



Strategic

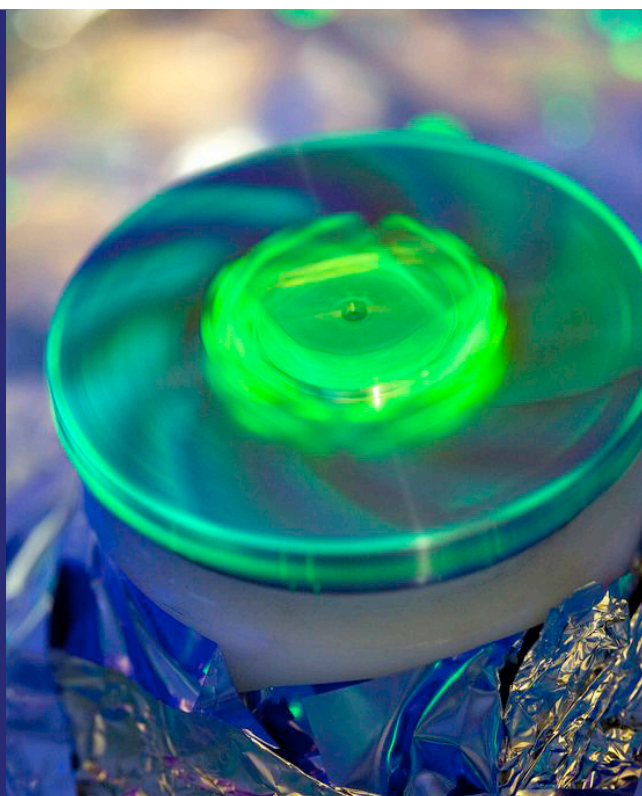


Interdisciplinary

Entrepreneurial



Commercial



KNOWLEDGE CENTRE
MATERIALS
CHEMISTRY

Annual Report 2014

Contents

- 3 Foreword
- 4 Executive Summary
- 5 KCMC at a glance
- 6 KCMC's role in the UK innovation landscape
- 8 KCMC Partner updates
- 10 Connect, Facilitate, Deliver...
- 12 Case Studies - Updates
- 14 Case Studies - New
- 17 Feature - SIG
- 18 KCMC Metrics

Collaboration that delivers....

Because the life-span of cutting edge technology is continually shortening we need to connect business with research in new and faster ways.

With the KTNs now together as a single company we can accelerate knowledge transfer and connect innovators more efficiently than ever before.

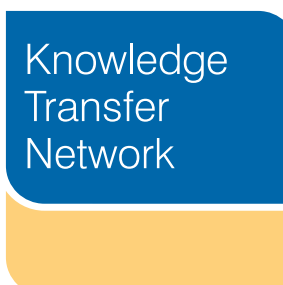
The application of materials chemistry is an excellent example of how the science base can boost growth across multiple industry sectors - and the Knowledge Centre for Materials Chemistry is a proven enabler of collaboration that delivers.

The interdisciplinary nature of innovation increasingly calls for connections to and between sectors which may not always be obvious. Accordingly, the new KTN will encourage more interaction at the interface between different communities.

With its national role across the innovation landscape – and most notably in advanced materials and high value manufacturing - KCMC is a key partner in realising the potential of scientific expertise and advances to aid UK innovation and growth.

“

Chris Warkup,
Chief Executive,
Knowledge Transfer
Network (KTN)



Foreword

KCMC delivers as UK innovation role widens....

KCMC's fifth year of service to the UK's innovation community, 2013-14 was the first for both its new funding partnership with the Technology Strategy Board and in taking a formal, nationwide role in the UK's innovation landscape.

Marking the start of this expansion - from 1 January 2014 for an initial one year period - Cardiff University became KCMC's fifth research partner, joining founders Manchester, Liverpool and Bolton Universities and the Science and Technology Facilities Council (STFC) at Daresbury.

Expanding the number and geographical footprint of KCMC research partners is already bringing benefits from increased engagement with industry nationwide, new strategic opportunities and extended research capabilities to meet industry needs.

These developments complement KCMC's new leadership of the Materials Chemistry Special Interest Group – and HVM focus to bring the research and business communities even closer together.

The widened KCMC remit – and the pivotal role of materials chemistry to innovation for high-growth markets and technologies – also link closely with other notable 2013 developments in the UK innovation landscape.

These included creation of the Chemistry Growth Partnership (CGP) between Government and industry to further accelerate the already strong growth of the chemical manufacturing sector – and simplifying collaboration processes through creation of a single nationwide KTN funded by the Technology Strategy Board.

Against this background, KCMC's proven business model has a natural role across chemistry-enabled innovation in new materials and in enhanced collaboration between industry and UK research capabilities especially for the SMEs so critical to long-term growth delivery.

Indeed, accelerating progress in graphene, composites and formulation were all features of 2013-14.

With 2013-14 reflecting the most positive economic climate since the Centre's creation in 2009, KCMC's momentum looks set to continue delivery well in advance of early projections.

Industry engagements progressed in early 2014 have built on the expanded capability in catalysis – and are now leading to active discussion of project possibilities in industry sectors ranging from the built environment, through aerospace to bio-based materials.

Finally, promising first steps towards addition of a further member to the KCMC research partner network were a fitting note on which to end the 2013-14 reporting period.

David Wright
Head of High Value
Manufacturing, Innovate UK



Innovate UK
Technology Strategy Board

KCMC **CONNECT** ► **FACILITATE** ► **DELIVER**

Materials chemistry is a vital enabler of the new advanced materials required for sustainable solutions for society and industry, especially in energy, health and transport.

