days of synthesis confirms stability of the NCs. The tuneability of PL between 460 nm-520 nm using only CsPbBr₃ NCs is realized in this work, without necessity to mix in different halides. Our work shows potential of scalable mechanochemical synthesis to achieve spectral tuneability in bright luminescent mono-halide perovskite NCs through quantum confinement

Preparation of Novel Magnetofluids

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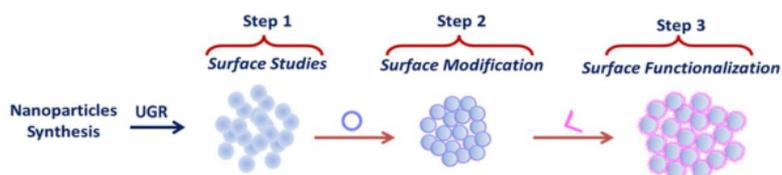
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Abstract

Magnetic particles are largely used for many different applications, including the preparation of magnetic fluids. Iron carbide (Fe_3C) is a largely unexplored magnetic material, despite being considered a valid alternative to currently used magnetic particles (mainly based on iron and iron oxide), thanks to its higher saturation magnetization and expected low toxicity. The main problems lie in the difficulties related to its preparation, especially as nanoparticles, and challenges in dispersing them, stably, in any liquid media.

The present project focuses on designing strategies for the surface modification of Fe_3C and metallic ceramic nanoparticles, in general, to

introduce selected functional groups finalized in the preparation of colloidal dispersions and magneto fluids. The modification is made in 3 steps, reported in the scheme.



Nanoparticles were synthesized¹ characterized by different techniques. Fe_3C nanoparticles showed a spherical shape with an average size of 40 nm in diameter. Different surface modification methods were tested. While neither thermal treatments nor chemical treatments gave the wished product, the addition of silica to the preformed nanoparticles was effective. The introduction of silica does not affect the magnetic properties of the nanoparticles but ease the functionalization step via the silica moieties. IR studies and EDS mapping showed that the silica is incorporated into the Fe_3C nanoparticles. Fig. 1 shows the difference of stability in ethanol between Fe_3C with and without silica.

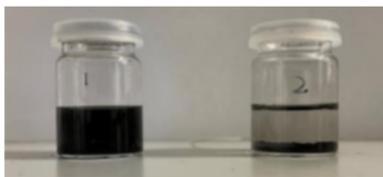


Fig. 1 Dispersion of $\text{Fe}_3\text{C-SiO}_2$ (left) and Fe_3C (right) in ethanol (stand still for 10 days)

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Engineering upconversion nanoparticles for non-invasive trans-tissue measurement of blood oxygen *in vivo*

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Abstract

Localised measurement of blood oxygen within biological tissues is essential for our understanding of how diseases such as cancer, diabetes, stroke, heart disease, and multiple sclerosis develop and progress. However, current technological limitations demand that biomedical researchers often turn to lethally invasive means (e.g., tissue staining/sectioning) to measure oxygen deficiency (hypoxia) in animal models. This is expensive, inefficient, and introduces large uncertainties into measurements due to inter-subject variability.

Can nanotechnology help biomedical researchers measure localised blood oxygen in a manner which is more efficient, more sustainable, and cheaper, whilst also reducing the ethical burden of biomedical research?

Upconversion nanoparticles (UCNPs) are unique in that they emit at visible wavebands but are excited by diffuse near-infrared (NIR) wavebands which can traverse several centimetres of tissue. This enables UCNPs to bypass the problems faced by conventional phosphorescent/fluorescent probes: i.e., UCNPs do not photo-bleach and do not induce autofluorescence from biological tissues. Further, UCNPs photonic and paramagnetic properties can be tuned by varying by dopant ions within the host crystalline lattice. UCNPs can be incorporated into functional nanoconstructs for drug/sensor loading and targeted cellular uptake. Red emitting UCNPs – typically constituting a cubic-phase NaYF₄:Yb,Er crystal lattice - can be excited and detected through more than 1 cm of tissue. These properties make UCNP constructs highly attractive for *in vivo* optical biosensing.

This talk will outline progress to producing UCNP constructs suitable for use as blood oxygen biosensors. Including a new method for producing strongly red emitting UCNPs with simple standard hotplate and beaker equipment instead of the more demanding and scale limiting UCNP synthesis methods currently relied upon. Future prospects and directions will be discussed.

Highly emissive lanthanide-doped gadolinium oxysulfide nanocrystals

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Abstract

Photonic materials based on rare earth oxysulfides ($\text{RE}_2\text{O}_2\text{S}$, where RE^{3+} : Sc, Y, La–Lu) are incredibly efficient and versatile, being applied in cathode ray screens and scintillator panels for X-ray tomography. Synthesizing $\text{RE}_2\text{O}_2\text{S}$ materials, however, can be a challenging task at bulk and nanoscales due to the chemical incompatibility of hard-acid RE^{3+} and soft-base S^{2-} ions. Numerous attempts were made to circumvent this issue and obtain monodisperse $\text{Ln}_2\text{O}_2\text{S}$ nanocrystals (NCs), e.g., using single-source precursors or employing large S/Ln molar ratios^{1,2}. Nevertheless, those strategies significantly increase the difficulty of the synthesis procedure, leading to several steps of precursor preparation, or even explosions during the reaction course.

To overcome such problems, this work reports a single-step preparation of highly luminescent Ln^{3+} -doped $\text{Gd}_2\text{O}_2\text{S}$ NCs. The synthesis procedure is based on Larquet *et al.*, which describes an efficient sodium-mediated template formation of $\text{Ln}_2\text{O}_2\text{S}$ NCs³. TEM image of $\text{Gd}_2\text{O}_2\text{S}:\text{Eu}^{3+}$ (4%) reveal monodisperse particles of 15–20 nm, which tends to self-assemble by the particles' edges (Fig. 1a). Under UV excitation (365 nm) the $\text{Gd}_2\text{O}_2\text{S}:\text{Eu}^{3+}$ NCs show bright red emission in colloidal suspension (Fig. 1b). Such red luminescence was assigned to the $^5\text{D}_0 \rightarrow ^7\text{F}_{0-4}$ electronic transitions of the Eu^{3+} ion.

The addition of oleic acid (OA) was demonstrated to influence the NCs formation, *i.e.*, a delayed OA addition to the synthesis caused the size of $\text{Gd}_2\text{O}_2\text{S}:\text{Eu}^{3+}$ NCs to decrease to <10 nm without losing monodispersity nor affecting the overall emission intensity. Furthermore, it is worth noting that these NCs were washed 3x simply with ethanol, *i.e.*, no post-synthesis treatment was employed. Finally, this work aims at growing an inert shell to reduce non-radiative losses at the NC surface, seeking highly efficient upconversion ($\text{Gd}_2\text{O}_2\text{S}:\text{Er}^{3+}, \text{Yb}^{3+}$) and scintillator ($\text{Gd}_2\text{O}_2\text{S}:\text{Pr}^{3+}/\text{Tb}^{3+}$) NCs.

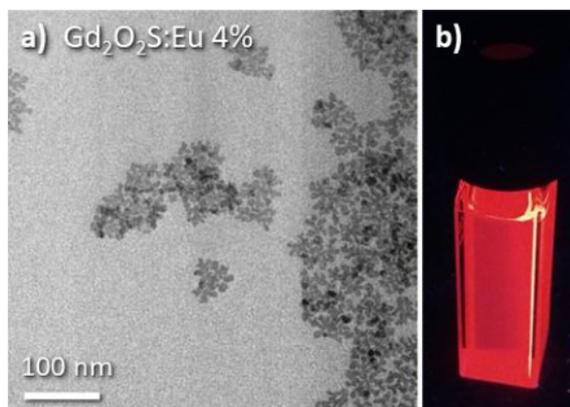


Fig. 1 (a) TEM image of $\text{Gd}_2\text{O}_2\text{S}:\text{Eu}^{3+}$ nanocrystals (NCs) synthesized by a single-step wet chemical route; (b) Intense red emission of a suspension of $\text{Gd}_2\text{O}_2\text{S}:\text{Eu}^{3+}$ NCs in cyclohexane under UV light (365 nm).

Acknowledgements: Ian P. Machado thanks the Brazilian Funding Research Agency – CNPq projects #141446/2016-1 and #204825/2018-0, for partially funding the research at IQ-USP – Brazil and UU – The Netherlands, respectively.

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Hydrophilic C flakes as electrode materials for aqueous Al batteries

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Abstract

Lithium-ion batteries are the dominant energy storage technology in the electric vehicles and portable electronics consumer markets. There is, however, much interest in developing alternative batteries due to the scarcity of Li and concerns about the safety of its systems. With respect to this, a more sustainable and (potentially) less expensive option would be the use of aluminium ions as the active species in rechargeable batteries.

