

Biomedical Materials

VISION: To accelerate the discovery, manufacture and translation of biomedical materials through a platform of state-of-the art equipment, enhancing the UK position as an international leader in the fields of biomaterials and biomedical systems and devices.

UK LANDSCAPE AND ROYCE FIT

Additive manufacture is becoming more and more important in the biomedical materials area with applications in patient tailored implants and increased ease of manufacturing ability of complicated 3D structures which will assist in optimisation and validation of *in silico* functional designs. To significantly improve our international standing in this area HRI will commission new state of the art equipment that has improved resolution, speed of printing and ability to print in novel composites.

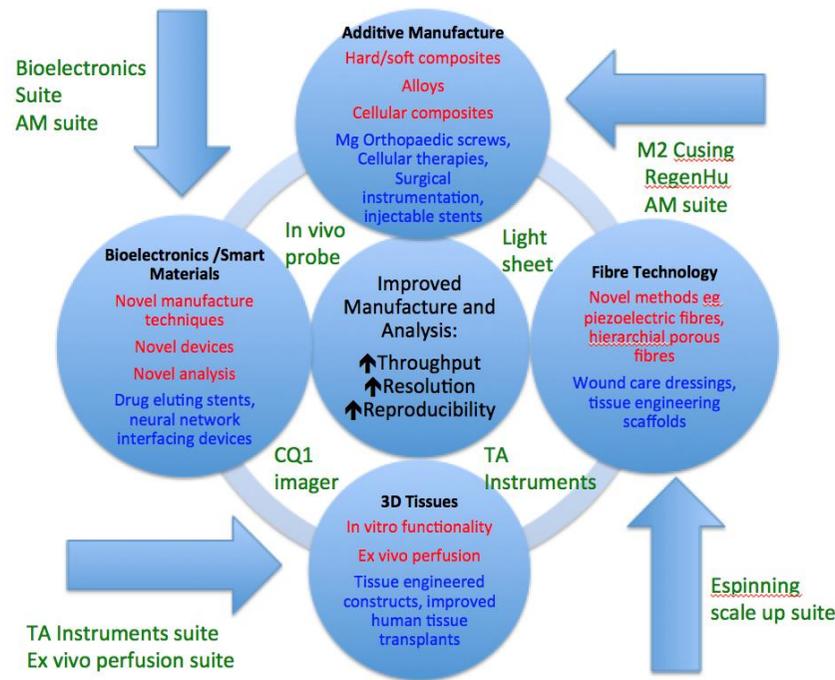
3D Printing / Additive Manufacturing

processes to include printing of hard materials (metals and ceramics), hydrogels/bio-inks, cellular materials, with improved resolution and speed of manufacturing.

Fibrous materials is a key growth area in biomedical materials due to its benefits ranging from increase in surface area and thus associated absorbency / controlled release profiles and its biomimicry relating to collagen fibre morphology. As an example, currently, for industry to scale up production of electrospun products for design validation, the manufacture has to be outsourced to companies outside of the UK such as Spain, South Africa or New Zealand. In addition, other

novel methods of fibrous material production are being developed and in particular UK SMEs would benefit from access to a novel suite in this area.

Fibre technology will also be a key focus, including process development of industrially scalable nanofibres



systems such as solution blow spinning, centrifugal, and electrospinning for hierarchical/graded structures. An underdeveloped but rapidly emerging research area in the UK is bioelectronics. In order to be a competitor in this area, bioelectronics and also development of smart materials that are able to adapt and respond

appropriately to their altering physiological environment are key growth areas.

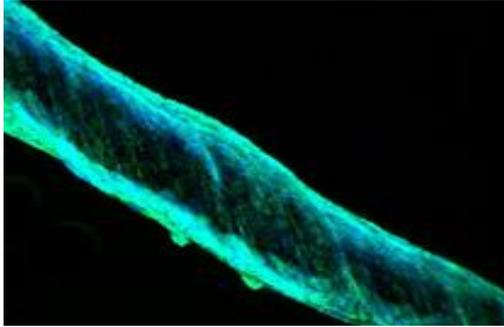
Bioelectronics and **Reactive/Smart materials** represents a step change from current biomedical reliance on 'non-smart' biomaterials (limiting longevity of medical implant) to 'smart' biomaterials for regenerative and precision medicine and remote sensing/monitoring (e-health). In addition, patient recovery is greatly enhanced when surgery is performed using keyhole rather than open surgery.

This clinically led move is an international focus in this field and thus to aid our UK position, a second focus of this HRI theme is:

Minimally invasive delivery of biomaterials and composites of soft/hard materials for tissue repair. This refers to surgical instrumentation as well as developing injectable biomedical materials such as novel hydrogels.

Within the UK there are many novel innovations in the field that are not translated or are very slow to translation (and thus not internationally competitive) due to the rate limiting step of

number of samples that are able to be manufactured, their reproducibility when being manufactured and also the rate at which these samples can be characterized (often n=1 sample at one time that takes one week for functional biological analysis).



Therefore one of the focuses of the biomedical materials theme are the following:

- **Scale up of novel biomaterials** currently being researched to 100-1000 sample production and their characterisation to aid their translation rate
- An improvement of **reproducibility of sample production** will also be a key area we will work on with our industrial partners
- Improvements of manufacturing processes to allow for **higher throughput** for material production, characterisation and testing, consider nanoscale to macroscale to create hierarchical structure

Many current animal models used by many biomedical materials scientists and pharmaceutical companies world-wide are not fit for purpose as they do not accurately reflect the physiological disease model or

Biomedical Materials

systemic configurations that occur in a human body. To address this, HRI will work with regulatory bodies and industry to develop improved models for this. A **3D tissue culture and functionality testing suite** will enable advances in this area. Another novel and internationally leading approach will focus on a **suite of perfused ex vivo systems** to sustain viability of both human tissues (eg lung, heart, liver, pancreas, kidney) and animal tissues (eg porcine limbs to emulate amputee patients).

KEY RESEARCH OUTCOMES/TARGETS

1. Bespoke hard and soft additively manufactured implants
2. New fibrous scaffolds for tissue regeneration
3. New bioelectronic systems
4. Faster biomedical device testing facility
5. Minimally invasive tissue repair
6. Smart materials for remote sensing/monitoring (e-health)

This novel suite will not only allow a fit for purpose testing suite on primary human tissue for our developing biomedical materials (thus aiding translation and impacting on improving regulatory

policy) but also will have a much wider impact on improving donor tissue morbidity and providing testing sites for pharmaceutical companies.

In addition it is anticipated that opportunity space discussions with larger companies will fall into the remit of **antimicrobial materials manufacture and testing facility**.



