UNIVERSITY OF LIVERPOOL

Delivering Innovation and Impact

Department of Chemistry

CONTENTS

WELCOME

Our research and approach to partnerships provide solutions that benefit the world. The Department of Chemistry at the University of Liverpool is outward looking, carries out world-leading research and has a strong record in delivering both innovation and impact.

We welcome the opportunity to work with new partners and to further develop our programmes of activity with our established collaborators.

We are proud of our excellent and impactful research. The Department of Chemistry ranked 2nd overall across the country during the last UK Research Excellence Framework process and we continue to build on this success through a strategic process of recruitment and institutional planning.

Our academics are internationally recognised experts in their fields and have access to state-of-the-art facilities which are described within. These include centres such as the Materials Innovation Factory, which combines knowledge leadership in advanced materials, unparalleled equipment and a dynamic support infrastructure – all of which is available to both academia and industry.

This brochure showcases some of our pioneering research that has also achieved substantial impact through our work with diverse partners. At the University of Liverpool, we take pride in being a global centre for fundamental science and technology development and here we highlight" the wide variety of engagement pathways possible.

Benefiting the world through our impactful research and by working in partnership is at the heart of our activities and we look forward to welcoming you to the Department of Chemistry at Liverpool.

Professor Rick Cosstick *(Dean of Physical Sciences)*

Dr Neil Berry *(Head of Department, Chemistry)*

Impact cases

DEVELOPING A GREEN AND LOW COST MANUFACTURING PROCESS – **CATALYSIS STUDIES**

The challenge

Methyl methacrylate (MMA) is the key monomer in acrylic plastics, used in windows, contact lenses, implants and paints. Around 3 Mtonne of methyl methacrylate is produced annually, with a factory gate value of ca. $9 bn. Historically this was done using toxic starting compounds in an energy intensive process.

Research at the University of Liverpool was critical in enabling the commercialisation of the green Lucite ALPHA process that has generated >$1.5 bn of new business in the first six years of operation for the partner.

A second ALPHA plant came on stream in 2018 and is the world's largest MMA manufacturing plant.

The research approach

The Lucite ALPHA process uses radically different chemistry from the conventional acetone cyanohydrin (ACH) process.

Research at Liverpool provided a detailed understanding of reaction intermediates and their relative stability and experimentally verified the thermodynamic model used for developing the chemical plant.

This helped provide key data to underpin a x30,000 scale up and gave an understanding of the chemistry that resulted in the use of counter-intuitive operating conditions that extended the catalyst life by several orders of magnitude, essential for commercialisation of the process.

Working in partnerships

Working closely with the industrial partner, Lucite, Dr Iggo's team used their expertise in Nuclear Magnetic Resonance (NMR) and high pressure systems to identify catalyst degradation pathways that were limiting the companies' technology.

This directed selection of a counter-intuitive operating regime and led directly to commercially viable catalyst turnover numbers (TON).

Outputs and outcomes

Liverpool academics continue to work on a range of industrially relevant catalysis providing expertise in NMR studies, catalyst design and product characterisation in order to deliver further improvements in the field of catalysis and full details of our team and expertise can be found at: www.liverpool.ac.uk/chemistry/research/energy-and-catalysis/

*Research at the University of Liverpool was critical in enabling the commercialisation of the green Lucite ALPHA process that has generated >**$1.5** bn of new business in the first **six** years of operation for the partner.*

PROVIDING A SMALL SOLUTION TO HUGE CHALLENGES – **NANOMEDICINE** FOR HIV AND OTHER INFECTIOUS DISEASES

The challenge

Globally, around 42.9 million people are living with HIV, while only 19.5 million people currently have access to the effective drugs used to suppress the virus and halt progression of the disease.

Pioneering research led by the University of Liverpool is accelerating global efforts to make more effective and cheaper HIV therapies available to more patients through the use of nanotechnology, more specifically, using Solid Drug Nanoparticles (SDNs).

Globally, around 42.9 million people are living with HIV, while only 19.5 million people currently have access to the effective drugs used to suppress the virus and halt progression of the disease.