Dating back to the 19th century, Al-based energy storage systems have come a long way. Still, the deployment of this technology continues to elude us. One major obstacle has been the lack of appropriate electrolytes. With Al plates acting as anodes, the need to counteract the passivating oxide layer that forms on their surface prevents the use of most liquids. In recent years, mixing AlCl₃ with ionic liquids (IL) has emerged as a preferred electrolyte, yielding promising performances when combined with carbon-based cathodes [1]. Whilst notable, this arrangement is hardly scalable due to the price, corrosiveness and moisture sensitivity of the IL. In these circumstances, reports of salt-water electrolytes employed alongside Al foils coated with a thin IL layer, brought much excitement to the field [2].

We present an Al-C battery that operates with an aqueous electrolyte and provides remarkable stability and capacity. In contrast to the graphite flakes that are commonly used as electrode materials, we employed a freeze-dried powder of reduced graphene oxide (rGO, **Fig. 1a**). Besides its hydrophilicity (when compared to graphite), the rGO contained bound-water and grafted organic moieties (**Fig. 1b**). These are all characteristics that contributed to the rGO cathode's compatibility with the 2M Al(OTF)₃ electrolyte (where OTF stands for trifluoromethane-sulfonate) and the unique charge storage mechanism proposed [3].

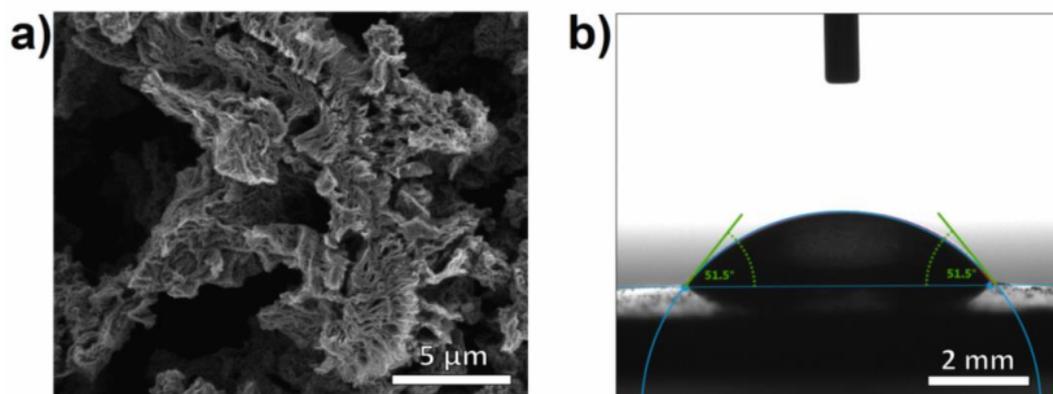


Figure 1. a) Scanning electron microscopy image of some freeze-dried rGO flakes. b) Contact angle of a water droplet with the rGO surface; generally, for graphite, the angle is >90° (hydrophobic).

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Magnetic quitine-based nanocomposite hydrogels

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Abstract

Structures and behaviours found in nature serve as an inspiration to engineering smart stimuli-responsive nanocomposite sustainable materials. Some of these structures are based in materials that self-assembly into liquid crystalline (LC) phase as DNA, chromosomes, collagen, chitin, cellulose (all originating cholesteric phases), proteins and lipids (in the membrane of living cells) just to state a few. The LC phase plays crucial role and impart essential functions in these natural systems, since it combines order and mobility required for self-organization and structure. LC phase confers, for instance, the necessary mechanical stability, optical communication, crypsis and aposematism [1-5].

In this work the combination of natural-based occurring products as nanochitin (NQ), alginate and iron nanoparticles (SPIONS) allows the production of magnetic hydrogels. The hybrid systems, prepared with different content of SPIONS, showed after freeze-drying a porous structure with nanoparticles homogeneously distributed within its assembly. Further microscopic analysis shows hierarchical organization that resembles the one derived from NQ LC aqueous suspension. Application of an external alternated magnetic field lead to an increase in the temperature of the hydrogel, paving the way to applications such as in cancer treatment and covert security features.

Acknowledgements (optional): This work is co-financed by FEDER, European funds, through the COMPETE 2020 POCI and PORL, National Funds through FCT—Portuguese Foundation for Science and Technology and POR Lisboa2020, under the projects PIDDAC (POCI-01-0145-FEDER- 007688, reference UIDB/50025/2020-2023), PTDC/CTM-REF/30529/2017 (Nano- Cell2SEC), PTDC/CTM-CTM/30623/2017 and Action European Topology Interdisciplinary Action (EUTOPIA CA17139).

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"Inverse vulcanisation" sulphur polymers and titanasilicate photocatalysts for water purification

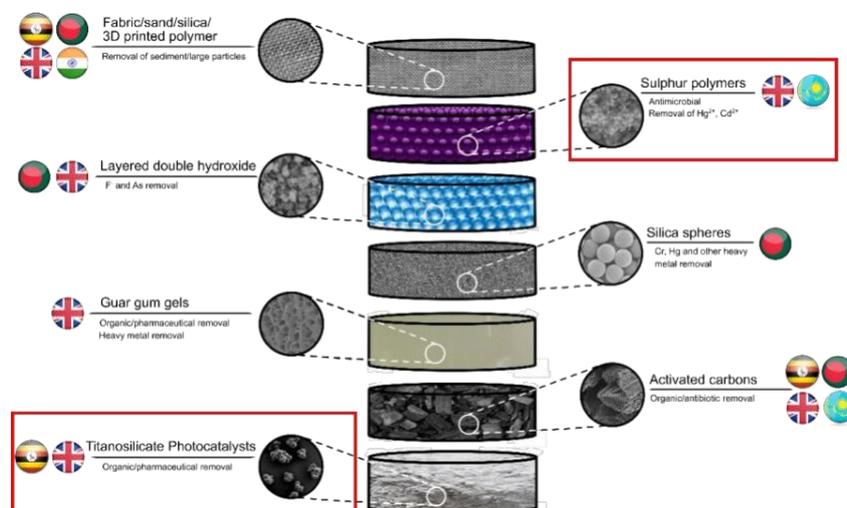
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Improving access to drinking water is Number #6 on the United Nation's list of Sustainable Development Goals. In order to address this in selected Development Assistance Countries (DAC), a consortium was formed at Kingston University (KU) in 2018 with the goal of producing a water filter with interchangeable layers that will be accessible and easily usable by local communities, and the poorest within them.

We have been working with several partner countries on this- thus far we have successfully gained collaborators in Kazakhstan at Al-Farabi (Almaty) and Nazarbayev Universities (Nur-Sultan), resulting in a burgeoning partnership with a spin-out company based at the Institute of Combustion Problems at Al-Farabi University who will be looking to manufacture the filter once the design is completed. Established collaborations with India and Bangladesh have resulted in various carbonaceous and silica-based materials and processes for the removal of heavy metal ions (arsenic, mercury chromium, cadmium, lead, fluoride) which are intractable problems in in Bangladesh and India (proof of concept completed). Further work with Uganda has allowed us to tailor materials for specific problems faced there, such as organic and bacterial contamination of water.

Our two newest filter materials, namely "inverse vulcanisation" **sulphur polymers** and a **titanasilicate photocatalysts** are the focus of the poster. Sulphur polymers have been shown to be able to remove heavy metal ions including Cd and Hg. They are synthesised by combining heated elemental sulphur (an abundant waste material from petroleum refining) with vinylic species (such as diisopropenylbenzene) to create a polymeric material. By changing the cross-linker, the properties of the resultant polymer can be tuned. [1] Proof of concept for the synthesis of new titanasilicate photocatalysts has been achieved and shown to be able to degrade model organic with visible light irradiation; [2] a key advantage in water filtration in areas with solar irradiation above AM1.5.



Scheme: A schematic of our water filter design showing contributions from our partner countries and joint research projects.

Acknowledgements: Global Challenges Research Fund (GCRF). **References** 1. "Nanoparticle-sulphur "inverse vulcanisation" polymer composites" - J. C. Bear, W. J. Peveler, P. D. McNaughton, I. P. Parkin, P. O'Brien, C. W. Dunn *Chem. Commun.* **2015**, 51, 10467–10470.; 2. "Optimization of mesoporous titanasilicate catalysts for cyclohexane epoxidation via statistically guided synthesis" – A.S. Perera, P. Trogadas, M.M. Nigra, H. Yu, M-O Coppens, **2018**, *Mater. Sci.*, 53, 10, 7279-7293.

Title: Novel Lipid Based Nanoparticles for the Stimulation of Plant-Fungal Mycorrhizal Symbioses.

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Abstract

The global population, under the cloud of a worsening climate, is expected to rise 11.2 billion by the end of the century. The twin pressures of a growing population and an environment less amenable to prodigious growth of crops challenges humanity's ability to meet the calorific needs of our contemporary, and near future, societies. The critical nature of this challenge compels us to develop more efficient, sustainable and effective agricultural praxis. Lipid nanoparticles (LNP) are a class of nanoparticles that hold promise for use in agriculture¹. These LNPs have certain advantages over typical liposomes such as a higher surface area and mechanical toughness for the delivery of bio-stimulatory active ingredients (AI). One process which may benefit from the delivery of vivifying AIs, is the promotion of the symbiotic relationship between plants and mycorrhizal fungi². Mycorrhizas are a symbiotic relationship between a fungus and a plant within the rhizosphere. Mycorrhizal symbioses can have both non-nutritional but primarily nutritional effects upon a plant that enhances plant survival and fitness. In exchange for the products of photosynthesis fungi, particularly, arbuscular mycorrhizal fungi spread throughout the wider terrestrial department to provide plants with mineral nutrients, water and an improved soil structure. This is particularly important for non-mobile nutrients such as phosphorus.