KCMC uniquely connects and networks academia and industry, facilitating collaborative R&D that can help companies to deliver accelerated innovation-to-market timescales.

Key highlights of KCMC achievements in the year to 31 March 2014 included:

Cumulative five year industry cash income is **£6.3m**, delivering in line with the original business plan (£6.3m).

Increasing focus on **“advanced materials”**, including composites and graphene, where materials chemistry is important to deliver industry growth strategies.

75% of businesses engaged are **UK owned** – this continues the upwards two year trend from 2011-13.

2013-14 saw **38 first time company introductions** to the five university partners – of which 40% were SMEs.

34 new projects were contracted and **220** industry engagements progressed in the year.

Continued expansion in capability to include catalysis with the accession of Cardiff Catalysis Institute to KCMC for an initial one year period.

59% of industry projects are **repeat business** – 62 companies have now benefited from multiple interactions with the KCMC research partners.

472 companies have engaged with KCMC since start-up in 2009 – and the total number of industry engagements is above **700**, **more than double** the original business plan (350).

KCMC **delivered ahead of five-year targets** in its original (2009) business plan. It is now **on track towards 2014-15 forecasts** in the three-year business plan agreed between the research institution partners and Innovate UK.

At the end of its fifth full year, KCMC has delivered projects to the value of **£17.8m** – **more than double the original government investment** and **75% above the original five year business plan**.

KCMC at a glance...

- KCMC's mission is to accelerate product and process innovation through collaborative R&D in materials chemistry.
- In a funding partnership with Innovate UK - aligned with the UK's 2013 Chemistry Growth Strategy – KCMC now takes a national role in the innovation landscape. The Centre links companies throughout the UK with a widening network of academic institutions offering materials chemistry expertise and facilities.
- Cardiff is the latest University to join the KCMC network, extending research capabilities, notably in catalysis science.
- KCMC collaborations bring added value to the materials science that translates advanced materials for high value markets into commercial opportunity and competitive advantage.
- KCMC is a virtual centre hosted by the UK Knowledge Transfer Network. KCMC provides highly flexible access to multi-disciplinary academic research by its partners – now the Universities of Manchester, Liverpool, Cardiff and Bolton and the Science and Technology Facilities Council (STFC) at Daresbury.
- Dedicated resources deliver competitive advantage for businesses in industrial timescales with reduced business risk.
- KCMC catalyses innovation in advanced materials across applications in energy, health, home and personal care, transport, construction and ICT. It offers companies single-point access to its research partners, rapid project start-up via dedicated scientists and ready access to support grants.

KCMC Leadership Team

Prof. Elias Siores,
University of Bolton

Prof. Matt Rosseinsky,
University of Liverpool

Prof. Stan Golunski,
University of Cardiff

Prof. Mike Turner,
University of Manchester

Dr. John Conti-Ramsden,
KCMC Director

Dr. Paul Sherwood,
STFC



“Chemistry enabled innovation in new materials is fuelling growth, with a strategic priority being to enhance and accelerate this innovation.

Collaboration between industry and the research base will drive the science and enable growth with multi-disciplinary working one of the keys to success....”

Ian Shott CBE
CGP Innovation Lead



KCMC's role in the UK innovation landscape



Introduction:

2013-14 brought a series of significant changes for the UK innovation landscape. From a KCMC perspective, key developments during the year signalled growing emphasis on “integrated solutions” and “collaboration” - where materials chemistry crucially contributes to application and market growth for advanced enabling processes and materials.

Securing quicker acceleration from concept to commercialisation was a driver in early 2014 for transition of the former 14 KTNs into a single company – Knowledge Transfer Network Limited - bringing faster connections across multiple technologies and market sectors.

And in the first full year of its funding partnership with Innovate UK, KCMC has added complementary capability in catalysis, through Cardiff University, and identified new cross-sector industry needs in composites.



High Value Manufacturing:

Helping to de-risk entry to high growth business sectors, KCMC continued to work closely with the High Value Manufacturing (HVM) Catapult. Launched in 2011 as a multi-partner collaboration to drive growth of UK “high end” manufacturing, “HVM” is distinguished by a high level of R&D intensity to drive significant growth.

With core funding from Innovate UK, the Catapult operates through seven elite technology and innovation founding centres, helping companies to incubate and develop new manufacturing technologies through to commercialisation.

KCMC research institution partners Liverpool and Manchester universities are two of the HVM Catapult's 42 university partners.

During 2013-14 KCMC has been active with the Catapult on more than five key capability developments. These include topics spanning the development of long fibre reinforced composites, atom scale surface engineering, formulation and materials for energy harvesting.

The Catapult is complementary to KCMC by helping customers to “de-risk” investment in new manufacturing processes at higher Technology Readiness Levels. Focused on key competencies identified as vital to future UK manufacturing, it provides a UK hub where companies can access the best manufacturing technologies, facilities and skills, working both cross sector and cross technology.

Chemistry Growth Partnership:

Complementing KCMC's role in collaborative materials chemistry research was the formal launch in Summer 2013 of the Chemistry Growth Partnership (CGP).

Focused on key work themes around energy, innovation and supply chains, this long-term collaboration between government and industry will further build on the chemical sector's impressive track record by addressing key challenges and opportunities.

Recognising growth of the chemical sector as a strategic priority, critical to the economy, social progression and the environment, the CGP is committed to delivery of ambitious growth – with the sector increasing GVA to £300bn. by 2030, a 50% growth.

Europe – the bigger picture:

A further – indeed crucial - context for KCMC's expanding remit is how UK innovation fits within and benefits from the wider, European picture and funding opportunities. Here too, 2013-14 brought key developments.