The research approach

SDNs are tiny particles that enhance drug absorption. Their diameter, usually as small 200-600 nm, means less drug is needed to provide the same blood concentrations as conventional tablets after oral dose. Using less drug means lower cost of treatment per patient, and better use of available supplies, making cutting-edge treatments available to more patients.

The cross-Faculty multi-disciplinary partnership accelerating this research encompasses members of our Department of Molecular and Clinical Pharmacology.

Honoured with a Queen's Anniversary Prize in 2017 for its work in improving the safety and effectiveness of medicines, and materials experts from our Department of Chemistry, who were awarded with a Regius Professorship in 2016 as part of the Queen's 90th birthday commemorations.

We utilise proprietary technology to generate libraries of nanoparticle candidates that are screened for pharmacological benefits. In recent programmes, it has taken as little as three years to progress new programmes through to first-in-human clinical trials using this approach.

Working in partnerships

Given it is the poorest countries that need these new medicines the most, the University has chosen a not-for-profit development pathway for HIV therapies, to license these medicines for charitable use in low- and middle-income countries through a partnership with the United Nations-backed public health organisation, Medicine Patent Pool.

The partnership is also working with other leading charitable partners such as the Clinton Health Access Initiative.

The technology may also be partnered for other oral, long-acting injectable and topical therapies.

Outputs and outcomes

Two, 2-stage first-in-human clinical trials have been conducted, representing the first studies of orally-dosed nanomedicines for HIV globally; the team are also actively targeting paediatric therapies. In other infectious disease research, for example long-acting injectable prophylactics have been developed for malaria and the team are also targeting TB.

Through direct engagement with regulatory authorities Medicines and Healthcare Products Regulatory Agency (MHRA) in the UK and Food and Drug Administration (FDA) in the US, we have accurate guidance for the route to approved therapies using our technology and are keen to partner development programmes which may benefit from long acting drug release or oral dosing optimisation.

Further details of our activites can be found at:
www.liverpool.ac.uk/chemistry/staff/steven-rannard/

PIONEERING THE DISCOVERY OF ADVANCED AND **FUNCTIONAL MATERIALS**

The challenge

New advanced materials are urgently required throughout sectors such as manufacturing, healthcare, energy and consumer products.

World-leading research at the University of Liverpool is accelerating the delivery of breakthroughs impacting across catalysis, solar fuels, filtration, thermoelectric, battery and fuel cell technologies.

Our current activities build on a long track-record of industrial partnership with recent examples of programmes including work that delivered new routes to advanced materials for the microelectronics industry.

The research approach

Chemical Vapour Deposition (CVD) is ideally suited to the deposition of thin films of highly pure materials for microelectronics applications. However, conventional techniques require precursor compounds with very specific properties such as appreciable volatility at atmospheric pressure.

Research led by Professor Helen Aspinall, in collaboration with colleagues in the Department of Engineering, has led to new, improved precursor compounds, as well as to pioneering low-pressure CVD techniques to develop new products and processes for thin film deposition.

Working in partnerships

The new, improved precursor compounds and CVD processes have been developed and optimised with SAFC Hitech.

The new products had a major impact on the growth of their silicon semiconductor business. The availability of the new oxide precursor compounds enabled SAFC Hitech to expand their customer base and help satisfy demand for increasingly diverse and exotic oxide materials.

Outputs and outcomes

Our award-winning research expertise in advanced materials is backed by excellent facilities that offer an unparalleled new opportunity for academic-industrial engagement.

The recently opened Materials Innovation Factory (MIF) hosts leading materials chemistry groups including those of Professors Andy Cooper FRS and Matt Rosseinsky FRS who are pioneering the acceleration of materials science discovery through the integration of expertise and experimental and computational models.

The MIF contains one of the highest-concentration of materials science automation robotics in the world, which is combined with a state-of-the-art instrumentation suite and expert technical support.

Details of how to work with us can be found at:
www.liverpool.ac.uk/materials-innovation-factory/

World-leading research at the University of Liverpool is accelerating the delivery of breakthroughs impacting across catalysis, solar fuels, filtration, thermoelectric, battery and fuel cell technologies.