The aim of this project is to elucidate the effects of LNP application on plant health and mycorrhizal symbioses and further to deduce whether the use of LNPs and an appropriate AI can efficiently stimulate this all important symbioses.

Acknowledgements (optional): This project is being funded by Engineering and Physical Sciences Research Council (EPSRC).

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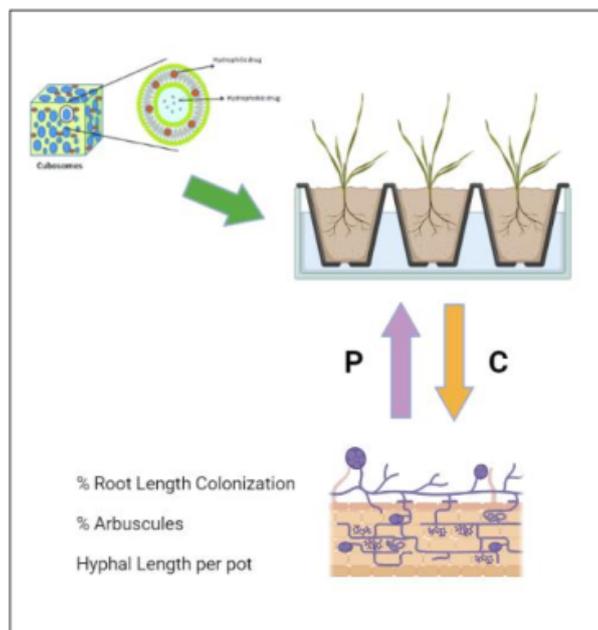


Figure 1: Deducing the impact of LNP application on mycorrhizal symbioses via qualitative measurements of percentage root colonization and quantitative measurements of carbon and phosphorus exchange via isotopic tracing.

Silver nanoparticle-polypyrrole nanocomposite treated linen textiles for personal thermal management

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^BDepartment of Engineering and Technology, University of Huddersfield, Huddersfield, United Kingdom

Abstract

Textile-based personal thermal management (PTM) devices provide a behaviourally aligned route to addressing societies' dependence on energy intensive heating and cooling systems. Most thermoregulating textile technologies currently available, such as phase change materials¹ provide enhanced thermal comfort but they suffer from limitations in their performance range and lack of wearer-control. Electronic textile (e-textile) strategies aim to overcome these limitations by electrically enhancing the properties of the textiles to deliver heating, cooling and / or sensing functionality that can be fully monitored and controlled by the user. Nanofunctionalised e-textiles facilitate exceptional electrical performance, with minimal impact on the comfort and wearability of the garment. Despite the rapid increase in PTM research to date, to the best of the author's knowledge, there is no published research demonstrating multifunctional PTM e-textiles based on nanofunctionalised linen using green synthesised silver nanoparticle-polypyrrole composite. Herein, a multifunctional silver nanoparticle-polypyrrole (AgNP-Ppy) treated textile has been developed demonstrating Joule heating (Figure 1), and motion, pressure and temperature sensing. Lime peel extract was used to synthesise AgNPs, and the synthesis process was optimized using a Plackett-Burman experimental design. The conjugated polymer, Ppy, was selected to enhance the adhesion of AgNPs to the linen textile through hydrogen bonding² and increase the conductivity. An in-situ polymerization process was used to polymerise the pyrrole on to the linen fabric and a Taguchi experimental design was used to optimize the polypyrrole@AgNP-linen production process. Characterisation and electrothermal analyses were carried out to confirm the successful synthesis of silver nanoparticles, electrical resistance, Joule heating and sensing capabilities. Further work is underway to fully characterise the electrothermal, mechanical and handle properties of developed PTM textiles.

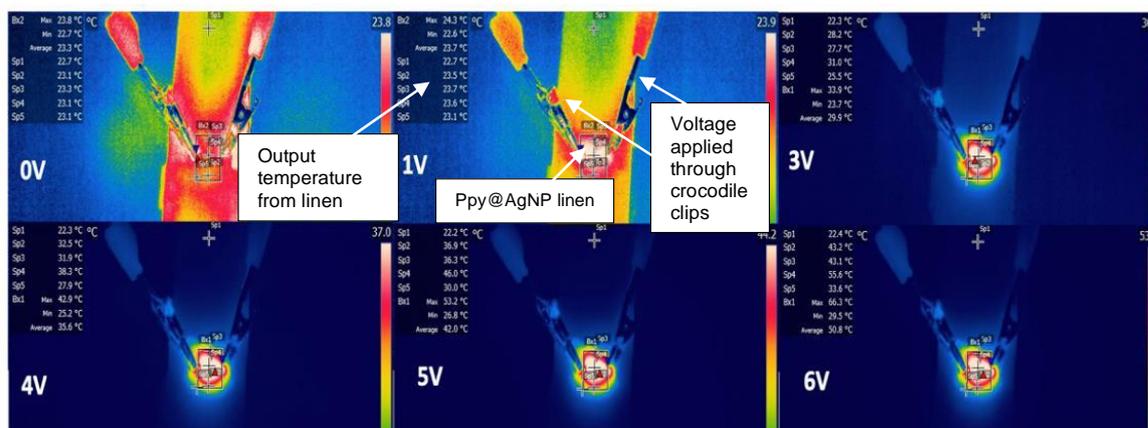


Figure 1 – Joule heating behaviour of silver nanoparticle-polypyrrole treated linen fabric (Captured through Thermal Imaging).

Acknowledgements: This research was funded by the UK Engineering and Physical Sciences Research Council (EPSRC) grant EP/T51813X/1 for the University of Huddersfield Doctoral Training Programme.

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Effect of BaTiO₃ polarisation on photocurrent generation and charge carrier dynamics in ferroelectric photoanodes for photoelectrochemical water splitting

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Solar-driven photoelectrochemical water splitting can provide a sustainable source of hydrogen as a clean and renewable form of energy. Semiconductors employed in water-splitting photoanodes can have large rates of recombination which ultimately reduces the amount of oxygen evolved and limits the solar-to-hydrogen conversion efficiency. Ferroelectric materials possess a permanent internal electric field which has been shown to increase the lifetime of charge carriers by an order of magnitude and has the potential to reduce recombination in ferroelectric semiconductors¹.

Here, BaTiO₃ is studied as a wide-bandgap ferroelectric semiconductor and the effect of enhancing the ferroelectric properties by a method of poling is explored. The impact of the ferroelectric field on photocurrent generation and charge carrier dynamics is examined using steady state and transient spectroscopic techniques.

Comparing as-grown films with little ferroelectric alignment to poled films, an increase of photocurrent from 30 to 145 μAcm^{-2} at 1.23 V vs RHE and an increase in IPCE from 3.5 to 34% at excitation wavelengths (325 nm) was observed after poling. Heating above the Curie temperature for BaTiO₃ to remove the polarisation was also shown to decrease the photocurrent in a reversible process. Transient absorption spectroscopy measurements demonstrate that the lifetime of probed electrons increases from $t_{50\%}$ from 0.1 ms to 4 ms after poling. Simultaneous transient photocurrent measurements show a corresponding increase in charge density extracted from 0.2 to 2 μCcm^{-2} , showing a link between electrons living longer and less recombination and more charge extraction. A model is suggested to explain how the orientation of ferroelectric dipoles and subsequent internal screening can influence surface band bending in a direction which favours the extraction of holes from the photoanode to the electrolyte. This study highlights the benefits of using ferroelectric fields to reduce recombination in photoanodes.

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Peptoid Nanosheets targeting Breast Cancer

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Breast cancer is the leading cause of cancer related deaths in women worldwide. In Pakistan, it kills nearly 40,000 women every year. Improvements in the diagnosis of breast cancer could be helpful in decreasing the mortality frequency. Nanotechnology deals with the matter at nanoscale ranging between 1-100nm¹. Applications of nanomaterials include ability to transport therapeutic or diagnostic materials in the body so that maximum molecular interaction and detection can take place in an efficient manner. We intend to extend the application of self-assembled "peptoid" nanosheets, which are like small pieces of cell membrane². Our Intended approach is multiplexed targeting which includes assembling sheets with coupling groups, then couple via bioorthogonal chemistry by utilizing different multiplexing methods E.g. alkyne-azide, oxime, thiol-ene, thiol-maleimide³. These nanosheets then could be selectively bind to certain receptors on the cancer cells that can be identified through spectroscopic techniques. In future, the nanosheets can also sequester cancer drugs for therapy.