First, early 2014 saw the launch of Horizon 2020, the biggest EU Research and Innovation programme ever, with nearly €80bn. in funding. Horizon 2020 couples research and innovation with emphasis on excellent science, industrial leadership and tackling societal challenges.

Succeeding the FP7 funding programme, it has a larger innovation component and prioritises challenges such as climate change and energy security.

Goals – closely complementing those of KCMC - include making it easier for the public and private sectors to work together in delivering innovation; to increase multidisciplinary and cross-sector working along value chains; to get new projects launched quickly - and achieve results faster.

Secondly, Horizon 2020 promises a key role for SusChem, the sustainable chemistry forum launched in 2004 to co-ordinate and improve industrial and academic engagement with EC research initiatives – and with which KCMC works closely in the UK.

An enhanced SusChem strategy has an even stronger emphasis on innovation – especially on novel options and technologies to benefit

the environment, economy and society overall.

Multidisciplinary working and the contribution of chemical technology and biotechnology to advanced materials have sharp focus in its 2020 strategy – again closely reflecting elements of KCMC's mission.

KCMC is notably aligned towards:

- Sustainable products and processes: Reduction and replacement of critical raw materials, bio-sourced materials, resource efficiency, materials recycling and reuse.
- Supporting SMEs and bridging the innovation gap “valley of death”.
- Creating innovative new materials: For electronics, photonics and sensors; lightweighting, catalysis, formulated products; biologically relevant materials; multi-functional materials; enabling new manufacturing technologies.
- Addressing societal challenges in energy, health and transport.
- Networking, facilitation and grant funding support for access to leading edge materials chemistry skills and capabilities

Composites – an exciting growth industry...

The composites industry is enjoying rapid growth, driven by the functionality and light weight properties of composite materials, and has a current global CAG of ca7.5%.

The UK has been a major player in development and application of composites across many industry sectors and has a strong track record in aerospace and automotive components since the 1930s.

In November 2009 the Government launched the UK Composites Strategy, highlighting the importance of composites to future UK manufacturing. These Industrial Strategies are supporting the UK capability to succeed in intensely competitive global markets. A further study was produced in June 2013 by the Composites Leadership Forum to scope the potential size and scale of the market and future investment required. The updated Composites Strategy is due for publication in autumn 2014.

“Materials chemistry has a vital role in delivering the products and processes required for this new growth phase of the industry”, said National Composites Centre (NCC) Collaborative Research Manager Dan Kells.

Key materials chemistry opportunities in composites were the focus of a KCMC industry meeting held jointly in Spring 2014 with the NCC at the High Value Manufacturing Catapult.



KCMC Partner Updates



University of Bolton

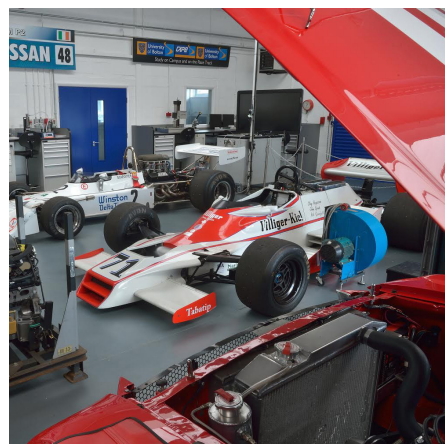


Materials research at the University of Bolton is furthering the state of the art know-how in smart and multifunctional materials.

Advances in nanofibres and thin flexible films and foams are benefitting biomedical applications such as tissue engineering and

antimicrobial wound dressing. Expertise in fire and retardant nanoparticles, responsive micro and nano gels, and polymeric piezoelectric fibre structures are all solving industrial and technological problems in advanced performance composites, technical textile design and renewable energy generation.

In 2013, the new Centre for Advanced Performance Engineering was launched to provide essential engineering skills and a learning experience with a strong emphasis on industry and practical experience, endeavouring to meet the current and future needs of the evolving UK automotive industry.



On the road to success...University of Bolton's Centre for Advanced Performance Engineering

University of Cardiff



Cardiff University: Cardiff's addition in early 2014 as KCMC's fifth research partner added significant competencies to the Centre's research capabilities.

With a track record of interdisciplinary working and collaboration, the internationally recognised strength of the Cardiff Catalysis Institute (CCI) is a natural fit with increasing industry focus on both sustainability and functionality in new product and process design.

CCI has a particular focus in the efficient utilisation of both conventional and renewable fuels and feedstocks, in the modification of existing catalysts and creation of new ones to deliver faster, cleaner and more economical transformations.

University of Liverpool



The University of Liverpool and Liverpool John Moores University will together create, attract and support new high-tech SMEs and provide larger multinationals with a new, creative centre for sensor research, development and commercialisation.

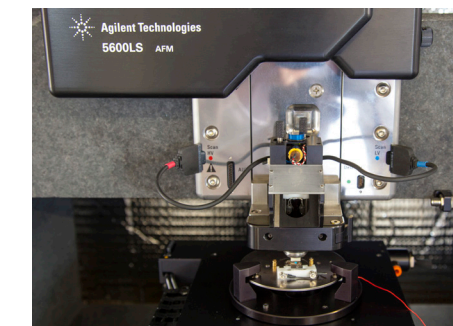
Sensor City will help inventions go from the lab to factory floor even

faster, allowing academics, private sector partners and investors to combine for the critical mass needed to establish a knowledge hub for sensor-related technology.

The incubator will include a bespoke, 2,500m² new building, providing co-working space; a technology development zone; an open innovation laboratory, entrepreneurship coaching and business mentoring.