Strategy Working Group

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Prof Brian Derby, School of Materials (Manchester)

Prof Jonny Blaker, School of Materials (Manchester)

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Nuclear Materials Research Landscape

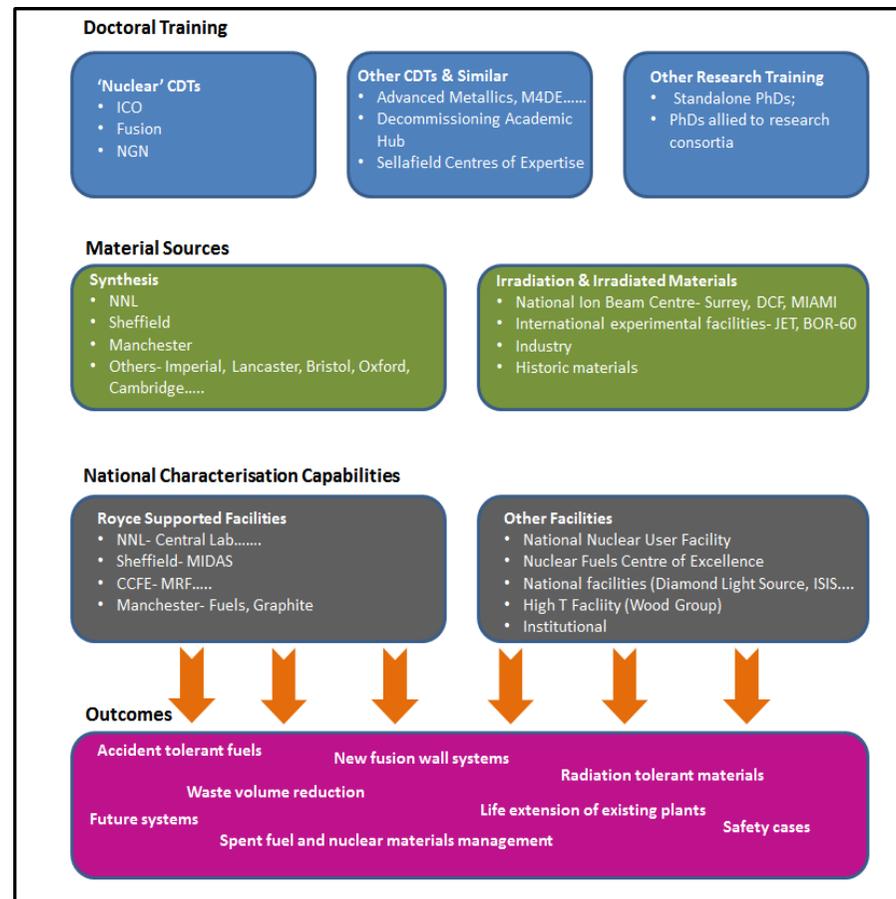
VISION: To facilitate experimental research on authentic irradiated and nuclear materials, particularly work which cannot be done in normal university facilities (e.g. with transuranics, high specific activity fission and activation products, irradiated materials).

UK LANDSCAPE & ROYCE FOCUS

The UK has a range of large nuclear programmes spanning the civil and defence sectors. Major elements include new build fission reactors (£ 50-60 bn for the first three stations alone; duration now to ca 2100), decommissioning and cleanup (£ 115 bn; now to ca 2030), geological disposal (£ 15 bn; now to beyond 2100), and fusion (in Europe, £ tens of bn over the next 30 years). There are also longer term options (e.g. Small Modular Reactors, Generation IV).

The nuclear core area will focus on whole-life management of materials associated with or originating in high neutron flux environments (e.g. in fission systems: reactor pressure vessels, the primary cooling circuit, in-core materials, used fuel and material derived from it; plasma facing materials in fusion). Within this broad area, two subsidiary themes can be identified.

- Improved fuels and fuel cycle materials;
- Structural materials for fission and fusion



both of which will need testing in active environments.

Challenges in Legacy and Current Systems- AGR and worldwide life extension of LWRs including Sizewell B; Spent fuel management, particularly AGR fuel and cladding being managed as waste; HLW glass disposability; Graphite waste management; Managing nuclear materials (Th, U and particularly Pu)
Challenges in Future Systems- Accident-tolerant and/or high burnup fuels and associated cladding; Small Modular Reactors; Fusion reactor materials; New build LWRs, particularly ABWR; Generation IV.

AIMS & BENEFITS:

- support experimental work relating to radioactive materials across the UK, and foster experiment-with-modelling studies to extract maximum value from expensive and difficult experiments;
- facilitate and support student and young researcher access;
- work with other national facilities (e.g. DLS, ISIS, NNUF) and key stakeholders in the nuclear sector (e.g. NDA, EdF Energy, Horizon, NuGen, Rolls-Royce, Westinghouse, ONR).

- position Royce as a partner in the nuclear materials research facilities; and
- broaden the Royce nuclear user community.

EXAMPLE OPPORTUNITIES

- Accident-Tolerant Fuel (with M4DE Core Area). In a loss of coolant accident, the zircaloy cladding in LWRs can react with water to generate explosive hydrogen, as in Fukushima. Development of modified, 'accident-tolerant' LWR fuels would greatly increase the resilience of fuel in a severe accident.
- Materials for the Plutonium Lifecycle (with

Nuclear Materials Research Landscape

community of international M4DE Core Area). The UK holds the World's largest stockpile of civil Pu, which will have to be stored as PuO₂ for some decades before end use. The container materials, the evolution of the PuO₂ itself, and the final form(s) of the Pu, whether waste or fuel, all present long term materials science challenges which have to be resolved in order to underpin stewardship of the material.

- Structural Materials for Advanced Fission and Fusion Systems (with M4DE Core Area). Future nuclear reactors may be very different from current ones, and structural

materials may be exposed to very high radiation doses and heat loads, and/or to novel coolants (molten salts, molten metals) for very long periods. If these reactor concepts are to be implemented, it is essential to build confidence in these structural materials.

KEY RESEARCH OUTCOMES/TARGETS

1. Radiation damage tolerant materials
2. Robust safety cases
3. Reactor life extension
4. Spent fuel and nuclear materials management
5. Future nuclear technologies



Strategy Working Group

Theme Champion Francis Livens, Dalton Nuclear Institute (Manchester)

Neil Hyatt, Department of Materials Science and Engineering (Sheffield)

Marin O'Brien (UKAEA)

Jonathan Hyde (NNL)

Other members to be added after the meetings on 9th and 10th January 2018

2D Materials Research Landscape

VISION: To develop a new paradigm of functional materials on demand and devices fabrication technologies based on atomically thin layers of two-dimensional (2D) crystals

UK LANDSCAPE AND ROYCE FIT

2D materials were pioneered in the UK, and are an area where the UK has internationally led the fundamental science. The EPSRC, EU Graphene Flagship and InnovateUK have built a strong science base in the UK through a series of dedicated calls. Activities in 2DM involve research groups at Manchester, Cambridge, Leeds, Oxford, ICL, UCL, Exeter, Lancaster, Warwick, Sheffield, Harriot Watt, Glasgow, Nottingham. In 2016-2017, UK community have run 8 events on various 2DM topics, involving both academia, industry and training (4 organised by HRI partners UoM and UoC).