NANOCHEMICAL SYSTEMS FOR GREEN TRANSPORT: **DELIVERING ENERGY EFFICIENCY** FOR MARITIME APPLICATIONS

The challenge

Shipping accounts for 1,000 million tonnes of CO^2 emissions annually and emissions are predicted to increase by up to 250% by 2050. Biofouling of ship hulls can increase fuel consumption, and hence CO^2 emissions, by up to 40% if left untreated.

The Department of Chemistry is a leading partner in the University of Liverpool's activities addressing global energy challenges. Our Stephenson Institute for Renewable Energy is pioneering research into energy conversion, storage and efficiency. Work led by Professor Dmitry Shchukin has delivered a low-toxicity, cost efficient class of antifouling materials that have the potential to greatly decrease the CO^2 emissions in this vital transport sector.

The research approach

Professor Shchukin's team have developed an innovative route to delivering a sustained low level of eco-friendly antifouling agent that can be painted onto existing ships.

The key is the careful design and control of nanocapsules that release the antifouling agent on demand over years, thus preventing the need for regular manual hull cleaning and reducing maintenance costs.

Working in partnerships

Working within a large EU consortium of academic partners and companies (19 consortium members) as part of the Byefouling programme the Liverpool team have been able to rapidly translate their fundamental advances into the paints industry.

The close interactions of the academic and industrial teams has ensured a focus on developing a product fit for real-world use.

Outputs and outcomes

The products designed by Liverpool academics are being carried forward by industry partners. They are currently undergoing field trials for testing antifouling activity on industrial shipping fleets.

The products are of interest for paint manufactures and can be applied not only on different types of ships but also in sea-farms, underwater oil platforms and pipelines.

More detail of our activities and activities in renewable energy can be found at:
www.liverpool.ac.uk/renewable-energy/

*Professor Shchukin's team have developed an **innovative** route to delivering a sustained low level of **eco-friendly** antifouling agent that can be painted onto existing ships.*

TACKLING BIOFILMS AND THE ANTIMICROBIAL RESISTANCE CHALLENGE - **SMART SURFACES**

The challenge

Microbial activity and biofilms on surfaces and interfaces cost UK industry billions of pounds each year due to product contamination, energy losses, and equipment damage. Affected sectors include:

- the healthcare and medical devices industry
- the foods, drinks and water industries
- consumer products
- paints and coatings
- the marine industry
- chemicals and the petroleum industries.

Biofilms are also implicated in the emergence of AMR

*Our team has worked with market **leading** companies including Boots UK Ltd, DePuy Synthes, Smith & Nephew, Ansell, Akzo Nobel, Croda and SMEs alongside NHS partners to **develop** a wide range of antimicrobial technologies.*

The research approach

The Open Innovation Hub for Antimicrobial Surfaces (OPIHAS) led by Professor Rasmita Raval provides leading capability in the design and engineering of next generation antimicrobial surfaces and materials, combined with characterisation from the nanoscale upwards.

State-of-the-art surface imaging and spectroscopic techniques are combined with advanced bio-imaging and microbiology techniques to evaluate antimicrobial performance from the single-cell to the population level.

There is a strong focus on:

- Antimicrobial technologies to prevent, control and manage biofilms
- Smart materials for targeted/triggered responses;
- Approaches that mitigate the threat of AMR

Working in partnerships

OPIHAS brings together academic, clinical and industrial partners for accelerated translation of research into industrial innovation.