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Creating High-Capacity Anode Materials from Barley Husks for Energy Storage

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Abstract

Because the demand of lithium-ion batteries (LIBs) is highly increasing, the development of high energy density electrode materials is being intensively studied ¹. The high theoretical capacity and low electrode potential of silicon makes it a promising alternative anode material to graphite that is being currently used. It has been widely reported that silicon has an exceptionally high specific capacity of 4200 mAh/g, especially when compared to the currently used graphite anode capacity of 372 mAh/g. However, stable cycling can be challenging due to poor electrical conductivity, sluggish electrochemical kinetics, and large volume change during lithiation/delithiation ^{2,3}. Mesoporous silicon structures can overcome these limitations and provide stable, high energy dense anodes for LIBs. However, the conventional production of these structures through electrochemical etching of single crystal silicon wafers is expensive and slow. Due to the high cost of pure silicon, SiO_x comes into consideration with a remarkable specific capacity of 1965 mAh/g ^{2,3}. Silicon is the second richest element after oxygen on the earth ⁴. All plants and animals may be impacted by this element. Silica is found in barley husk (BHs) which is the waste after the barley is processed. In this project, porous silicon anode material was synthesized from barley husk. BHs have a rich content of amorphous nanostructured SiO_x (14wt%) which is coated by organic carbon component. Moreover, BHs are readily available, cheap, and sustainable ⁴. The following picture shows how the active material was obtained through a low-cost procedure:

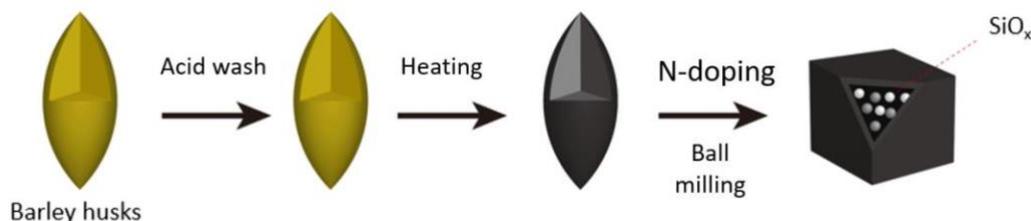


Figure 1. The procedure taken place to obtain porous silicon from barley husks

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Developing and Understanding Nanoscale Design Features in Nanostructured MRI Contrast Agents

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Abstract

Magnetic resonance imaging (MRI) is a crucial medical imaging technique that is useful in non-invasive diagnostics due to its well established spatially resolved images. To aid this diagnostic tool further, contrast agents have been designed to improve the quality of the images, with nanostructured MRI contrast agents showing exceptional promise in image enhancement at extremely low doses. Relaxivity is the term used to assess the effectiveness of an MRI contrast agent on signal enhancement. Taking advantage of their generally high surface areas, nanostructured contrast agents often host large numbers of paramagnetic centres thereby increasing sensitivity through increased local concentration. There is also increased evidence that nanoscale design features, such as pore size and surface chemistry can influence water mobility and hence affect the ultimate capability of these nanostructures as MRI contrast agents.^{1,2} Importantly, their bulky size improves relaxivity by contributing to increased rotational correlation time, resulting in longer T_1 relaxation times.³ However, the understanding of the structure-property relationship of the behaviour of nanostructured contrast agents is still relatively poor and therefore a more thorough investigation is required in order to improve their potency.

Surface modifications can impact water diffusion, and as such, the objective of our work is to explore how such modifications could influence the relaxation of Gd^{3+} -chelate loaded mesoporous silica nanoparticles (MSNs). We seek to gain a better grasp of how a gadolinium complex interacts with neighbouring functional groups, to understand water accessibility and ultimately to improve relaxivity. Taking this concept a step further, switchable contrast agents, which exploit water gating to internalised Gd^{3+} -chelates using bulky 'stopper' materials based on azobenzene photochemistry, have also been developed. Irradiation allows the capping and de-capping of pores with β -cyclodextrin *via* a conformation change, producing controlled 'switching' of MRI signal as a result of water access to the internalised Gd-chelates. A full characterisation of these potential MRI agents has been conducted to highlight their unique properties. Importantly, single field relaxometry has been used to analyse water exchange behaviour and the water gating capabilities of these composites. Such materials have potential applications for diagnostics and sensing.

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Acknowledgements

The authors thank the EPSRC and SFI Centre for Doctoral Training in Advanced Characterisation of Materials (EP/L015277/1).

Hydrophilic C flakes as electrode materials for aqueous Al batteries

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Abstract

Lithium-ion batteries are the dominant energy storage technology in the electric vehicles and portable electronics consumer markets. There is, however, much interest in developing alternative batteries due to the scarcity of Li and concerns about the safety of its systems. With respect to this, a more sustainable and (potentially) less expensive option would be the use of aluminium ions as the active species in rechargeable batteries.

Dating back to the 19th century, Al-based energy storage systems have come a long way. Still, the deployment of this technology continues to elude us. One major obstacle has been the lack of appropriate electrolytes. With Al plates acting as anodes, the need to counteract the passivating oxide layer that forms on their surface prevents the use of most liquids. In recent years, mixing AlCl₃ with ionic liquids (IL) has emerged as a preferred electrolyte, yielding promising performances when combined with carbon-based cathodes [1]. Whilst notable, this arrangement is hardly scalable due to the price, corrosiveness and moisture sensitivity of the IL. In these circumstances, reports of salt-water electrolytes employed alongside Al foils coated with a thin IL layer, brought much excitement to the field [2].

We present an Al-C battery that operates with an aqueous electrolyte and provides remarkable stability and capacity. In contrast to the graphite flakes that are commonly used as electrode materials, we employed a freeze-dried powder of reduced graphene oxide (rGO, **Fig. 1a**). Besides its hydrophilicity (when compared to graphite), the rGO contained bound-water and grafted organic moieties (**Fig. 1b**). These are all characteristics that contributed to the rGO cathode's compatibility with the 2M Al(OTF)₃ electrolyte (where OTF stands for trifluoromethane-sulfonate) and the unique charge storage mechanism proposed [3].

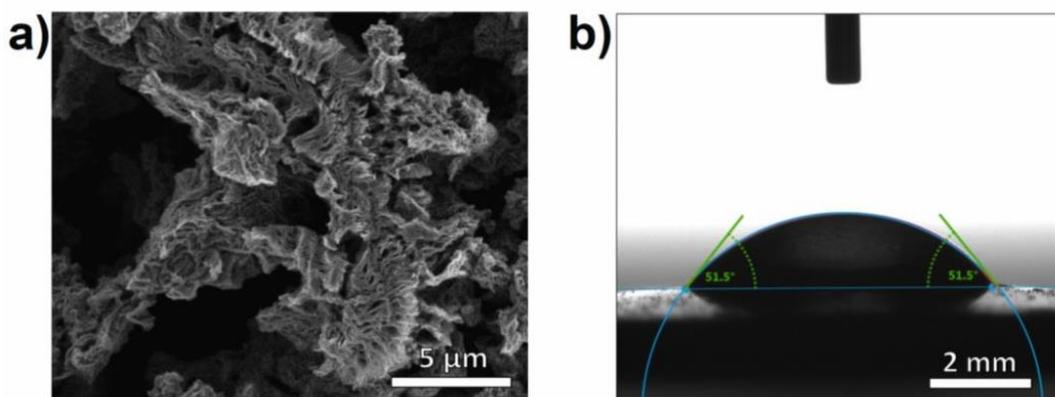


Figure 1. a) Scanning electron microscopy image of some freeze-dried rGO flakes. b) Contact angle of a water droplet with the rGO surface; generally, for graphite, the angle is $>90^\circ$ (hydrophobic).

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Amorphous nanoparticles for the electrocatalytic reduction of CO₂ into added-value chemicals

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Abstract

A world-wide more growing concern is the rising levels of CO₂ that leads to devastating consequences to our environment. Beside reducing the level of CO₂ emissions, one alternative strategy is the conversion of CO₂ into added value chemicals, such as CO, HCOOH, C₂H₅OH, CH₄, and many more.

CO₂ is a stable molecule, and its electrochemical reduction requires a suitable catalyst. Despite many noble and non-noble metal-based catalysts have been investigated, the difficulty achieving a high selectivity and faradic efficiency towards specific products, especially hydrocarbons, are still a challenge, alongside the concern over cost and scarcity of the metal catalyst. The present research project focuses on the synthesis of Cu, Ni and CuNi nanoparticles, prepared using different strategies based on a green, cost-friendly, and facile method, called the urea glass route.¹ The goal is to prepare targeted products, such as Cu-based alloys and core/shell structures *via* different strategies (CuNi, Cu@Ni, and Ni@Cu).

The final products were characterised using X-ray diffraction (XRD) and scanning electron microscopy (SEM). Pure Cu⁰ and Ni⁰ nanoparticles, crystalline and homogenous in size, were also prepared and used both as a comparison and as component to synthesize core/shell structures. For the CuNi system, changing the strategies and methodologies had an influence on the final structures. Remarkably, tuning factors such as heat treatment, metals ratio, urea content and precursors' composition were shown to influence the composition, size, and morphology of the final product.

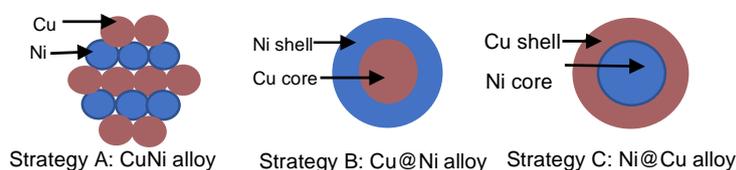


Figure 1: Schematic illustration of desirable outcomes expected for each strategy. The Cu (brown) and the contribution of the second metal Ni (blue) indicated by colours.