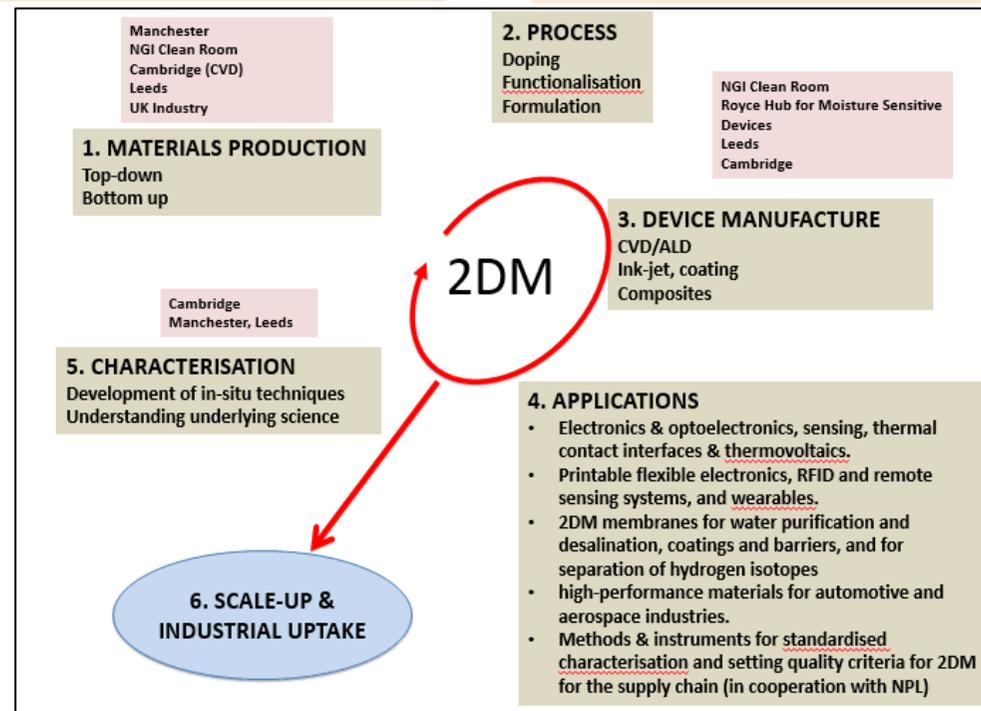
Over 70 UK and multinationals companies from the following sectors have expressed interest in developing technologies based on the use of 2D materials:

- Aerospace (ATI)
- Automotive (especially, mobile energy systems)
- Bio-Medical and Healthcare

- Chemical
- Electronics (including printable flexible, packaging, heat management systems)
- Optoelectronics (incl communications systems)
- Membranes for water desalination
- Instrumentation and tooling

Characterisation and device fabrication facilities at Manchester, Cambridge, Leeds, Oxford, ICL, Warwick, Sheffield in HRI and UCL, Exeter, Lancaster, Harriot Watt, Glasgow, Nottingham beyond HRI. Outside HRI, suitable spectroscopic facilities are available at Diamond.

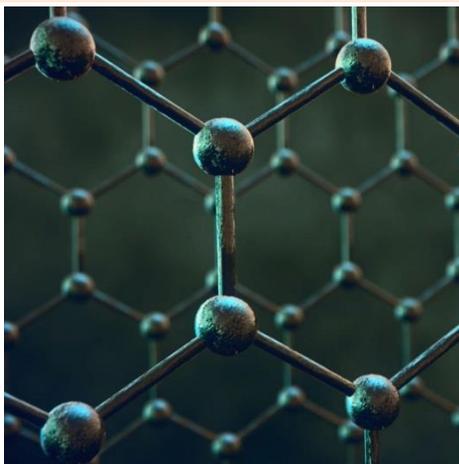
In general, UK lacks dedicated growth effort of materials beyond graphene. While UoM, UoC and Nottingham have facilities for CVD and even MBE growth of graphene, UK capability to grow other 2DM (those with optical functionalities) are almost absent and are definitely inferior to the capabilities built in China, South Korea, and USA.



2D Materials Research Landscape

FUTURE OPPORTUNITIES

- A good chance to develop new generation of electrodes for batteries (graphene-based).
- Niche application of graphene, hBN and other 2DM membranes for H/D/T isotope separation.
- Use 2DM to offer new electronic devices for applications in quantum technologies.
- Collaboration with graphene and 2DM research Centres in China would offer an access to a complementary materials base.



KEY RESEARCH OUTCOMES/TARGETS

1. To fabricate and characterise atomically thin (2D) materials and their heterostructures, aiming to identify their properties suitable for applications in electronics, optoelectronics, and sensing.
2. To develop new prototype electronics and optoelectronics devices based on 2D materials.
3. To create nanocomposites where such two-dimensional materials are implemented to enhance properties of materials already used on products and manufacturing processes (polymers, epoxy, resins, enamels, etc.).
4. Develop new materials for energy mobile storage, energy harvesting, water desalination and separation of gases.
5. To use 2D materials to develop inks and new printable flexible electronics technologies, and functional coatings.

Theme Champion Vladimir Falkos, School of Materials (Manchester)
Prof Ian Kinloch, School of Materials (Manchester)
Sir Prof Konstantin Novoselov, School Physics & Astronomy (Manchester)
Prof Rahul Raveendran nair, School of Chemical Engineering & Analytical Science (Manchester)

Prof Robert Dryfe, School of Chemistry (Manchester)
Prof Andrea Ferrari, Cambridge Graphene Centre (Cambridge)
Prof B Hickey, School of Physics and Astronomy (Leeds)

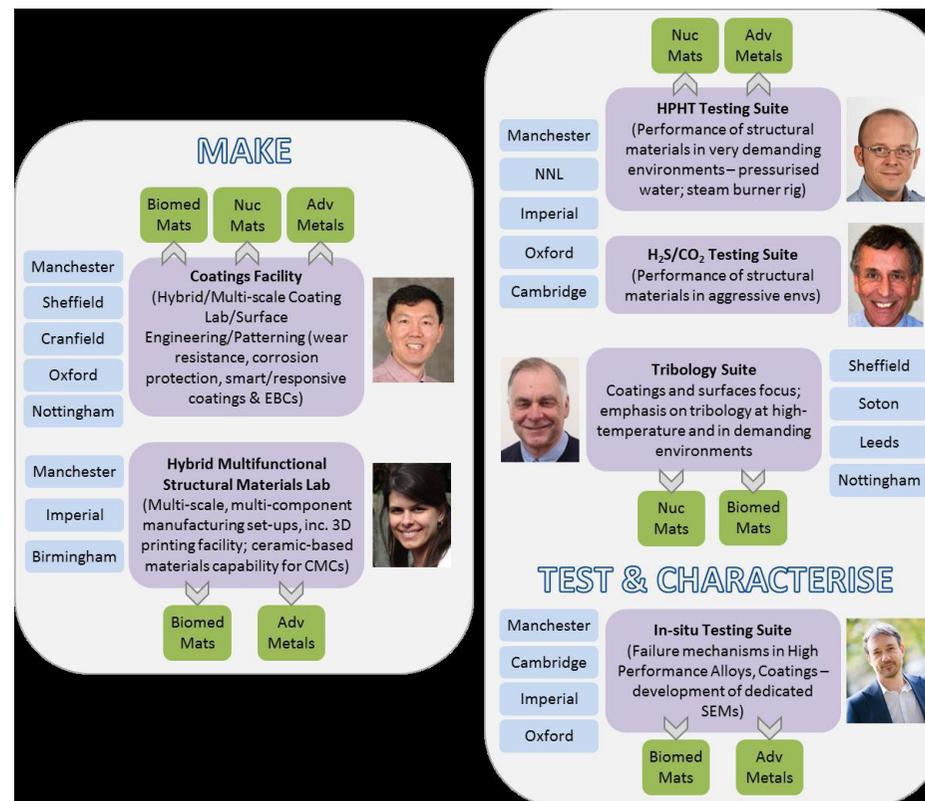
Material Systems for Demanding Environments Research Landscape