Sensor City has a clear technology focus to develop and implement novel sensor systems integrating sensors, firmware programming and advanced algorithms. Sensor systems and measurement

technologies are integral to the science-based economy, supporting innovation across sectors ranging from manufacturing to healthcare.



"A wide range of expertise and equipment such as this multi-mode Atomic Force Microscope are available for the characterisation of materials at the University of Liverpool"

University of Manchester



The University of Manchester

As part of the £1bn. investment in the campus the University of Manchester is investing £200m. in the Engineering Campus Development. The development will include new accommodation for several Schools including Materials and Chemical Engineering & Analytical Science.

Phase 1 of the development is well underway with the construction of the £61m National Graphene Institute and an investment of over £18m in state-of-the-art Multidisciplinary Characterisation Facility for advanced materials.



The National Graphene Institute

Science and Technology Facilities Council (STFC)



The Council is well known for its computational science expertise in modelling and simulation, including the high performance computing

(HPC), Big Data and Visualisation capabilities of its Hartree Centre.

Officially opened in 2013, STFC's Hartree Centre is the UK's largest supercomputing facility dedicated to industrial-led applications.

HPC capabilities are currently being used in a joint initiative – with Unilever, Syngenta and Infineum - to develop new software tools that can shave months or years off product development (See case study on p. 16).

Providing cutting edge and cost-effective research techniques, STFC's world class facilities carry out over 2,000 experiments annually across a wide range of the physical and life sciences.



Professor John Womersley, Chief Executive at STFC, and Jim Crilly, Senior Vice President, Strategic Science Group at Unilever

2013-14 marked KCMC's first full business year in its widened, national innovation role in funding partnership with Innovate UK.

The addition of Cardiff University as a KCMC partner in early 2014 notably expanded the range of capabilities in catalysis available to industry by connecting with the research institute network.

Cardiff's work gives emphasis to the drive for more sustainable products and processes, while KCMC's

growing involvement with composites points to the crucial role of materials chemistry in advanced materials for high-value markets.

KCMC progressed 220 industry engagements in 2013-14, connecting companies with more than 30 senior academics from the five research partners. There is a trend to an increased proportion of UK businesses engaged (up from the prior year's 72% to 75% in 2013-14) - see **Figure 1**. Altogether, 38 new companies have been introduced to

the KCMC of which 40% were UK SMEs.

Industry sectors supported are led by chemicals and materials companies working across a broad range of end application. There is an approximately even split between this sector and companies which are specialised in other industries eg in energy, health, fast moving consumer goods and electronics (**Figure 2**).

KCMC's collaboration business model has been refined in the last five years by the successful management of a diverse range of dialogues between many industry sectors and the Centre's research partners.

The experience across hundreds of collaborations enables KCMC to uniquely add value and focus in the field of materials chemistry – and

often to save time - through each stage of the facilitation template.

In practice, projects are managed through four key stages, albeit with a high degree of customisation to suit client circumstances and the nature of the materials chemistry innovation. These are:

- (1) Detailed clarification of company requirements/expectations

- (2) Agreeing confidential disclosure protocols
- (3) Supporting generation of project description/cost
- (4) Assisting in contract development, including:

- IP ownership
- Project financing (eg options such as KTP, SMART and SBRI etc.)
- Contract negotiation

Project portfolio:

The project portfolio continued to grow in 2013-14 with 34 projects contracted during the year and overall research income of £4.2m (**Figure 5**). Cumulative five year research income now stands at £17.8m, 75% above the original business goals for KCMC.

Cumulative 5 year industry income is £6.3m, exactly in line with original business plan projections of £6.3m. Strikingly, in 2013/2014 all the smaller industry projects (< £50,000 value) were contracted with SMEs (eight projects, see below)

- Energy
- Health (woundcare and sensors)
- Lightweighting and composites
- Resource efficient manufacture
- Next generation thin film
- manufacturing technology

A notable trend following the launch of STFC's Hartree Centre has been the continued growth of a pipeline of industry projects exploiting the use of High Performance Computing in the development and exploitation of new materials.

Grant awards from 2013-14 included topics focussed on health (sensors, imaging and woundcare), energy (modelling of materials), lightweighting (fire retardant composites and power electronics), novel processing for electronics and photonics, sustainable manufacture and formulation.

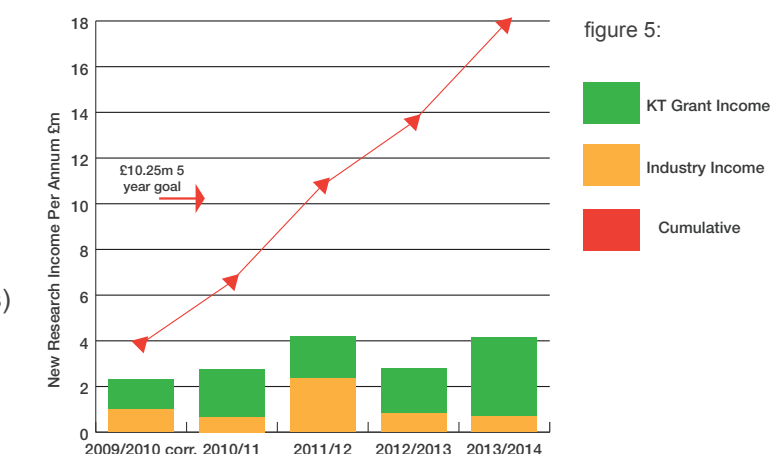


figure 1:

Company by Type

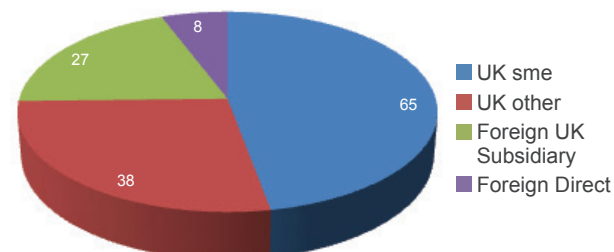


figure 2:

Companies by Sector

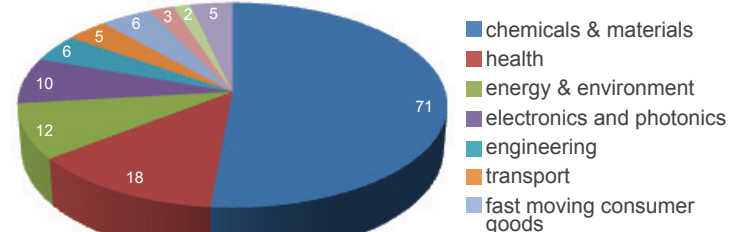


figure 3:

SME by Industry Sector

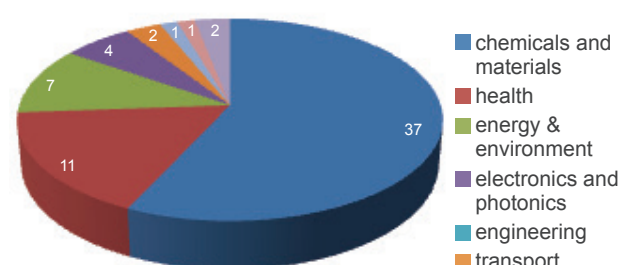
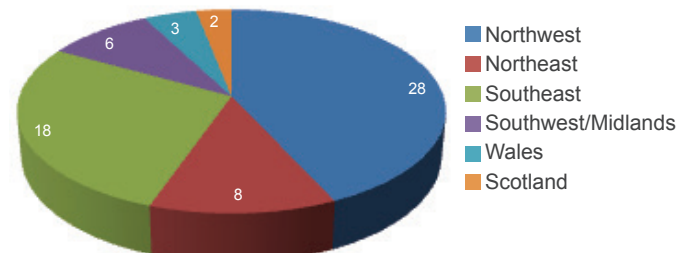


figure 4:

SME by Region



SMEs: key innovation drivers...

A major source of innovation in the development of new materials, SMEs are a priority for KCMC support, through networking and timely collaborative R&D.

Significantly, the number of SME engagements in 2013-14 (43%) has increased as a proportion of total engagements compared to 2012-13 (34%). The absolute number of SME engagements increased to 96 in 2013-14 (79 in 2012-13).

Since the number of SMEs remained constant at 65, this reflects an increased repeat activity and relationship building with selected companies (ca 15 companies). The industry spread of SMEs engaged remains broad, **Figure 3**.

The geographic spread of SMEs engaged has broadened further to reflect KCMC's increasing national role. Just over 40% of SMEs were from the Northwest; 28% from the

SouthEast, 12% from the Northeast and the balance from other regions. **Figure 4**.

The role of SMEs in driving broad front innovation is illustrated by the range of collaborative research topics covered. These included low carbon energy (fuel cells, photovoltaics); healthcare (materials for assisted living); energy harvesting; next generation materials and chemical processing (impacting multiple

industry sectors) and advanced materials for bio-processing.

Significantly, SMEs are more strongly represented in the development of new materials with cross cutting applications ("chemicals and materials", 57%) than larger companies (47% working in this way). **Figure 2** Larger companies involved in new materials development are more heavily weighted to sector-specific businesses.

The majority of SME projects are short term responsive projects, carried out using the flexible KCMC model. For larger projects, Innovate UK awards - including SMART, KTP and Collaborative R&D Feasibility funding - have been used, augmented by impact funding from EPSRC and STFC in selected areas in line with programme criteria.

Case Studies

Five new KCMC case studies for 2013-14 showcase sectors where advanced materials and technologies benefit a range of key industries - from transport and energy generation to food, consumer products development and advanced display technology.

Progress updates on earlier case studies re-visit fire resistance in composites for transport and fuel and emissions savings for applications in the aerospace and automotive sectors.



Biocomposites evolving FR capabilities for transport applications:

Safety and weight-savings are key

Challenge:

Biocomposites contain natural fibres and/or resins derived from plant sources. Therefore they are combustible and this presents a significant barrier to wider application.

The FRBioComp project aims to produce biocomposites with fire retardant qualities for use in construction and mass transportation applications.

Partners in this Innovate UK-funded project are NetComposites, Sam Weller & Sons, Exel Composites, Drake Extrusions Tilsatec and the University of Bolton.

Solution:

FRBioComp is investigating intrinsically fire retardant biobased materials (such as polyfurfuryl alcohol resins) and treating fibres/fabrics or matrix polymer resins with environmentally friendly flame retardants.

Continuous treatments of fibres/fabrics and/or resins with flame retardants are being explored, while fire retardant biopolymer fibres incorporating synergistic flame retardants and polymer layered silicates are also being developed.

Benefits:

Biocomposites' weight-saving is key in transport applications - delivering reduced emissions, rail track wear and stopping distances. Lightweight panels allow for faster buildings construction. Inherent fire retardance is an essential safety feature.

Update:

Various strategies to develop flame retardant flax/polypropylene (PP) and flax/polylactic acid (PLA) composites have been adopted:

- (1) Applying flame retardants (FR) to flax/PP or flax/PLA woven fabrics using conventional pad-dry technique commonly used for textiles;
- (2) Use of FRs in thermoplastic matrix by developing FR-PP or FR-PLA fibres for potential use in woven fabric and use of FRs in furan resin as additives; and...
- (3) Development of composites by either introducing FR on fibres, in polymer matrix, or both components.