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Concentration-dependent optical properties of Indium Phosphide Quantum Dots

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Abstract

Colloidal semiconductor nanoparticles, commonly known as quantum dots (QDs), have emerged as an attractive class of optoelectronic materials with increased potential for biological applications. Their small size allows for the existence of quantum confinement effects that confer them unique optical properties. Indium phosphide core QDs with zinc sulphide shells (InP/ZnS) have been reported with a maximum photoluminescent quantum yield of 85% in organic solvent and 57% in aqueous solvent.¹ Toxicity reports show that these materials are safer alternatives to the traditional toxic cadmium-based nanoparticles.²⁻³

With the aim of further investigating the optical properties of InP/ZnS QDs, the effect of core growth time and sample concentration were tested using different indium precursors following a typical hot-injection synthesis. Preliminary results show that InP/ZnS QDs exhibit a concentration-dependent fluorescence emission profile, independent of the indium precursor used.

Analysis of the emission profile within the same batch of QDs shows that with increasing concentration, the emission peak redshifts, accompanied by a decrease in the intensity. In addition to absorbance and emission analysis, time-resolved fluorescence measurements allowed to gather evidence of energy transfer mechanisms in more concentrated samples of InP/ZnS QDs. The increase in average lifetime and longer decay components are characteristic of polydisperse samples of QDs where there is transfer of energy from the smaller donor QDs to the larger acceptor QDs.

The observed results provide important insights on how the control of the synthetic conditions of InP/ZnS QDs affects the optical properties of the nanoparticles. This study on the concentration of InP/ZnS QDs provides a better understanding of the optical behaviour of these nanoparticles, enabling us to define an upper limit value and validate the concentration range to use in biological experiments.

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Guest Mediated prevention of Quantum Dot Aggregation by Surface Bound Cucurbit[7]uril

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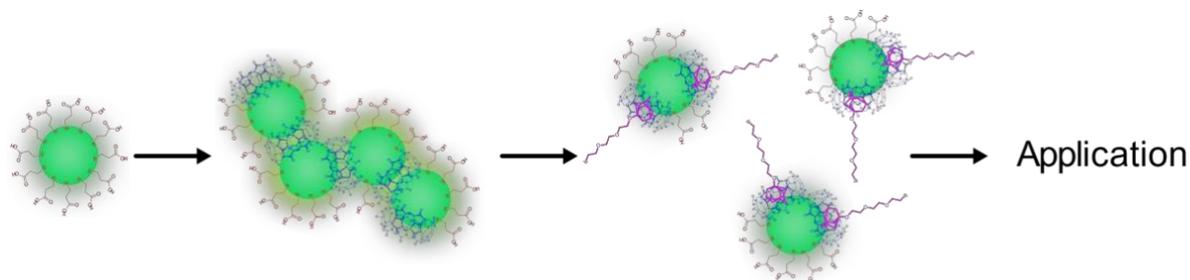
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Abstract

Switchable nanoparticle (NP) surface ligands produce the possibility to create novel sensors and smart materials by providing versatility at the NP surface. Attempts have been made to supply this type of material but normally lead to a non-flexible, non-adjustable material.¹⁻³ The use of a supramolecular host-guest (H/G) complexes at the NP surface allows for formation of a flexible and swappable surface through guest binding affinity manipulation.⁴⁻⁶

Here we present our initial results utilising hydrophilically modified adamantyl guests on electrostatically surface bound cucurbit[7]uril (CB[7]) at the surface of CdTe quantum dots (QDs).⁷ We demonstrate the prevention of aggregation of QDs through the bound CB[7] by the formation of 1:1 inclusion complexes. Monitored by optical spectroscopy, we show that this modular system is dependent on factors such as the total and relative concentrations of added host and guest, as well as the order of addition. We explore the potential for chain-length variation and switchable chemistries for further control assembly.

Preliminary data is shown of the envisaged route of long-term novel sensing opportunities for a variety of sensing applications.



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Development and Optimization of Dual Drug loaded Nanolipidic Carriers for Effective Management of Diabetic Foot Ulcer using Box-Behnken Design

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Abstract:

Diabetic foot ulcer is a serious complication of diabetes, associated with poor glycemic control, neuropathy, chronic inflammation and extremely slow wound closure resulting in amputation or losses of limbs, high health care cost and poor quality of patient's life. The usage of bioactives, in this regard, is documented to exhibit diverse pharmacological activities that have proved to be quite useful in the management of diabetic wound healing. However, their low and inconsistent bioavailability primarily pose serious impediment against their potential therapeutic usage. Therefore, the present research work was carried out to explore the untapped potential of nanolipidic carriers (NLCs) for co-delivery of tetrahydrocurcumin (THC) and folic acid. NLCs will aid in improving the low bioavailability and poor stability issues associated with THC and folic acid, respectively. The nanocarriers were prepared by hot emulsification method employing the principles of Quality by Design. Factor screening studies were performed using 7-variables-8-runs Taguchi design to select "vital few" critical method/process parameters, influencing critical material attribute (CMAs). Subsequently, response surface optimisation studies were conducted on the identified critical method/process parameters, viz., solid lipid concentration (X1), liquid lipid concentration (X2), and sonication time (X3), with chosen CMAs, viz., particle size, polydispersity index, zeta potential and entrapment efficacy, employing a 3-factors-17-runs, Box-Behnken design. Further, the design space demarcating the optimal formulation conditions was identified using numerical and graphical optimisation with optimised conditions of 4% solid lipid concentration, 1.2% liquid lipid concentration and 17 minutes sonication time. The final formulation depicted an average particle size of 181.6 nm, PDI of 0.21, zeta potential of -23 and entrapment efficiency of 90% for THC and 72% of FA. In a nutshell, the application of QbD has aided in developing a robust, reproducible and nanosize formulation for the co-delivery of THC and FA. Future research will be focused on evaluating its safety and uptake potential in human dermal fibroblast (HDF) and normal human epidermal keratinocytes (NHEK) cell lines.

Acknowledgments

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Development of multifunctional mesoporous silica nanoparticles for treatment and diagnosis of hepatocellular carcinoma

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Abstract

Hepatocellular carcinoma (HCC) is commonly diagnosed in the late stages which limits the treatment options to only the FDA approved drug sorafenib. However, its low efficacy, poor solubility, and the toxic side effects are all obstacles that limit its performance. In addition, the lack of a proper diagnostic tool for either detecting the tumour in the early stages or to monitor the disease progression represents another barrier toward effective HCC treatment.¹

Our work aims to solve these problems by producing mesoporous silica nanoparticles (MSNs) that can enhance the therapeutic performance through high drug loading.² Sorafenib-loaded MSNs have been prepared and the effect of the pore size, hydrophilicity and solvent polarity on both drug loading and entrapment efficiency was studied. It was found that the lower the solvent polarity, the higher the drug loading and entrapment efficiency. However, both pore size and surface chemistry did not affect the results significantly. In term of diagnosis, MRI active MSNs have been prepared by incorporating the MRI contrast agent gadolinium 1,4,7,10-tetraazacyclododecane-N,N',N'',N'''-tetraacetic acid (Gd-DOTA) chelate to internal surfaces, at locations where water gating can be exploited to provide an 'on/off' MRI signal switch for disease diagnostics. The diagnostic MSNs showed a higher r_1 relaxivity values (*i.e.* higher relative signal enhancement) when compared to the commercial Gd-DOTA chelate (Dotarem©) at 1 T.³

As a final step, theranostic MSNs will be developed with a thermo-responsive polymer grafted on the surface that prevents water access to the internalised Gd-contrast agent and effectively caps pores preventing the drug release. Upon mild hyperthermia, the grafted polymer will change its conformation resulting in opening of the pores, with simultaneous release of the loaded drug as well as switching of the MRI signal to 'on'. In this way, we have developed an all-in-one theranostic vehicle for this difficult to treat disease.

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Amphiphilic Self Assembly of Fatty-Alcohol in Silica-Salt Hydrogels. Implications for Abiogenesis

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Abstract

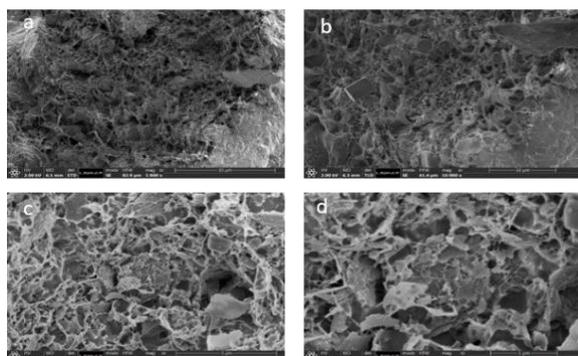


Figure 1b. cryo-SEM images of silica hydrogel matrix.