VISION: To design, *make*, *characterise* and *test* new materials systems for demanding environments, supporting energy, transport and other sectors. Emphasis will be placed on developing protective/smart coatings, and hybrid material systems, with the ambition of widening the parameter space in which structural materials can be used.

UK LANDSCAPE & ROYCE FOCUS

The vision is that M4DE will enhance the broader UK demanding environments R&D landscape in the following three key areas:

Make. Providing additional coating and hybrid material manufacturing capability to the UK. Planned procurement in this area focuses on adding to, and complementing, existing UK capabilities, with a view to creating unique facilities without duplication. The exact nature of the facility is being developed through close, continuous community and stakeholder engagement. For this reason, for example, certain large-scale items of plasma spray equipment have been agreed as unnecessary due to existing capabilities at Oxford (HRI partner institution) and Nottingham.



Test. Providing an extensive range of test environments to replicate demanding environment conditions. These will focus on testing at high temperature and high pressure, and in H₂S and CO₂ environments, as well as through the development of high-temperature tribological testing capabilities. Manchester already has leading testing capabilities, including a large autoclave suite and a bespoke H₂S laboratory. Investment here will expand this capability considerably, creating a UK user facility for demanding environments testing.

Characterise. Lead in the development of new/novel in-situ testing capabilities. This will be undertaken in close collaboration with microscopy OEMs, and so will be of benefit not only to industrial (and other) stakeholders, but will also put the UK at

the forefront of equipment development. The capability developed will be of

Material Systems for Demanding Environments Research Landscape

benefit to a range of research partners in the M4DE theme and beyond, in other themes and at a range of institutions.

ANTICIPATED OUTCOMES AND PRODUCTS:

A unique UK facility for the production, deposition and testing of coatings.

Key focus on new coatings for components exposed to demanding environments, stimulating a critical mass of people and research in the area, focused around HRI. Example product: Thermal and Environmental Barrier Coatings (TBCs/EBCs) for power generation and transport applications (to TRL-4).

Development of a **novel, bespoke tribology suite**, for the testing, analysis and development of coatings and surface treatments, distinguished from current UK capability by the emphasis on tribology at high-temperature and in demanding environments. Example products: high-temperature fretting in jet engines (e.g. Fir tree root); valve seat surfaces in power generation (high temperature galling, such as in a nuclear plant).

Set-up of a **hybrid multifunctional structural materials Lab**, exploiting the latest developments in multi-scale, multi-component and 3D printing to design and make hybrid materials solutions across the themes of *M4DE*, *Biomedical Materials* and *AMP*. Example product: corrosive media filters for petrochemical plants made of hierarchical ceramic-based hybrids, giving improved filtration efficiency, durability, reduced costs and optimised plant performance.

Significant expansion of **HPHT testing and H₂S/CO₂ labs**, in order to create a

UK centre of capability in testing for harsh and demanding environment. Example product: improved understanding of degradation mechanisms of reactor pressure vessel (RPV) steel enabling life extensions of future reactors.

In-situ testing and degradation characterisation capabilities. Developing in-situ testing stations that enable a new approach to imaging during mechanical

loading in various environments. Example product: Develop damage tolerant microstructures for aerospace, nuclear and oil & gas sector, support development of coating for accident tolerant fuel cladding that can sustain dimensional instability of Zr cladding substrate.

The engagement working groups will be formally kick-started with forthcoming workshops on: Coatings; Tribology (possibly to be combined with the above); Hybrid Multifunctional Materials; Materials testing in demanding and aggressive environments; In-situ testing and characterisation.

KEY RESEARCH OUTCOMES/TARGETS

1. To develop **structural material solutions and systems**, and **improve existing materials** to enable a 'step-change' in component development, for application in aggressive environments.
2. To develop materials systems that will **exceed the capability** of advanced metals, or protect these.
3. To provide/develop **testing and characterisation capabilities** for the evaluation of structural materials in demanding environments.
4. To provide fundamental **understanding of degradation mechanisms**.

Strategy Working Group

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Prof Anne Neville, School of Mechanical Engineering (Leeds)

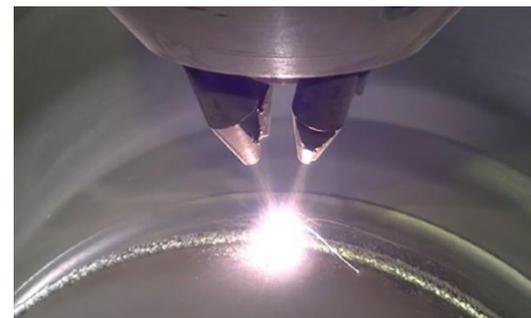
Advanced Metals Processing Research Landscape

VISION: To provide a step change in the discovery, manufacture and translation of new resource efficient metallic alloys to enhance the UK position as an international leader in metals processing.

UK LANDSCAPE AND ROYCE FIT

The UK has considerable strength in metals processing. Metallurgy and metals processing is going through period of rapid change driven by the need to improve their performance in-service but also by the socio-economic drivers of reducing process waste and emissions. To address these challenges the overall objective of the Advanced Metals Processing theme is to establish a world leading facility for metals discovery, processing, characterisation, upscaling and manufacturing. The focus will be on metals process innovation in the "missing gap" between small-scale laboratory metals processing and the industrial scale. It will address the key themes of materials discovery, resource efficient materials manufacture, light weighting, flexible manufacturing, prototyping and production scale-up.

The SHRI partners have long-standing international research strength in metals processing and manufacture and industrial translational strength through our ca. 45 major industrial partners and through the links with the HVM Catapults, namely the AMRC, NAMRC, MTC and AFRC. Both the Sheffield and Manchester branches of the SHRI will be in a purpose-designed facility for materials processing and characterisation and will deliver unique integrated facilities around the following themes:



Materials Discovery and Prototyping: Materials discovery has largely progressed through trial and error; this approach is being challenged by large scale activities such as the Materials Genome project in the US. We will combine Computational Materials Design, High-Throughput (HT) materials discovery and rapid scale-up and material property screening to deliver a step change in the way that novel materials are developed for specific applications.