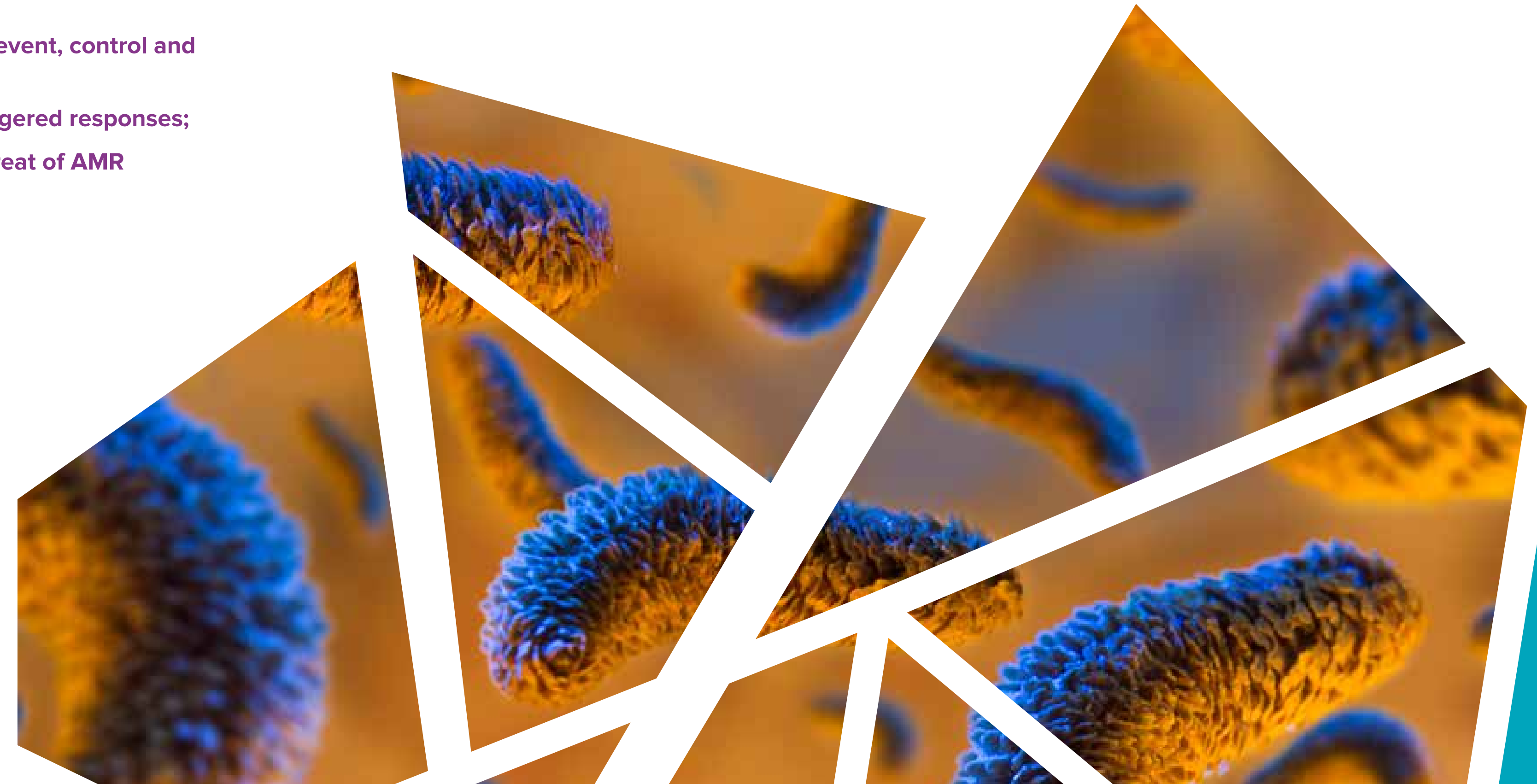
The Hub is actively working on innovative antimicrobial and anti-biofilm products via collaborative R&D projects involving partnerships with multinationals and SMEs in a number of sectors (healthcare, marine, food security, consumer products) via a portfolio of EU and Innovate UK Projects range from proof of concept through to Translation (TRL) 6/7 levels.

Outputs and outcomes

Our team has worked with market leading companies including Boots UK Ltd, De Puy Synthes, Smith & Nephew, Ansell, Akzo Nobel, Croda and SMEs alongside NHS partners to develop a wide range of antimicrobial technologies.

This innovation activity has led to patents and to a number of products progressing towards users.