In attempting to understand the emergence of biological life, both top-down and bottom-up approaches aim to converge at some primitive cellular system. Therefore, tracking of amphiphile and polymer emergence can lead to an understanding of the molecular evolutionary process relevant to the emergence of life. As part of this, amphiphilic and polymeric molecules are important.¹ However, what may have been less widely recognised is that a cellular cytoplasm is not just an aqueous salt solution but a hydrogel environment. Indeed, Trevors and Pollack had realised the potential importance of hydrogels to life emergence in 2005, arguing that “a primitive hydrogel was a more suitable environment for the assembly of pre-cells, and ultimately cells capable of growth and division”^{2,3}.

Therefore, we have been examining hydrogel environments which may have been plausible within the early earth Haden period, such as silica hydrogels, and specifically how important processes as molecular self-assembly may be different in the gel to aqueous phase. Prebiotic experiments in gel-phase media are still very few in number and nature. The benefits of hydrogels can easily be seen when compared with aqueous media. In this poster we present some unpublished work exploring the effects of organic additives such as alcohol on amphiphilic self-assembly in the hydrogel phase and comparing these to aqueous systems with the same additives.

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Synthesis of magnetic biochar composites for enhanced soil toxic metal pollution adsorption

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Abstract

Magnetic biochar composites were successfully fabricated by pyrolysis of siderite and Sawdust under N₂ condition. The results of a variety of characterization implied magnetic biochar displayed porous structures with larger specific surface area. CHN Elemental analyzer (Vario EL c) was used to analyze total carbon, nitrogen, oxygen and hydrogen content. Chemical composition of natural siderite was measured using an X-ray fluorescence (XRF) spectrometer (Shimadzu XRF-1800). The morphology of magnetic biochar was examined by scanning electron microscopy (JEM-2010, Japan) with dispersive X-ray spectroscopy (EDS). The mineralogy of magnetic biochar was analyzed by an X-ray diffractometer (Dandonghaoyuan 2700) equipped with a rotation anode using Cu K α radiation at 300 mA and 45 kV. The surface structural groups of magnetic biochar were characterized using a Fourier transform infrared spectrometer (VERTEX-70). The zeta potential of each suspension was measured by a Malvern Zeta Potentiometer (Nano-ZS90). SBET was measured using N₂ sorption using TriStar II 3020 instrument by Brunauer–Emmett–Teller (BET) method. Magnetization curve was examined by a magnetometer (Lakeshore Cryotronic, USA).

The batch adsorption experiments showed high adsorption properties of magnetic biochar composites toward soil toxic metal pollution, whereas adsorption was significantly influenced by pH, temperature and time. Owing to the simple synthesis procedure, low cost, high adsorption efficiency, easy separation and environmental friendly, magnetic biochar can be considered as a potential adsorbent for the purification of toxic metal-bearing wastewater after soil washing process in environmental remediation.

Acknowledgements (optional): Financial and Characterization tests support from The Earth Research Institute, Geological Survey & Mineral Explorations of Iran (GSI), TEHRAN - IRAN are acknowledged.

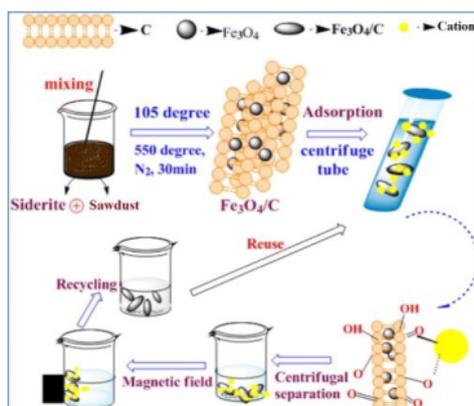


Figure 1 – schematic of Synthesis of magnetic biochar composites for enhanced soil toxic metal pollution adsorption and desorption-recycling

Development of highly fluorescent Carbon Dots from abundant non-commercial weeds for environmental remediation

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Abstract

Rapid industrial and urban development is a major source of environmental stress and poor health with the unprocessed release of harmful species from various manufacturing, agricultural and domestic sectors [1]. While this is a world-wide issue, it is particularly acute in low to medium income countries with high population densities where government regulation is also lacking. Processes such as waste-water treatment typically involve a costly multi-step process requiring significant infrastructure. As a starting point, it would significantly benefit those living in the at most high-risk regions to have access to low-cost solutions for both monitoring and small volume water remediation. Functionalized nanoscale materials offer exciting new opportunities to address these environmental challenges [2]. It is also essential that suitable candidate materials are produced as sustainably as possible with green methodologies for the synthesis of nanomaterials using biomass considered as a more desirable alternative to existing techniques [3].

In this poster, the application of functionalized carbon dots (C-dots) sourced from an environmental waste species with no commercial value is described. **Ragwort (*Jacobaea vulgaris*)** is a toxic biennial weed found throughout the United Kingdom, especially on open, sunny sites such as pastures and on roadsides [4]. Consumption of ragwort can sicken or even kill cattle, horses and pets. Due to its toxicity and widespread presence, ragwort was investigated as a source of controlled environmental waste that could be sustainably used to produce a valuable tool for environmental sensing. C-dots were prepared from different parts (leaves, flowers, stem) of locally sourced ragwort and their properties compared. A variety of analytical methods including UV-visible spectroscopy, photoluminescence spectroscopy, life-time fluorescence, FTIR and HRTEM imaging were utilized to demonstrate their excellent absorption and emission behavior and uniform size distribution. These properties were also compared to C-dots produced from more conventional sources. Furthermore, surface-functionalization of the ragwort derived C-dots will be described to improve the specificity and efficacy of pollutant adsorption on the nanomaterial surface for both sensor and remediation purposes.

Acknowledgements: This work is supported by a Commonwealth Split-site PhD scholarship to Pooja Chauhan.

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Photocatalytic decolourization of a new water-insoluble organic dye based on phenothiazine by ZnO and TiO₂ nanoparticles

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Abstract

A new water-insoluble organic dye, namely, 2-((10-decyl-10H-phenothiazin-3-yl)methylene)malononitrile, was synthesized and fully characterized. It was envisioned that photocatalytic decolourization of a dye-containing long chain would pave the way for the photocatalytic remediation of wastewater containing toxic hydrophobic organic pollutants. Two commercially available nanoparticles, ZnO and TiO₂, were selected, and their photocatalytic decolourization of the dye from aqueous medium were compared. The black UV light irradiation of the colored samples in the presence of TiO₂ (P25) or ZnO resulted in their decolourization and the photocatalytic activity observed for TiO₂ (P25) was better than that of ZnO. The kinetic of decolourization indicated that the process was first-order from which the rate constant was calculated. Also, the effect of pHs on the kinetic of decolourization revealed a negligible effect, indicating that the pH, although it affects the catalysts but has no effect on the organic-based hydrophobic dye and thus no effect on the photocatalytic process

Acknowledgements (optional):

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Morphology control of silk fibroin nanoprecipitation under bulk and microfluidic mixing regimes

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Abstract

The control of silk fibroin multiscale structure by shear processing is fundamental to the biopolymer function in the natural world and can be harnessed in nanoprecipitation. Here, we report the modulation of silk fibroin primary–tertiary self-assembly by varying factors which control shear and mixing during nanoprecipitation in semi-batch and micro-mixers. Under high shear regimes and bulk mixing conditions, the size and polydispersity index of assemblies decreased with mixing time, as stirring rate ($800, 400 < 0$ rpm) and feed addition height ($3.5 < 0$ cm) increased. Using the optimised conditions for low bulk mixing times, moving from low to high shear processing increased the extent of self-assembly ($0.017 < 16.96$ mL min⁻¹) for 0.5, 2 and 3% w/v silk. Finally, in conditions of high shear and low mixing time, the feed concentration controlled the assembly shape, size, and polydispersity index in microfluidic ($0.5, 3.0 < 2\%$ w/v) and semi-batch format ($3.0 < 0.5\%$ w/v). Although the multiscale structure was varied with silk precursor concentration in high shear, fast bulk mixing, mixtures of spherical nanoparticles with nanofiber, lamellar and gel-like assemblies were formed. Due to the sufficiently low micro-mixing times in high shear, microfluidic format, the particle morphology was tuned from monodisperse, worm-like to spherical nanoparticles by increasing concentration from 0.5 to 3% w/v silk precursor. This comparative work provides new insight into morphology control of silk nanoparticles using silk concentration as a controllable input factor.

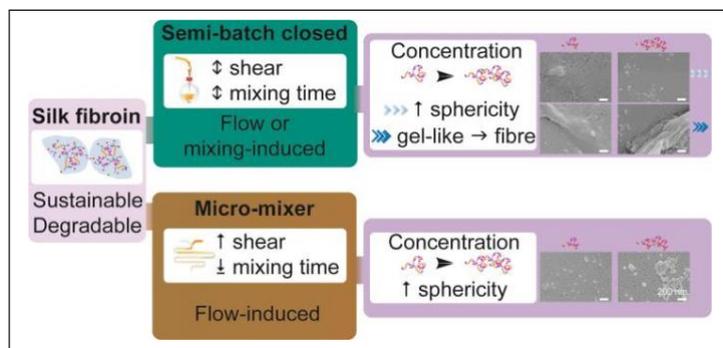


Figure 1 - The silk feed shear and solvent-antisolvent mixing time influences nanoprecipitation of the silk biopolymer. Assemblies were characterized from low and high shear semi-batch nanofabrication platforms and a high shear micro-mixer.