Powder production: Many of the key near-net-shape manufacturing technologies of the future are becoming increasingly dependent on alternative feedstock forms, such as powder and wire, where the quality of the feedstock material is a major factor in determining the product quality. Near Net Shape technologies will require alloys designed specifically for these resource-efficient process routes. This will require the production of bespoke alloys in the form of small powder batches, which can then be evaluated directly in the various NNS processing technologies.

Advanced Metals Processing Research Landscape

Near-net-shape manufacturing technologies: Net and Near Net Shape (NNS)

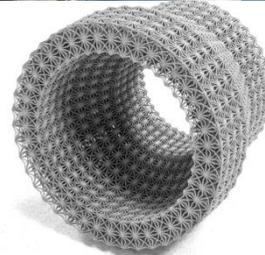
manufacturing technologies have the potential to disruptively displace

existing technologies. A move towards NNS methods, for example, through Additive Layer Manufacturing will be a critical part of this strategy to help conserve raw materials, reduce the material/energy per unit volume and improve competitiveness. ALM now covers many technologies, including powder bed, blown powder, wire feed etc., which allows manufacturing on-demand. The Royce facility will be absolutely at the front of this technology.

Advanced Materials Manufacturing: The focus is on the introduction of new resource efficient, sustainable, lightweight materials and processes for modern manufacturing technologies. The research will sit at the interface between manufacturing technology and materials processing science to better control material form, integrity and function and hence economic value. It will exploit the ability to locally tailor microstructure and therefore properties by embedding materials engineering in the process.

Agile forming technologies: Agile manufacturing requires the production of complex shapes without fixed tooling. There are a number of processes that are being developed in this area that have the potential to be disruptive. Topics targeted include: High temperature incremental forming of

titanium aerospace components; Precision guided flexible warm forming of high strength Al and Mg sheet; 3D Roller forming with thermal assistance; Near net shape forging with adaptive tooling.



Working with Low Cost and Scrap Material Streams: There is a need to devise “cradle-to-cradle” strategies for high value materials streams. As an example, for additive processing to realise its full economic potential, high-cost metal powders, such as titanium, gradually pick up contaminants such as oxygen. This degraded material could be used to produce a more impurity-tolerant part, such as through the use of continuous rotary extrusion to obtain high quality wire, for applications such as low cost, low density springs for automotive applications.

Theme Champion Prof W Mark Rainforth, Department of Materials Science and Engineering (Sheffield)
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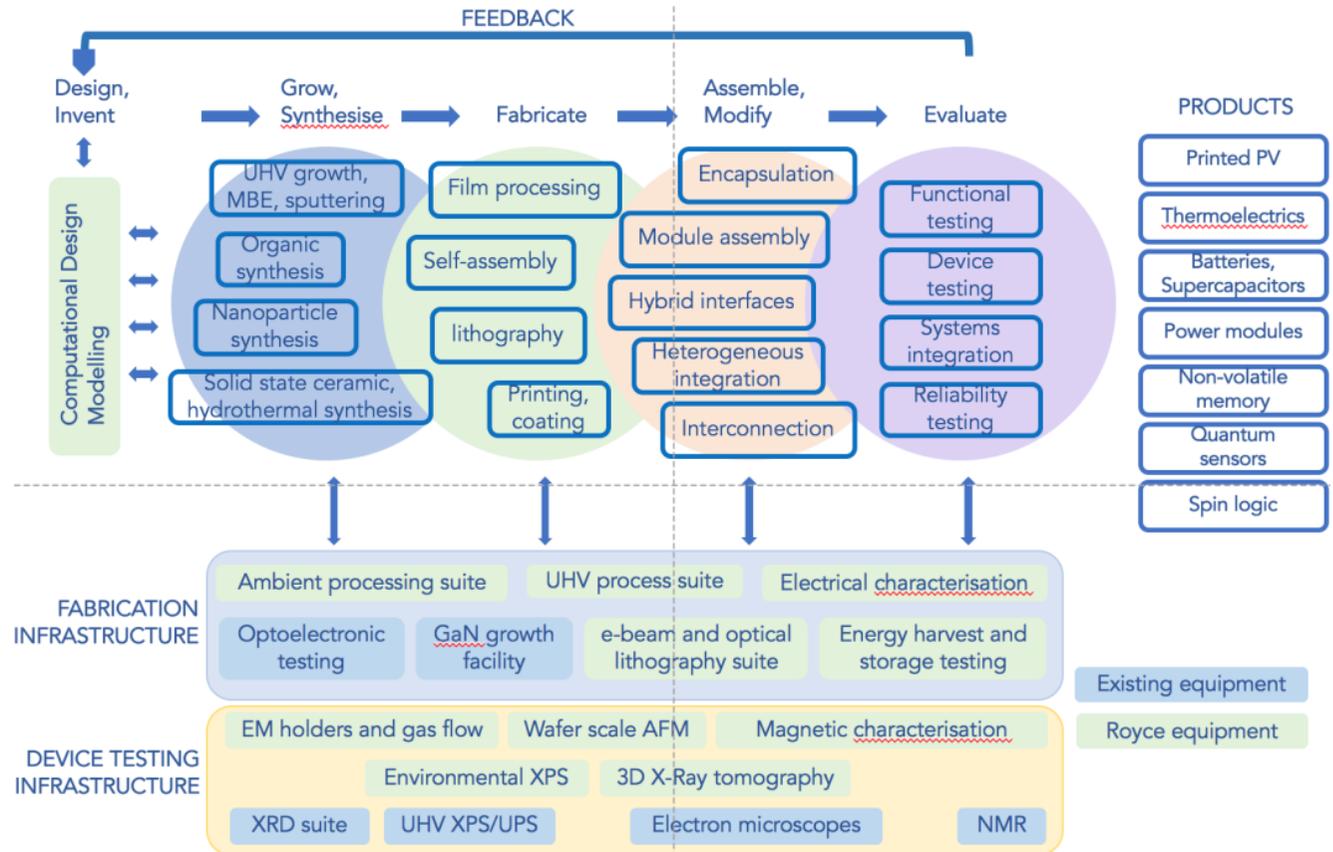
Materials for Energy-Efficient ICT Research Landscape

VISION: Development of new materials and integrated materials systems to lead to breakthroughs in efficient energy generation, energy storage, and energy use, to power the next generation of ICT devices

UK LANDSCAPE AND ROYCE FIT

The field of ICT offers a tremendous opportunity for radical technology changes, most of which will be driven by energy efficiency. Current technologies for energy usage, energy generation, and energy storage all operate way below fundamental limits set by thermodynamics. There is huge potential to introduce radical changes in energy materials systems. The Cambridge Royce facilities act as a national centre for Materials for Energy-Efficient ICT.

Materials for Energy Efficient ICT is one of the University of Cambridge's Energy Grand Challenges, and efficient generation, storage and use of energy is the performance metric for most emerging ICT technologies, ranging from very large data farms to autonomous 'internet-of-things' remote sensor devices. Cambridge Royce will provide and support a broad user facility for materials growth and characterisation, for novel materials device fabrication and testing, and for system level demonstration of new ICT functionalities. Materials for Energy Efficient ICT will go beyond our traditional focus on new



materials/devices and take steps towards system integration. This will allow a more rigorous evaluation of the performance and capabilities of new materials/device technologies within an

energy efficient ICT system, aid the identification of application opportunities and accelerate their industrial exploitation.