Details of how to engage with OPIHAS are at:
www.liverpool.ac.uk/antimicrobial-surfaces/



Our Expertise

OUR FIELDS OF EXPERTISE

Energy and Catalysis:

Catalysis research in the Department ranges from industrially-sponsored applied programmes to catalyst discovery and fundamental studies on catalytic mechanisms.

Our expertise spans homogeneous, heterogeneous, photo, electrochemical and bio-catalytic systems and we utilise cutting-edge capabilities in Chemistry, the Materials Innovation Factory and the MicroBioRefinery. Energy is a key research theme, and strength of the University of Liverpool.

Chemists based in the interdisciplinary Stephenson Institute are playing a leading role in renewable energy research by developing the underpinning knowledge and new materials that are required for both energy storage and conversion with expertise across battery materials, solar fuels and thermal energy materials.

Our academics have specific expertise in the following areas: molecular and asymmetric catalyst design, mechanisms of catalysis, biocatalysis and biomass conversion including high throughput catalyst synthesis and screening, photocatalysis, electrocatalysis and electrochemical interfaces, heterogeneous catalyst design, energy storage (thermal and electrical).

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Functional Interfaces:

In Liverpool we are engaged in a wide range of projects in physical chemistry ranging from understanding the properties of nano-materials, achieving nanoscale control, design and assembly of function at surfaces to how proteins fold and to developing new energy technologies.

Our work ranges from fundamental understanding of physical chemical processes at the molecular and atomic level to developing new processes and products together with industrial partners.

We cover a wide range of applications including the control of functional interfaces for energy harvesting, catalysis and antimicrobials, the use of nanoparticles for medical diagnostics and therapy, single molecule electronics, electrocatalysis for energy applications and high-pressure and fluid processing research.

Our academics have specific expertise in the following areas: nanoparticles for use in medical diagnostics and therapy, high pressure chemistry and spectroscopy capabilities, molecular and nano-electronics, characterisation and study of molecules at surfaces, femtosecond processes at surfaces, surface modelling.

Contact: Professor Mathias Brust
M.Brust@liverpool.ac.uk

Medicinal and Bio-nano Chemistry:

The Medicinal and Bio-nano research cluster impacts many important areas of drug discovery, drug delivery and formulation research with targeted projects on the development of new drugs for infectious diseases, including malaria, TB, filariasis and Cryptococcus neoformans, and new therapies using existing drug compounds.

Recently the group has also expanded into medicinal chemistry programmes focused on chronic pain, pancreatitis, viral acute respiratory disease and breast cancer. The majority of these programmes include industrial partners.

The organic nanotechnology and nanomedicine group utilise exciting advances in controlled polymer synthesis techniques, liquid manipulation/ processing, and the generation of complex molecular architectures, organic nanoparticle dispersions and active/triggered particles within the Materials Innovation Factory.

These techniques are being applied to the design and synthesis of nanomedicines for the treatment of diseases such as HIV and cancer, aiming at improved oral delivery, long acting dose delivery and prophylactic approaches. These programmes are supported by global charities and industry. On-campus collaborations with the MRC Centre for Drug Safety Science, Life Sciences, Structural and Chemical Biology, Institute of Integrative Biology, Institute of Translational Medicine and the Liverpool School of Tropical Medicine further strengthens the group's impact.

Key academics across these collaborations have co-founded the British Society for Nanomedicine and the Wiley Journal of Interdisciplinary Nanomedicine. The cluster also has synthetic organic chemistry at its core including organometallic chemistry, development of enzymes for important industrial biotransformations, nucleic acid chemistry and peptidomimetic chemistry.

Our academics have specific expertise in the following areas: drug design and synthesis, chemical probe design and synthesis, synthetic organic chemistry, cheminformatics and molecular modelling, nanoformulation, organic materials design, materials chemistry, novel polymer design and synthesis with capabilities including ambient anionic polymerisation, atom-transfer radical polymerization (ATRP), RAFT polymerisation, branched vinyl polymerisation and conventional free-radical polymerisation, organic nanoparticle formation (solid drug nanoparticles and polymer-derived nanocarriers), characterisation and application.