Selected solutions have shown great commercial potential for development through the consortium.



Victrex growth through collaborative R&D

New polymer would bring weight and fuel savings

Challenge:

A leading global player in high performance polymers, Victrex plc, targets growth through product leadership, translating innovation into high performance, market leading polymer-based solutions.

Yet speedy, cost-effective R&D with rapid project start-up can pose investment and timeline challenges.

Solution:

A Knowledge Transfer Partnership (KTP) with the University of Manchester (OMIC) has been a focused and highly cost-effective R&D route, contributing to rapid innovation in extreme temperature plastics.

The KTP approach accesses University expertise and resources, freshening and broadening scientific perspectives to address the challenge.

KCMC introduction to OMIC triggered collaboration leading to

current development of a new polymer – polyaryletherketone (PAEK). Easily extruded and welded, PAEK potentially has exciting weight-saving applications in the aerospace and automotive sectors, which would bring benefits in both fuel and emission savings.

The project model ("small is beautiful" collaboration) ensured retention of focus on delivering objectives – avoiding compromises impacting on efficiency, timeline and value-for-money.

Benefits & Update:

The successful partnership resulted in an IP filing in novel, high temperature plastics, which have applicability across a number of Victrex's strategic markets.

In-house prototype manufacturing studies are planned for the near future in order to determine future commercial exploitation. Victrex was also pleased to be able to recruit the Knowledge Transfer Associate on a full-time basis at the completion of the project.

williamblythe

Excellence in chemistry

developments in fire resistant materials

Supporting new product development

Challenge:

Meeting the polymer industry's aspiration to use non-hazardous and environmentally benign products, William Blythe Ltd. wished to understand effectiveness of their Flamtard flame retardant ranges in greater detail – to support promotion and new product development.

Solution:

With KCMC facilitation, the company sponsored a work programme at the University of Bolton.

Flame retarded polymer compounds, based on commercial formulations, were prepared and Flamtard product effectiveness established using measurement techniques including Cone Calorimetry.

For halogenated and halogen-free systems, work has identified flame retardants with which Flamtard S and Flamtard H can show synergistic activity in commercial polymer systems.

Novel, non-toxic environmentally benign, synthetic inorganic compounds are also being researched. These can impart fire retardance and smoke suppression to selected high performance polymers without use of halogen-containing flame retardants and synergists.

Benefits:

Project data is being used to advise on the most effective ways to use Flamtard and to assist sales expansion of into new applications.

Update:

Project is ongoing into 2016 - to build on these experiences, understand the mechanisms of action of the existing systems and develop new systems through two inter-related PhD programmes.

The first PhD funded by William Blythe is to investigate the mechanisms of synergism of zinc stannates and other metal metallates with conventional flame retardants in different polymer systems using modern methods. The second PhD programme, partly funded by Cotton Industry War Memorial Trust UK, is to develop novel, environmentally sustainable surface coatings for textiles.

SunChemical[®]

a member of the DIC group 

keeping it fresh

New solutions in food packaging

Challenge:

The world's largest supplier of printing inks, pigments and coatings, Sun Chemical is a leading source of innovation to various industries including publication and packaging.

The primary function of packaging is contents protection - for example, keeping a food product fresh - by separating it from external environmental factors such as moisture and oxygen.

Clay particles show promise as an effective, inexpensive candidate to use in coatings to improve this barrier. For Sun Chemical to implement new packaging solutions, they naturally require efficient, cost effective testing of potential new materials.

Solution:

STFC's Hartree Centre, alongside partners Durham University and University College London, conducted a pilot study, introducing Sun Chemical to computational modelling as a new materials testing method. The project, part-funded by METRC, allowed researchers to observe how clay particles disperse in a solvent-polymer mixture at the molecular level.

Researchers designed new dispersions or packaging candidates in-silico, and were able to accurately predict their behaviour prior to real-life testing.

Benefits:

With computational chemistry modelling, scientists can gain an insight into not only the "what" but also the "how" and "why" of a process. Along with more useful results, this method is more time/cost effective, reducing the need for physical prototyping and experiments.

Introducing savings to just 5% of the global food barrier packaging market with an environmentally friendly clay-polymer technology would be worth around £150m. of new business to Sun Chemical.

The partners proved the value of computational chemistry and simulation to Sun Chemical, who now have the potential to utilise the method in future R&D.

acal
energy

Clean affordable power

taking fuel cell technology further

Predicting candidate catalyst properties

Challenge:

Fuel cells are a leading contender in the battle to find green, emissions-free power sources. ACAL Energy has a novel patented technology that replaces most of the costly platinum catalyst used inside every PEM fuel cell.

ACAL Energy's liquid catalyst is much cheaper than using platinum and vastly improves fuel cell durability. Fuel cells can now be a practical, affordable option for mass-market adoption.

ACAL Energy wanted to investigate some catalyst materials' capability to react with oxygen, to determine opportunities for performance improvement. STFC's Hartree Centre has provided supercomputing capability to gain a better insight into fuel cell technology.

Solution:

In its R&D phase, ACAL Energy collaborated with Hartree over a three-year period to gain deeper understanding of the fundamental processes controlling candidate catalyst materials performance.

The aim was to reduce the number of molecules needed to synthesise and test as potential catalysts.

The Centre's computational simulations - which model results on an atomic scale not possible in a lab - enabled ACAL Energy to understand the in-depth chemistry in fuel cell performance.

ACAL Energy calculated redox properties of intermediate reactive stages of chemical reactions for a range of candidate material types. This provided useful insights into key properties and reaction mechanism features that can affect fuel cells performance.