Materials for Energy-Efficient ICT Research Landscape



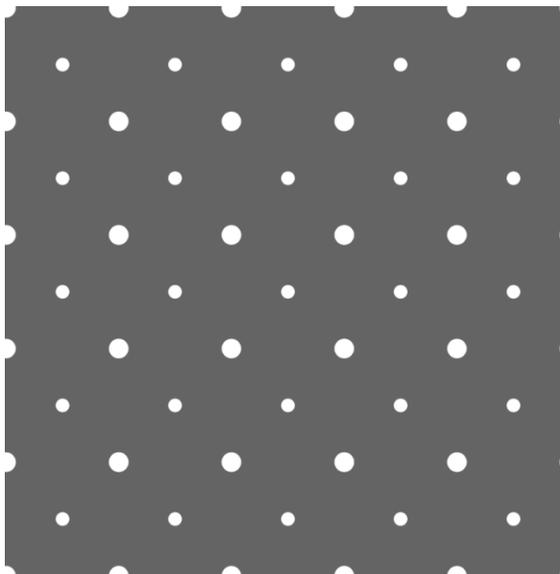
Cambridge Royce facilities act as a national centre for Materials for Energy-Efficient ICT.

Efficient energy generation, energy storage, and energy use is the performance metric for most emerging ICT technologies, ranging from very large data farms to autonomous *Internet of Things* remote sensor devices.



Cambridge Royce comprises ten equipment suites:

1. UHV deposition/processing suite
2. Wafer-scale scanning probe suite
3. Ambient processing cluster tool
4. Environmental XPS/UPS suite
5. Electron beam/optical lithography
6. *In situ* electron microscopy
7. High-resolution 3D X-ray CT
8. Energy harvest/storage test suite
9. HV/HF device testing suite
10. Magnetic characterisation suite



Cambridge Royce supports a broad user facility for materials growth and characterisation, for novel materials device fabrication and testing, and for integrated system-level demonstration of new ICT functionalities.

The facilities are selected to provide versatility so that new and unexpected areas can gain fast traction to accelerate commercialisation.

Energy Storage Research Landscape

VISION: To enable and stimulate significant advances in high quality basic science and will accelerate the generation of important technologies for translation to industry.

UK LANDSCAPE & ROYCE FOCUS

Across the globe, automotive companies and those countries whose economies rely on them are addressing the challenge of the transition to all electric vehicles in order to drive reductions in local and global pollution. Those economies who manage this transition effectively will secure their prosperity and generate new export opportunities for wealth creation and growth. The UK automotive industry provides 800,000 jobs, 25% of Europe's electric vehicles and hybrids and £25bn of exports, and the UK has the opportunity to become Europe's leader in electric propulsion. Many of the same energy storage technologies will also enable greater penetration of renewables onto the UK energy grid, which has strategic and economic benefits as an island nation with significant wind and wave energy capacity. However, the UK faces fierce international competition in the race to develop these energy storage technologies and is currently too reliant on non-UK battery manufacturing expertise and facilities. Insufficient diversity of training and skills in energy storage materials and related technologies will also increasingly undermine UK competitiveness. The Royce Institute research will focus on electrochemical energy storage technologies

(batteries and supercapacitors) as well as thermoelectric and piezoelectric devices. Advances in these technologies are particularly dependent on advances in underpinning materials science, and their related synthesis and manufacturing technology. This focus recognises that we cannot be world

leading in every area of energy storage but we can in electrochemical energy storage technologies, thermoelectrics and piezoelectrics, where we can build on a track record of world-class excellence.

AIMS & BENEFITS

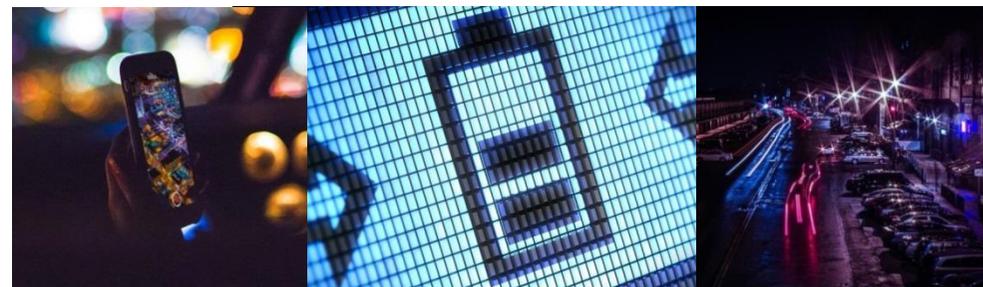
- Integrate UK research excellence in energy materials
- Critical mass of inter-linked science, technology, manufacture and translational
- Collaboration and co-ordination across university and commercial sectors
- Sharing and accessing state-of-the-art facilities and know-how

	Materials discovery	Materials properties & characterization	Electrode, electrolyte & device optimisation	Scale-up & testing	Industrial partners, end-user pull-through
Li-ion, Na-ion batteries	New solid electrolytes & electrodes (Liv, Ox)	Conductivity, voltage, capacity, stability, cycle & calendar life (All)	Composite electrolytes, hierarchical/ graded electrodes (ICL, Ox)	A5 cells & electrode manufacture, cycle life (ICL, Ox)	Innovate UK Automotive Council
Beyond Li-ion batteries	Materials, electrodes & electrolytes (Ox, Liv, Cam)	Capacity, stability, cycle & calendar life (Cam, Ox, Liv, Man)	Porous gas diffusion & protected electrodes (ICL, Ox, Cam, Liv)	Lab-scale demo stacks, rate testing, fading & life (ICL, Ox)	Advanced Propulsion Centre
Redox flow batteries for the grid	Materials, membranes, redox couples, electrolytes (ICL, Ox)	Separator cross-over, redox potentials, solubility, stability (Cam, Ox, Liv)	Membrane conductivity & transport, electrolyte flow (ICL, Ox)	Lab-scale electrode & separator manufacture, life (ICL)	Supergen ES Hub Industry
Thermo-electrics	Thermoelectric materials (Shef)	Seebeck, transport and energy props (Shef)	Ceramic processing, bulk/gb properties (Shef)	Device manufacture (Shef)	Faraday Challenge
Super-capacitors	Metal oxides, MXenes, electrolytes (Ox, Shef)	Surface props, high power testing (Ox, Shef)	Asymmetric-hybrids, layered electrodes (Ox, Shef)	A5 cells (Ox)	Faraday Institution JCESR (US)

Timeline

- Beacon for UK energy storage materials
- Innovation pipeline for UK industry

Energy Storage Research Landscape



Areas of anticipated breakthroughs enabled by the Royce Institute are:

- Electrode materials for lithium and sodium batteries delivering advanced performance at lower cost Structured electrodes for lithium and sodium batteries
- All solid-state batteries
- Electrode/electrolyte interfaces
- New electrode structures for redox flow batteries
- Novel redox flow architectures
- Electrode manufacture for supercapacitors and batteries
- Thermoelectric materials and devices
- Establishing state-of-the-art facilities for the characterisation of battery materials and interfaces, including many operando characterisation facilities, NMR, XRD, TEM, SEM, mass spectroscopy.