Contact: Professor Paul O'Neil
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Materials Chemistry

The Liverpool Materials Chemistry group is a vibrant, internationally leading activity spanning the entire range of modern materials chemistry, publishing regularly in top journals such as *Science* and *Nature*.

We have made core fundamental advances in the discipline with the discovery of high-surface area porous molecules, the discovery of the highest transition temperature molecular superconductors, the discovery of new classes of oxide ion conductor and the demonstration of computationally-assisted materials discovery.

Our academics have specific expertise in the following areas: porous materials (including polymers, metal-organic frameworks, porous molecules), superconductivity, nanomaterials for biological and medical applications, unit cell by unit cell assembly of new solids as thin films, polymers for organic electronics, peptide-based materials, materials for energy applications (fuel cells, photocatalysis, batteries), polymer synthesis.

Contact: Dr John Claridge
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Theoretical and Computational Chemistry

Theoretical and Computational Chemistry research covers virtually all classes of problems regularly encountered in molecular science, namely, organic and inorganic materials and small molecules, interfaces involving molecular, metallic, semiconducting and insulating materials, biomolecules and drug discovery, soft-materials and polymers.

The methodologies used include high-level quantum chemical methods, solid-state physics method, classical atomistic simulation methods and coarse-grained approaches. The main applications reflect the current strength of the University of Liverpool and the interest of its collaborators, eg surface science and catalysis, materials discovery and energy research.

Our academics have specific expertise in the following areas: *models of interfaces (adsorption of molecule, reactivity, magnetic properties); computation of optical/magnetic/electronic properties of materials and biomaterials; high-throughput calculations of large dataset of hypothetical materials/compounds; cheminformatics and drug discovery; polymer simulations; materials oriented data-science and machine learning.*

Contact Professor Alessandro Troisi
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Our Facilities

OUR FACILITIES

Materials Innovation Factory (MIF)

Directors: Professor Andy Cooper & Simon Longden

The MIF aims to develop next generation functional materials for science and industry, accelerating the R&D process by up to 200-fold.

The unique nature of the MIF, created through a unique suite of state-of-the-art, open access facilities, provides a new template to allow researchers to work together and meet society's grand challenges whilst driving the UK's competitive advantage.

With computer aided materials science (CAMS) and high-throughput (HT) automation, new approaches to materials science and novel applications will be sought bringing materials chemistry into the 21st century; it is our belief that the benefits of large scale aggregation of automation, control and cognitive computing are limitless.

The MIF activity spans Organic Materials, Inorganic Materials, Nanomedicines, Sustainability, Genomic Sequencing and High Throughput Formulation/ Automation. It houses the Leverhulme Research Centre for Functional Materials Design to drive a design revolution for functional materials at the atomic scale by fusing chemical knowledge with state-of the-art computer science.

The MIF also houses the Liverpool contribution to the Henry Royce Institute, a national institute for materials science research and innovation underpinning the UK government's industrial strategy to drive economic growth.

For more information visit:

liverpool.ac.uk/materials-innovation-factory/about/

Surface Science Research Centre (SSRC)

Director: Professor Rasmita Raval

The SSRC was first established as a UK Interdisciplinary Research Centre (IRC) in 1989.

Our cutting-edge research aims to achieve nanoscale control, design and assembly of function using a broad equipment base comprising over 25 sophisticated spectroscopic and imaging techniques that allow surface events to be mapped at the nano lengthscale and down to the femtosecond timescale.

The research themes of the SSRC cut across the disciplines of chemistry, physics, biology and materials science, and combine the efforts of both experimentalists and theoreticians. The overarching ambition of our work is to achieve nanoscale control, design and assembly of function.

For more information visit:

liverpool.ac.uk/surface-science/

The Stephenson Institute for Renewable Energy (SIRE)

Director: Professor Laurence Hardwick

As a specialist energy materials research institute targeting leading edge research towards sustainable energy, SIRE focuses on the physics and chemistry that will transform the future of energy generation, storage, transmission and energy efficiency.