Acknowledgements (optional): The authors thank Professor Andrea Ducci (University College London,), Professor Nigel Mottram (University of Glasgow,), Dr Alice Turner, Dr Deborah Bowering and Dr Maider Olasolo (University of Strathclyde) for providing training and technical advice. The authors acknowledge that this work was carried out in part at the EPSRC Future Manufacturing Research Hub for Continuous Manufacturing and Advanced Crystallisation (CMAC) (EP/P006965/1). S.A.L.M. is supported by a Medical Research Scotland Ph.D. Studentship (PhD-1292-2018).

Templated Growth of Nanoparticles to Indicate the Reductive Potential of Whisky

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Whisky is the number one internationally traded spirit, with Scottish Whisky exports reaching £3.8 billion in 2020.¹ Currently, around 22 million whisky filled casks are maturing in Scottish warehouses, by law, for a minimum of 3 years. It is during this resting stage that the flavour profile develops. Congeners are responsible for the flavour of the whisky, these are residual chemicals from the distillation process and molecules such as aldehydes, ketones, and catechols that have leached from the cask. With time congener levels increase, owing to the deeper flavour profiles, and in turn their increased commercial value.

Factors such as wood source or treatment will contribute to the rate at which the whisky matures in the cask. Whisky manufacturers look to investigate the 'agedness' of a whisky before deciding if it is ready for bottling or blending. Typically, expensive HPLC-MS instruments or experienced whisky sommeliers are required to make this decision. Therefore, a simple, colorimetric test for checking the whisky aging process is desirable within the industry. We propose a metallic nanoparticle-based test, which can detect key chemical changes in the aging whisky compared to 'new make' spirit.

The reducing potential of a whisky increases with maturation, leading to a predictable formation of Au or Ag nanoparticles. The rate and plasmon position can suggest the chemical composition of the whisky. This templated growth could indicate to distillers the agedness of a whisky and barrel pairing. Multiple shop-bought whiskies were shown to form AuNPs (Figure 1) and a trend in the aging of a single cask was also demonstrated.

Further investigations are being carried out to identify the congeners from the wood that are responsible for the reducing effect, with ketones already demonstrated as likely contributors.²

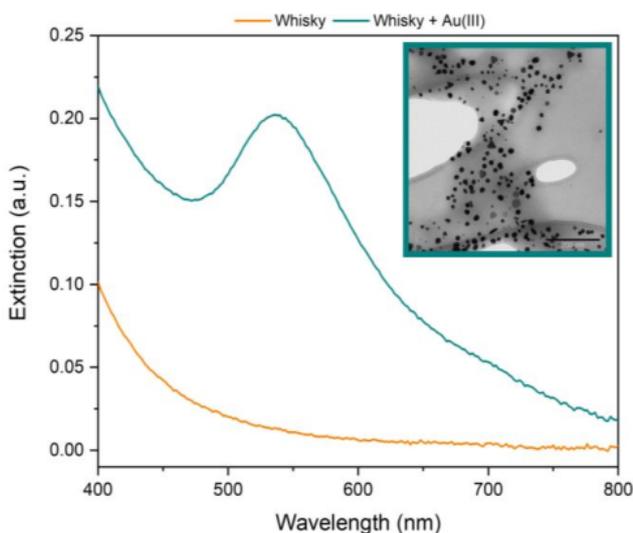


Figure 1. Whisky reduced AuNPs. TEM insert shows predominantly round nanoparticles, scale bar 200 nm.

Acknowledgements: The Scottish Whisky Research Institute for supplying the aged whisky sample series.

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Protocol for the Rapid Detection of Salmonella by using Antibody Functionalized Immuno-magnetic Iron Oxide Nanoparticles

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Abstract

Rapid detection of pathogens by using functionalized nanoparticles coupled with antibodies provides advantages to detect bacterial pathogens in food and drinking water samples¹. The study was aimed to develop an immuno-analytical assay to detect Salmonella by using magnetic iron oxide nanoparticles (IONPs) conjugated with the mouse anti-salmonella enteritidis LPS antibody. The IONPs were synthesized by reducing iron chloride and stabilized by using trisodium citrate. The morphophysical analysis of nanoparticles by using the TEM technique manifested that the nanoparticles are spherical and exist in the size range of 10-15 nm. A Williamson-Hall plot analysis of the XRD peaks gave a crystallite size of 9.9 nm. The magnetization of IONPs was recorded as $61 \text{ Am}^2\text{kg}^{-1}$ at 1 T by performing the vibrating-sample magnetometer analysis. Magnetic iron oxide nanoparticles were carbodiimide conjugated to mouse antibody (8209-5349) by using N-Hydroxysuccinimide (NHS) and 1-Ethyl-3-(3-dimethyl aminopropyl) carbodiimide (EDC) at room temperature². Size distribution analysis of IONPs, EDC-NHS associated IONPs and carbodiimide antibody conjugated nanoparticles showed the gradual increase in the hydrodynamic diameter of IONPs after their conjugation with NHS, EDC, mouse antibodies, and finally with the bacterial pathogens. A magnet was used to sequester the Salmonella conjugated immuno-functionalized nanoparticles from water samples. Confocal microscopic images of Salmonella conjugated immuno-functionalized IONPs showed the association of immuno-magnetic nanoparticles with Salmonella. The findings of the current study confirm the potential of immuno-functionalized IONPs to separate and detect Salmonella successfully from contaminated samples.

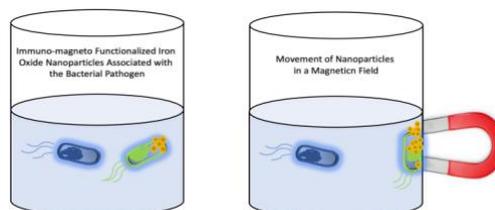


Figure 1: Movement of IONPs associated Salmonella bacterium toward a magnet

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Investigation into the use of microfluidics in the manufacture of metallic gold coated iron oxide hybrid nanoparticles

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Abstract

The ever-increasing interest in incorporating hybrid nanoparticles in novel nanomedical, photonics and energy storage applications demonstrates a clear need to improve their synthetic scalability and reproducibility¹. Successful synthesis is partially attributed to skill and experience and current procedures suffer in quality at higher scales, likely caused by inadequate mixing, which is crucial in maintaining uniform particle size.

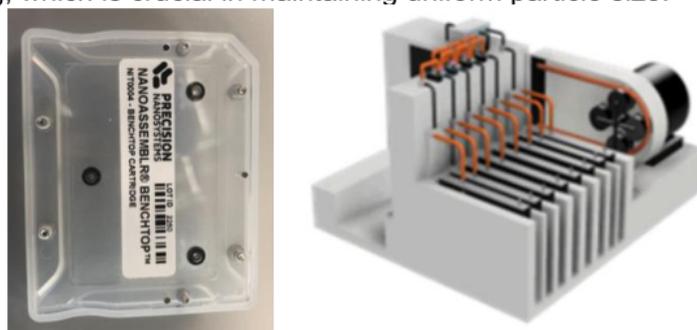


Figure 1: NanoAssemblr cartridge where reagents are efficiently mixed via two inlets (left) and proposed microfluidic setup for continuous manufacture of hybrid nanoparticles.

Recently, there has been a surge in the successful scale-up and continuous manufacture of liposomes using microfluidics and we aimed to determine the feasibility of using these systems for hybrid nanoparticle synthesis². Within this study, we utilized a Precision NanoAssemblr Benchtop® system to construct 60nm hybrid nanoparticles with Fe/Au ratios of 1:0.7, in comparison to standard benchtop derived hybrid nanoparticles (Fe/Au – 1:0.6). This demonstrated that this process was suitable for the synthesis of hybrid nanoparticles with the next steps for optimisation being to construct a continuous flow system³.

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Spherical polymer nanoparticles and nanocomposites, their biofunctionalization and proposed applications

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Abstract

Polymer nanoparticles have considerable advantages for applications in drug delivery systems, biosensors, etc. Therefore, it is of great importance to find environment-friendly, efficient methods to synthesize and functionalize polymer nanoparticles. The synthesis of different types of polymer nanoparticles was achieved using aerosol photopolymerization – an integrated and continuous method that produces highly pure dry polymer particles without using surfactants, heating, or hazardous solvents. Polymer nanoparticles with thiol-functional groups can be obtained by combining the aerosol photopolymerization process with thiol-ene chemistry. Thiol-mediated biofunctionalization can be applied to functionalize these nanoparticles via the reactive -SH groups.

Production of nanocomposite materials via aerosol photopolymerization can be achieved by introducing inorganic nanoparticles into the process. We established a procedure for the synthesis of nanocomposites with silver nanoparticles (of mean size 50 nm) finely distributed inside the polymer nanoparticles (of mean size 300 nm). Fluorescence-labeled streptavidin was conjugated on the surface of the nanocomposites via a two-step bioconjugation: 1) maleimide-biotin conjugation onto -SH groups accessible on the polymer surface via thiol-maleimide reaction, 2) conjugation of fluorescence-labeled streptavidin via streptavidin-biotin binding. These functionalized nanocomposites can be used as biosensors in cancer diagnostics and treatment when appropriate biomolecules are conjugated onto the polymer.