KEY RESEARCH OUTCOMES/TARGETS

1. UK facility for synthesis and characterisation of air sensitive materials for Li and Na ion batteries
2. Improved redox flow batteries for the grid
3. Materials for solid-state batteries; prototype devices
4. Higher energy density supercapacitors for automotive and other applications
5. Improved thermoelectrics
6. Strategic alignment with emerging Faraday Institution for UK battery research
7. New generation of energy storage materials and energy storage device scientists and engineers

Theme Champion Prof Peter Bruce, Department of Materials (Oxford)

Atoms to Devices Research Landscape

VISION: To deliver significantly enhanced and novel properties, with their utilization in devices enabling new technologies. The functional materials, films and device application areas cover almost all industrial sectors and particularly ICT, Healthcare and energy.

UK LANDSCAPE and ROYCE FOCUS

The UK has very strong research in the general area of functional materials. In the Royce core partners EPSRC current grants in the A2D area exceed £80M.

Functional materials are found in all classes of materials: ceramics, metals, polymers and organic molecules. Functional materials are often used in electromagnetic applications from KHz to THz, and at optical frequencies where the plasmonic properties of metals assume particular importance. Functional materials are also of critical importance in materials for energy such as electro- and magnetocaloric materials, for energy storage and for solar harvesting functions. The term is very broad and practically every industrial sector – automotive, marine engineering, aerospace, electronic – rely on functional materials to deliver products.

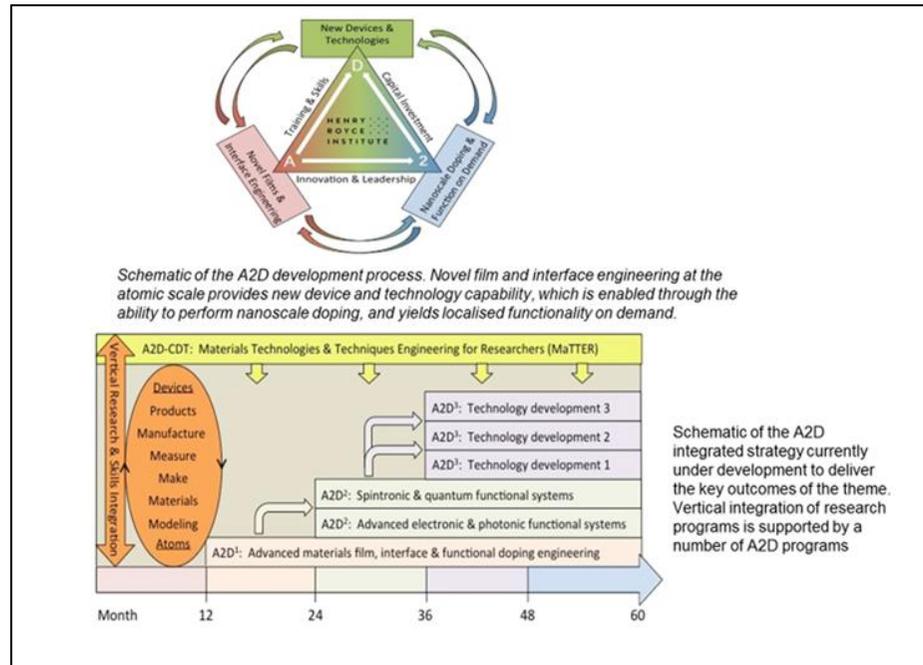
Smart materials (a subset of functional materials) have properties that enable them to adapt or mitigate a change in their environment and communicate that a change has taken place. This means that one of their properties can be changed by a stimuli from an external environment e.g. pressure, temperature, light, chemical, magnetic or electrical. These stimuli then trigger a pre-designated course of action such as, but not limited to, self-healing

through a smart coating. Increasingly the triggering stimuli which causes the pre-designated course of action is linked to some form of sensory capacity which enables the material to signal that a change in the environment has

taken place audibly, optically or electronically, or a combination of these. For a good overview of nanomaterials/nanotechnology in particular see the Genesys report <http://www.nanowerk.com/nanotechnology-report.php?reportid=136>.

The range of application sectors is correspondingly large, including: information and communications, and electronics, health and energy. Perhaps the greatest contribution in the area of functional materials is in Information and Communication Technologies (ICT) but of course the areas extend well beyond ICT. The market size for this area alone is in the region of \$4 trillion with AGR (annual growth rate) of around 4.8%. The UK's Photonic Leadership Group report (2013) estimates photonics to be worth £10.5

billion to the domestic economy; plasmonics and metamaterials are cited as key new technology enablers. Finally, A2D will engage with the UK effort on Quantum technologies both at low temperature and at room temperature. Indeed, A2D is well placed to take advantage of forthcoming investments in Quantum Technologies.



Atoms to Devices Research Landscape

ROYCE A2D: RESEARCH TARGETS

Oxide or Nitride/Metal Heterostructure systems:

- prediction of improper ferroelectrics with novel spin structures (theory leading, growth demonstrating)
- control and modelling of ferroelectric domain walls (growth with characterisation input to develop materials systems and methods for later demonstrator device development).
- ferroelectric based memristors for cognitive computing (growth supporting device fabrication for demonstrator/prototype devices).
- development of magnon spin current devices (materials growth supporting characterisation and device design).
- refractory nitrides for temperature tolerant routing and manipulation of light at the nanoscale
- energy efficient ICT exploiting giant piezomagnetism in spin frustrated Mn nitrides

KEY RESEARCH OUTCOMES/TARGETS

To coordinate A2D research across Royce and other UK partners

1. To ensure that the capital equipment within Royce partners and beyond can deliver the structures required
2. To make new materials and device discoveries capable of translation to industrial partners
3. To protect intellectual property and to assist industrial partners to develop new technologies
4. To take advantage of new funding streams in the A2D theme (e.g. Quantum Technologies)

Oxide/Organic Systems

- ferroelectric/semiconductor hybrids with high PV effect & high stability/long lifetime (theory lead, growth demonstrating for potential future development to devices).
- integration of organics and inorganics – controlling and coupling charge transport across organic/ferroelectric interfaces – leading to programmable emergent phenomena

(growth leading with theory and characterisation support).

- Organic maser media

Metals/Organic Heterostructure Systems

- hybrid materials, e.g. low spin orbit coupling in organics (theory and growth to produce demonstrator materials for future incorporation in device structures).
- improving Coercive fields in non-rare earth magnetic materials (growth and characterisation with input from theory).