During our lifetimes, we can all expect to see major changes in the availability, price and supply of energy. SIRE is a group of twelve physics and chemistry academics and approximately 20 postdoctoral research staff plus nearly 60 PhD students. At any one time, we command about £18m of active research funding won competitively from the UK Research Councils, the European Union, scientific societies and from industry.

The SIRE researchers work to (i) develop enabling techniques and theory for the elucidation of underpinning mechanisms of energy materials (ii) discover new materials and catalysts for energy capture and conversion and (iii) identify improved materials and devices for energy storage.

For more information visit:

liverpool.ac.uk/renewable-energy/what-we-do/

Ultra Mixing and Processing Facility (UMPF)

Academic Lead: Professor Dmitry Shchukin

Emulsions offer an important product delivery format across a diverse range of market sectors from personal care and food to pharmaceuticals and paints.

The UMPF provides a world class facility with a unique capability to explore a broad range of alternative emulsion processing regimes that may minimise energy consumption and help reduce raw materials in feedstocks.

UMPF can generate pressures that are orders of magnitude higher than those used in conventional mixing technologies (up to 5000 bar). These are combined with innovative modifications of operational modes and geometries that exceed the scope of conventional rotor-stator devices (accessing speeds up to 50,000 rpm). This places the UMPF at facility the leading edge of emulsion science and sets new standards in fluid processing.

For more information visit:

liverpool.ac.uk/physical-sciences/facilities/facilities-and-services-for-hire/

MicroBioRefinery (MBR)

Director: **Professor Tony Lopez-Sanchez**

The MBR aims to identify and design the next generation of sustainable chemicals derived from agricultural, forestry and food residues and waste including the by-products of crops like wheat, corn, sugar, beet and other biomass sources.

The facility brings together academic and industrial expertise to bridge the gaps between identifying new sustainable chemicals in the laboratory, transforming and testing them in small quantities with the ambition of seeing them used by industry.

The facility consists of three laboratories with advanced capabilities and expertise in heterogeneous catalysis, biocatalysis, material sciences, biomass conversion, polymers and analytical chemistry. This is combined with high-throughput synthesis and characterisation equipment with full integration between capabilities.

For more information visit:

www.liverpool. ac.uk/micro-bio-refinery/facility/

Open Innovation Hub for Antimicrobial Hub Surfaces (OPIHAS)

Director: **Professor Rasmita Raval**

The Open Innovation Hub for Antimicrobial Surfaces (OPIHAS) is a dynamic multi-disciplinary initiative to develop new processes and technologies that will tackle the detrimental impact and economic burden of microbial activity on materials, surfaces and interfaces in UK industry and the urgent societal problem of increasing microbial resistance to existing antimicrobial treatments.

The Hub brings together a range of expertise, ideas, and resources to create a nucleation point for academic, clinical and industrial partners to share knowledge and innovation in the science of antimicrobial surfaces.

The primary focus of the Hub is the design and engineering of a new generation of intelligent surfaces and materials that are capable of inhibiting bacterial, viral, and fungal attachment and proliferation. A key goal for the hub is to stimulate growth and support business driven innovation in the UK economy and deliver sustainable antimicrobial innovation that has global societal impact.

For more information visit:

https://www.liverpool.ac.uk/antimicrobial-surfaces/about-us/

Radio Materials Laboratory (RML)

Director: **Professor Steve Rannard**

The RML is a bespoke laboratory able to work with long half-life radionucleides (mainly ^{3}H and ^{14}C).

The facilities allow either the synthesis of bespoke radio materials (organic compounds and polymers) or the handling of purchased radiolabelled materials.

RML activities include radiopurity analysis, the monitoring of materials in complex biological environments, monitoring pharmacokinetics in collaboration with colleagues from the Department of Molecular and Clinical Pharmacology, the study deposition or competitive deposition, of active ingredients in fully formulated products.

The facilities include radioTLC, radioHPLC, radioAF4, radioGPC, radioDLS, freeze drying, scintillation counting, quantification by sample oxidation and a class II bio cabinet to handle biological samples.

For more information contact:

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