Benefits:

ACAL Energy has made significant savings on R&D, allowed it to simulate and predict the properties of candidate catalyst molecules.

Based on the results, ACAL Energy was able to eliminate a range of potential catalysts and finalise the structure of FlowCath®, the company's patented liquid catalyst, in its own laboratory.

datalase 

"next generation" digital printing

High-speed packaging sees the light...

Challenge:

To develop "next generation" materials for DataLase Infinity full-colour, in-line, high speed digital printing – especially with regard to light driven colour change reactions.

A market leader in colour-change materials for laser coding and marking (consumer products, packaging and labels), DataLase is focused on developing digital print solutions that are scalable across multiple platforms, media and applications.

Solution:

(1) Study by UOM and STFC Daresbury of polymorphic properties of Infinity materials, including material analysis and molecular modelling. (2) UOL study of reduced indium tin oxide NIR absorbers (r-ITOs) to assist r-ITO development for highest efficacy in DataLase applications, and to underpin IP generation.

KCMC has been supporting DataLase since 2011-12. The Centre identified partners for (1) molecular modelling and (2) expertise in complex metal oxides, facilitated engagement and provided financial assistance.

Benefits:

Clarity on the presence of low energy unreactive and reactive configurations and ability of a molecule to convert from unreactive to reactive form. Data feed into R&D programmes.

The PhD based programme with UoL is being used to steer in-house development of high efficacy NIR absorbers based on complex metal oxides. This next generation of NIR absorbers will help the optimization of the light-based digital print engine for labelling on high speed packaging lines.

HPC

speeding products
to market



The Hartree Centre's IBM Blue Gene Q supercomputer helping to provide innovative solutions to wide-ranging materials chemistry challenges for UK companies

A week's work in just 40 minutes...

Challenge: Against a highly competitive market environment, speed-to-market is critical, especially for UK companies creating new products every year.

To accelerate and support development of new ways of designing, improving and manufacturing complex, high-value formulated products, high performance computing (HPC) can now shave months or even years off product development and therefore cost.

Solution: Unilever, Syngenta and Infineum selected the expertise and facilities at STFC's Hartree Centre within a joint initiative to develop a range of new software tools, being funded as part of a £1m. grant from the Technology Strategy Board.

A week's experimentation on a new product formulation can now be done in just 40 minutes through advanced computer modelling, simulation and 3D visualisation.

An 'app' - developed by Hartree in association with IBM - is connected to the Centre's Blue Joule supercomputer, capable of more than 15 trillion calculations per second. It can accurately predict the behaviour and structure of different concentrations of liquid compounds and how they will interact, both in the packaging, throughout shelf-life and in use, helping researchers plan fewer, more focused experiments.

Benefits: Manufacturers – rather than computational scientists – are enabled to routinely run predictive simulation tests through the 'app', with speed-to-market for new product designs potentially being reduced by up to 80%. Environmentally friendly cleaning products; cleaner, more efficient lubricating oils and fuels; more sustainable crop protection products and breakthrough personal care products are just some of the consumer and industrial products that will benefit from the three-year initiative.

Flexible collaboration with UOM supports innovations

Challenge: Cambridge Display Technology (CDT) leads the development of solution processable light emissive technology based on organic light emitting diodes (OLEDs). The company expects to see the technology used increasingly in mobile applications, televisions and lighting.

As a leader in organic light emitting materials and devices CDT has developed a number of important relationships which help to maintain its leading position and accelerate identification and realisation of promising new technologies. One of these relationships is with the University of Manchester (UOM).

Solution: CDT and the University of Manchester have been collaborating for a number of years on the development of a range of novel materials for uses in and related to CDT's display technology.

The relationship has flourished on the flexible approach both partners have taken to clarifying the requirements and developing the most appropriate mechanism for a specific collaboration based on the objectives, timescales and deliverables. The portfolio has included EPSRC CASE and fully funded PhD studentships, feasibility studies and full collaborative R&D projects across the Schools of Chemistry, Physics and Electrical and Electronic Engineering.

Benefits: The close relationship between CDT and the University of Manchester is supporting a number of innovations within CDT.

This has been achieved through access to considerable expertise in novel methods for use in synthetic organic chemistry, new materials for use in CDT display technology, insight into possible new opportunities for the underpinning technology and connection to application expertise.



Materials Chemistry SIG

Accelerating Innovation

Led by KCMC and funded by Innovate UK, the goal for the Materials Chemistry Special Interest Group (SIG) is to help turn leading edge UK capabilities in materials chemistry into industry competitive advantage.

The strategy is to accelerate innovation in development and commercialisation of new/novel materials to meet future industry needs. This recognises both KCMC's focus to support and drive growth in high value manufacturing industry, and its increasing role as a national centre.

The SIG looks to build on KCMC's track record in delivering value from collaborative research and its proven business model: aligning university capability with industry need in transferring research to market.

Targeted benefits from SIG involvement include shorter time-to-market for innovation dependent on materials chemistry; better connection of industry need to leading edge university research and enhanced connection of universities' materials chemistry expertise to manufacturing innovation – including to the High Value Manufacturing Catapult.

In a key 2013-14 step, leading UK capabilities in materials chemistry and their impact on industry growth and innovation were highlighted at the event "New Materials: Fundamental to Growth", held jointly with KCMC and Innovate UK in London in December 2013.

This demonstrated the power of materials chemistry as a vital enabler, driving innovation in renewable energy, electronics and advanced materials - and how the KCMC business model facilitates new approaches to the collaborations required.