The application of polymer nanoparticles produced via aerosol thiol-ene photopolymerization for the immobilization of enzymes was also considered. β -galactosidase was immobilized on the surface of biotin-functionalized polymer nanoparticles (mean size 300 nm) by affinity binding immobilization technique using a two-step bioconjugation technique. The immobilization was carried out with high efficiency, 62% of enzyme introduced into the reaction was bound onto the surface of nanoparticles. The nanoimmobilized enzyme was stable at room temperature for 28 days. Furthermore, a 15% increase in enzyme activity was observed. Enzyme-conjugated nanoparticles were also encapsulated inside the hydrogel microparticles (~400 μ m in diameter) via microfluidic devices to maintain the reusability. We discovered that the encapsulation process impacts β -galactosidase and certain chemicals can cause significant reduction in enzyme activity, whereas other compounds protect and prolong enzyme's activity.

In conclusion, a set of new polymer nanoparticles and nanocomposites was obtained by combining aerosol photopolymerization technique with thiol-ene chemistry, and possible applications of the new systems were studied, introducing a prospect of multifunctional polymer nanoparticles.

Organogels as versatile biomaterials for skin-delivery

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Abstract

Organogels (ORGs) are semi-solid systems, widely investigated for pharmaceutical and cosmetic applications. In these systems, an organic phase is immobilized by a three-dimensional lattice composed of a self-organized aqueous phase. In this context, this study targets at the development of Poloxamer (PL) based ORGs, comprising different compounds for a diversity of topical delivery applications¹. ORGs were prepared associating an aqueous phase (AP) of PL407 (20 and 30% w/v) with different organic phases (OP) such as fatty acids, long-chain esters, and waxes. The OP:AP ratio was 1:4 w/w¹. Characterization of the formulations was performed by physicochemical techniques including rheology, differential scanning calorimetry, and scanning electron microscopy. First, this work investigated the relationship between different oil phases and structural changes in ORGs. Thus, ORGs were synthesized with OP based on mineral oil and twelve different organic compounds. The chemical nature of compounds affected the ORG morphology (figure 1) and rheological parameters. For example, unsaturated fatty acids increase the G'/G'' ratio 2-fold compared the ORG with mineral oil OP. Then, isopropyl myristate ORGs were evaluated for topical co-delivery of lidocaine (LDC) and curcuminoid derivatives (CURs) to treat topical lesions. Results revealed that LDC and CURs insertion into ORGs increases viscosity and elastic/viscous moduli (G'/G'') ratio, modifying the cubic ORGs supramolecular organization². Furthermore, these ORGs were also tested as formulations to sanitize hands against the COVID-19 virus. In this case, ORGs were prepared with oleic acid and TiO₂ nanoparticles (NPs)³. The thermoreversibility of poloxamer was maintained after the NPs addition, displaying a sol-gel temperature transition around 16 °C. The combination between ORGs and inorganic NPS is an innovative purpose since such ethanol-free formulations avoids the dehydration and damage of the skin tissues. In summary, results pointed ORGs as promising formulations for skin delivery with potential different pharmacological applications.

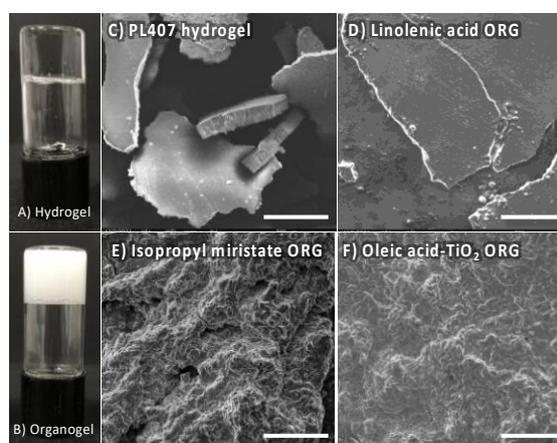


Figure 1 - (A) PL407 hydrogel, (B) Organogel and Scanning electron micrographs of the PL407 hydrogel (C), Linolenic acid ORG (D), Isopropyl miristate ORG (E) and Oleic acid-TiO₂ ORG (F). Scale bar = 500 μm.

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Acknowledgements: FAPESP (2019/14773-8, 2019/20303-4), CNPq (307718/2019-0), CAPES e CEM-UFABC.

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Green synthesis, textural and magnetic properties of water dispersible gold coated superparamagnetic iron oxide nanoparticles

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Abstract

Gold coated magnetic nanoparticles have received a lot of attention in recent years due to their multifunctional attributes and their prospective unique characteristics in environmental and biomedical applications¹. This paper reports the synthesis and characterization of gluconic acid capped gold-coated superparamagnetic iron oxide nanoparticles (SPION@Au) via a greener co-precipitation approach. The textural and magnetic properties of the as-synthesized nanoparticles were thoroughly analysed. The as-synthesized nanomaterials were characterized using scanning electron microscopy (SEM), energy-dispersive X-ray spectroscopy (EDX),

transmission electron microscopy (TEM), powder X-ray diffractometry (XRD), thermal gravimetric analysis (TGA), Brunauer–Emmett–Teller (BET), and superconducting quantum interference device (SQUID) magnetometry. The XRD, SEM and TEM measurements showed that the gluconic acid capped magnetic core was coated with gold with cubical spinel crystalline structures. TGA results revealed the thermal stability of the nanoparticles. Textural properties indicated that the gold coated nanomaterials were mesoporous in nature and exhibited the type IV isotherm with H₂ hysteresis loop. The estimated surface area and maximum pore diameter of SPION@Au were 134.02 m²/g and 3.33 nm respectively. Furthermore, the SQUID results showed the nanocrystals were superparamagnetic with a blocking temperature (TB) of 214 K at 500 Oe and saturation magnetization of 11.38 emu/g. These noteworthy results demonstrated that the as-synthesized SPION@Au are promising nanomaterials for biomedical and analytical applications.

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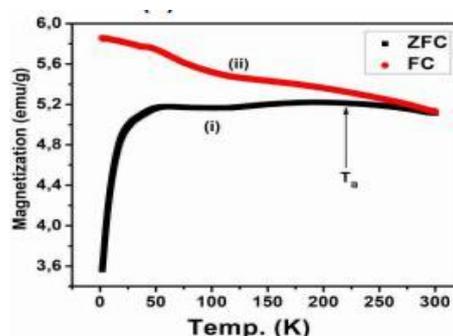


Figure 1: SQUID analysis of SPION@Au

Fabrication of nanosilver imbued polymer wafers

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The application of nanomaterials in healthcare has been very prominent since its development, with nanometals such as nanosilver being heavily utilised in the aspect of wound care and antibacterial activity. One of the issues with nanosilver, especially in the case of wound care is that it can permeate through wounded skin and systemically accumulate within the host body, which can lead to complications such as liver, lung, nervous system, and reproductive toxicity¹.

To combat such an issue, we are working to develop a multifunctional polymer system for wound healing that can help to expedite the wound healing process, whilst facilitating the antibacterial effects of nanosilver without it leeching into the host, thus avoiding gradual systemic accumulation.

Current experimental work is focussing on the one pot synthesis method of developing nanosilver within a polymer solution and then physically locking into the polymer microstructure, thereby allowing the nanosilver to elicit its antimicrobial effects through ion release without it physically detaching from the polymer matrix. Prior to that, past experimentation focussed on the development of the base polymer system itself, with regards to its mechanical strength and physical characteristics which needs to be optimised for its application in wound healing.

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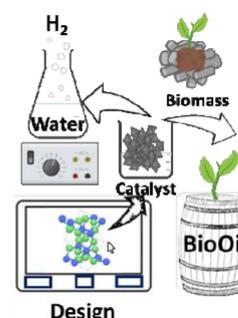
Metallic Ceramics: the New Generation of (Elettro-)Catalysts for Sustainable Energy Production

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Abstract

The worldwide request to find renewable sources of energy and chemicals to face the global warming and energy crisis, alongside the constant increase in terms of energy demand, urges for sustainable solutions. Governments worldwide have imposed clear actions to reduce the burden on future generations, and among widely accepted “green process” alternatives, the electrochemical *water splitting* (specifically the hydrogen evolution reaction, HER, to produce H₂ as a clean fuel) and the *biomass valorisation* (to convert waste into biofuels) cover a predominant role. However, those processes are currently limited by several factors, including unstable catalytic materials and complex reaction engineering.

To face these challenges, we designed and formulated resilient metallic ceramic-based catalytic materials imbedded on functional support, and have validated them by lab scale reactors, specifically designed to facilitate rapid optimization, improve performances and minimise waste. Results on these specifically designed metallic ceramic based nanocomposites will be presented, together with examples of their applicability in (electro)-catalytic processes (including biomass conversion¹, ORR², HER³⁻⁴ and more), alongside the strategies to control their structure and properties.



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