Inorganic Functional Systems

- Diamond/SiC/ZnO defect states for quantum technologies

Metals/Topological Materials Systems

- hybrid materials, e.g. high spin orbit coupling into superconducting and magnetic systems to develop materials for quantum technology applications – strong interaction with 2D materials theme in Royce and into Quantum Technology hubs (requires significant materials development as well as characterisation and theory input).

Theme Champion Prof Neil Alford, Department of Materials (Imperial)

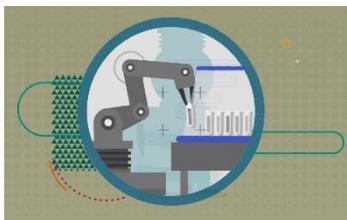
Theme Champion Prof Edmund Linfield, School of Electronic and Electrical Engineering (Leeds)

Prof Richard Curry, School of Electronics and Electrical Engineering (Manchester)

Professor David Ritchie, Department of Physics (Cambridge)

Chemical Materials Design Research Landscape

VISION: To drive scientific excellence, strongly integrated with industrial exploitation, and link together the world premier groups in the UK to maximise return on investment. By creating sustainable international leadership in chemical materials design allowing the UK to discover new step change functional materials, thus driving inward investment and economic growth.



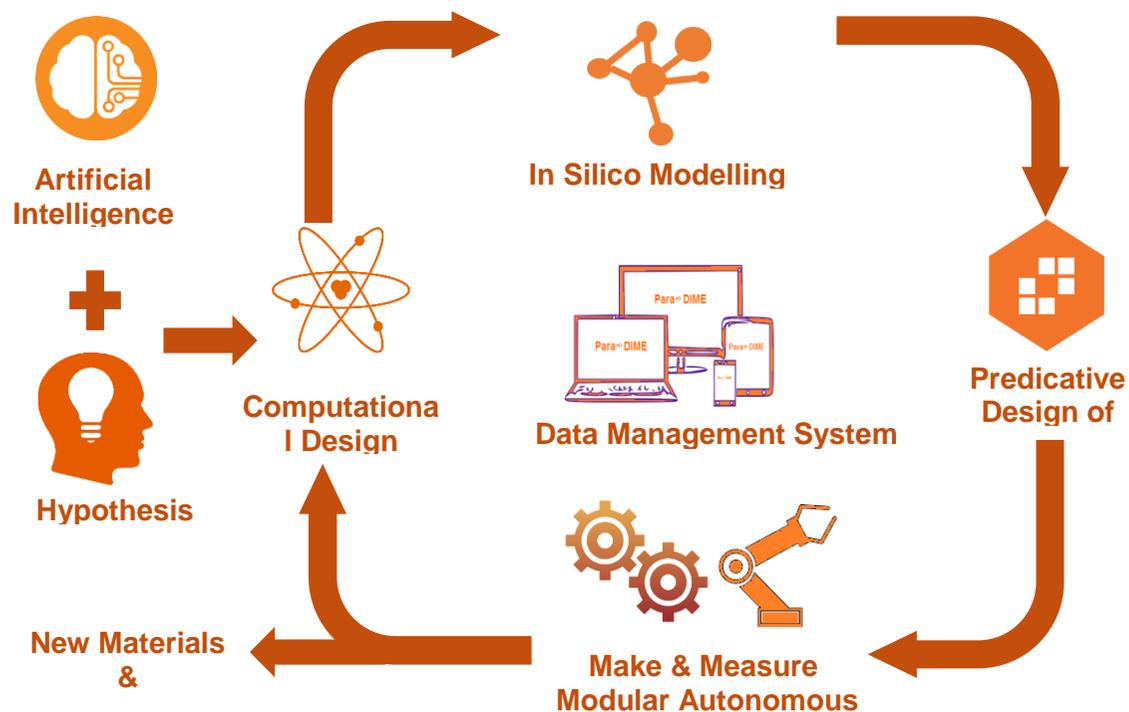
UK LANDSCAPE AND ROYCE FIT

The Royce Laboratory in Liverpool addresses one of the key components of the UK's present industrial strategy Advanced manufacturing. The UK's global economic competitiveness is, and will remain, underpinned by the ability to innovate in materials, new systems and technologies which can be applied to a wide range of specific manufacturing sectors.

Potentially, this is as revolutionary as the original invention of the factory at the end of the eighteenth century. But in the twenty-first century, the concept of a 'factory' will need to be quite different to that established by the pioneers of the Industrial Revolution if wealth creation is to be sustained against global Competition and in the face of environmental and sustainability pressures. This also presents the UK with a great opportunity to reinvent its concepts of advanced manufacturing.

The concept of Computer Aided Materials Science will greatly reduce new product discovery times and driving economic growth and international competitiveness.

There is a strong synergy between the imperative of academic research and new product development. In both cases, being 'first to market' with a good 'product' may define success, and hence accelerating and streamlining the research process, through instrumentation, well-designed facilities, and excellent researchers, is of pivotal importance to the competitiveness of both parties, and hence to our potential to contribute to economic growth.



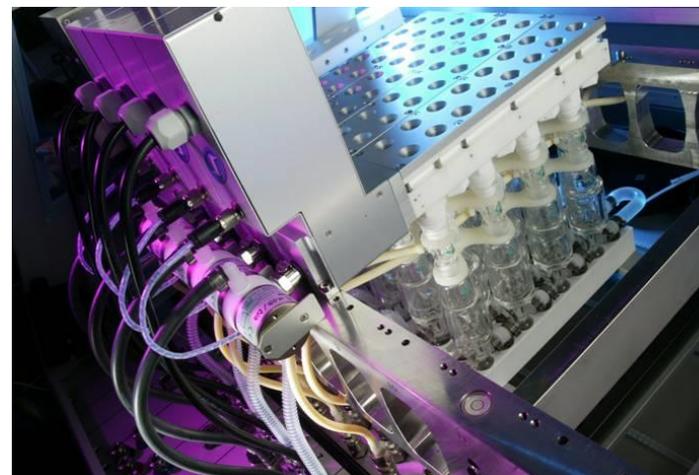
Chemical Materials Design Research Landscape



The Royce at Liverpool will be housed within the Materials Innovation Factory which is staffed by dedicated technical personnel, particularly suited to short- to mid-term access by multiple partners. This will facilitate open access to organisations who wouldn't ordinarily have access to this technology, from SME to large multinational.

KEY RESEARCH OUTCOMES/TARGETS

1. Underpinning research in Functional materials design using computer aided technologies
2. Soft materials, high throughput – shortening development time for stable emulsions, dispersions, high shear mixing, stability
3. Catalysis - Liquid Fuels from CO₂, photocatalysis of H₂
4. Energy - Organic Mixed Matrix Membrane Technologies for Post-Combustion CO₂ Capture
5. Energy storage - development of new battery technologies



Prof Andy Cooper (**Theme Champion**)
Prof Laurence Hardwick
Prof Alessandro Troisi



Dr Kim Jelfs
Prof Jenny Nelson
Prof James Durrant



Dr Martijn Zwijnenburg
Prof Furio Cora
Prof Ben Slater



Prof Graeme Day



Prof Mike Turner