Priorities:

Priorities for related KCMC expansion of capability in 2013-14 have included catalysis - impacting industry priorities in resource efficiency, environment, and product design for functionality - and composites. Here, materials chemistry has a vital role in helping to deliver the promise of lightweight, functional structures for future needs, especially in the aerospace, automotive, construction, marine and energy sectors.

Strategic expansion of the KCMC into added capabilities was notably marked by the accession in early 2014 of the Cardiff Catalysis Institute. This has triggered new KCMC industry engagements to meet diverse industry needs, ranging across low carbon manufacturing, automotive and aerospace.

Similarly, and recognising the vital role of materials chemistry in composites, the year saw KCMC working closely with several leading industry players involved with "next generation" composite materials. (Key materials chemistry opportunities were the focus of joint KCMC/National Composites Centre meeting in Spring 2014, feeding into the Government's evolving UK Composites Strategy).

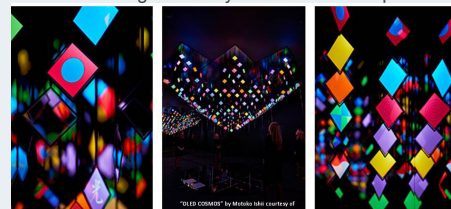
With its contribution to the progression and application of new materials, the Materials Chemistry SIG is an important partner in realising the potential of the UK chemical sector to deliver ambitious growth targets over the next 15 years.



novel materials in light emissive technology



Panasonic 4k2k Printed Curved OLED Screens at CES 2014. Image courtesy of Panasonic Corp.



Ink-jet printed designer lighting installation by Sumitomo Chemical Co. at Light and Build 2014. Centre: OLED COSMOS" (W3.8mxD2.5mXH1.9m) Designed by Motoko Ishii. Left/right: Detail of OLED COSMOS



KCMC is a vital catalyst, with a proven business model helping to link innovation in advanced materials with exciting commercial opportunities in high value industry sectors....

John Grasmeder
Chair, KCMC Industry Steering
Group and Technical Director,
Victrex Polymer Solutions

KCMC Metrics

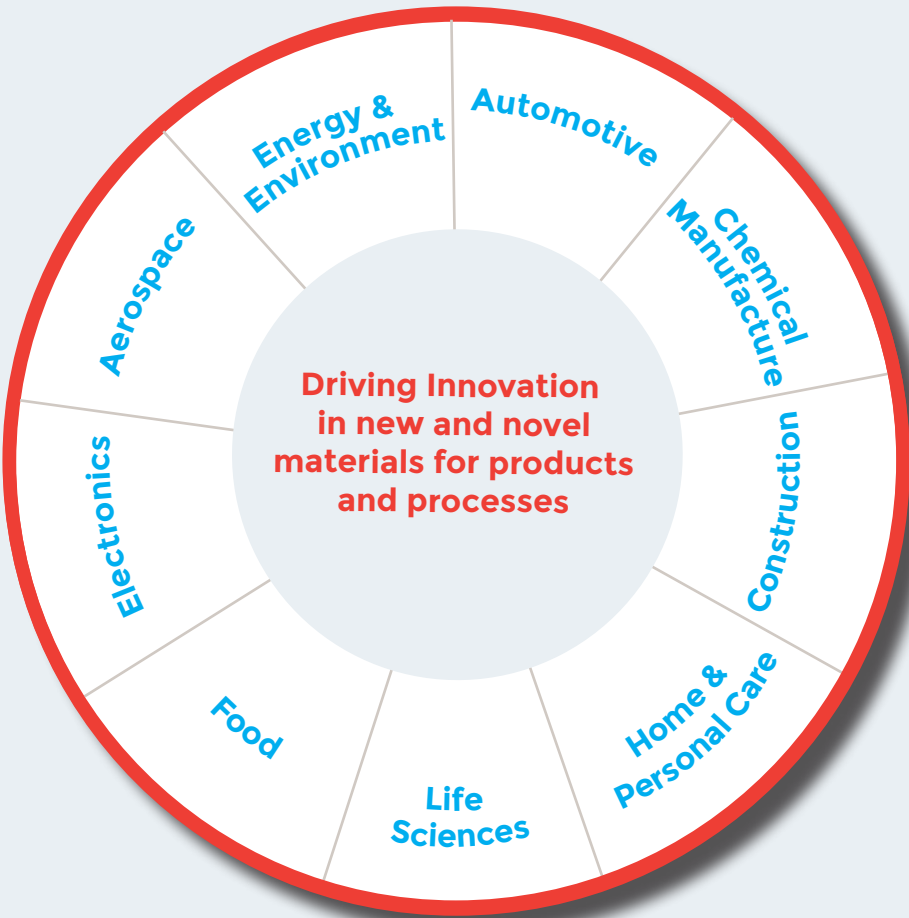
Key goals for KCMC in the new partnership with Innovate UK reflect priorities for supporting growth in UK high value manufacturing. These include strategic growth in materials chemistry capability, robust financial performance, SME engagement, collaboration with Catapults, and publication of case studies to highlight economic impact.

Key metrics to support delivery of these goals are:

Metric	2013/2014 Actual	Comment from Business Plan
Strategic growth in capability	Catalysis - CCI	-
Financials: collaborative research income	£4,178,218 (Industry income £691,000)	Ahead of budget
SME Engagement	96 (total engagements 220)	7% above plan
Meetings held with Catapult	3 (CPI, NCC)	On plan
Case Studies	7	Ahead of target

Materials Chemistry: External World

Driving Innovation in multiple sectors





KNOWLEDGE CENTRE
MATERIALS
CHEMISTRY

**The Heath
Runcorn
WA7 4QX**

01928 511824

www.materialschemistry.org