



KNOWLEDGE CENTRE
**MATERIALS
CHEMISTRY**

Annual Report 2019–21

Climate
change

Environment

Energy
saving

Industry

CO_2

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KCMC Knowledge Transfer Team



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Dr Christophe Brodin
Knowledge Transfer Manager

Cultivating a Network of Innovation and a Pipeline of New Opportunities with KCMC

While 2020 brought a number of challenges, over this period the relationship between CPI and KCMC has only strengthened. This strengthening has brought several benefits, including the fortification of CPI's connections with KCMC's academic network. By joining the dots between academic research, innovation, scale up, and eventual commercial translation, KCMC provides CPI with invaluable opportunities to connect with academic partners. There is a rich pipeline of opportunities available within academia and by picking up these innovations at an early, proof-of-concept stage they can be better translated towards commercial reality.

KCMC sits at the heart of both CPI's academic engagement and materials strategies. Materials chemistry is an underpinning capability that feeds into multiple industries downstream, and within the materials

industry as a whole there has been an increasing focus on sustainability and the role of sustainably sourced materials. This focus is both a way to contribute to the global efforts to reduce the impacts of climate change, but also to help the UK meet its net zero target by 2050. Through CPI and KCMC's network, combining academic, government and industry partners, we can unlock the potential within materials innovation.

KCMC and CPI are both driven by the goal of a healthier society, a cleaner environment and a more vibrant UK economy, with a purpose to ensure that every great idea or invention has the chance to turn into a commercial product. By combining these goals with cross-sector connections and advanced capabilities, we are creating innovative outputs that can help solve some of the world's biggest challenges.

As we complete our third full year of hosting KCMC within CPI and the High Value Manufacturing Catapult, we are seeing several benefits and lasting connections through the evolution of this partnership. KCMC is an integral part of CPI's strategy moving forward, and we are excited to see the amazing innovations that come out of it over the next few years.



Dr Arun Harish
Strategy Director, CPI



Faced with a difficult set of circumstances and multiple challenges ahead, both as a country and an industry, the goal at KCMC is to continue to keep the innovation pipeline flowing. In order to achieve this, we will be building on our strong working links with CPI, and more widely within the High Value Manufacturing Catapult, to better understand the industry needs and opportunities for materials chemistry in the UK. We will be looking to evolve what we do to meet these needs. By growing the interaction between industry partners, universities and the Catapults, we can take advantage of this challenging, but opportunity-rich environment.



Professor Rick Cosstick

Chair KCMC Governing Board,
University of Liverpool





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**MATERIALS
CHEMISTRY**



**Dr John
Conti-Ramsden**
KCMC Director

KCMC executive summary

2020 has been a challenging year for many, with lockdown restrictions threatening the development of our innovation pipeline. Despite these challenging circumstances, the materials chemistry industry has adapted and responded to multiple challenges and opportunities within the sector. Our partners, those in industry and especially those in universities, have had to adapt to very different ways of working but have found ways to continue their activities and maintain outputs to bolster our collaborative pipeline.

Over the past year, we have seen exciting progress in several areas. This includes the development of new sensor technologies and materials discovery for advanced manufacturing technologies, as well as starting the journey towards materials chemistry solutions for waste valorisation in the circular economy. In addition, the project pipeline surrounding digital approaches to materials chemistry innovation has strengthened, with COVID-19 challenges bringing these approaches to the forefront. This is an area that will continue to grow and become more embedded in everyday materials chemistry, so understanding how to envision and implement application of these techniques will be crucial in realising their potential. Another area that has grown in importance is the relationship to our network of start-ups and spin-outs. We have been building these links and involving CPI Enterprises to support the innovation pipeline and help to bring in new ideas, whilst providing these companies with more opportunities.

An overarching goal for KCMC is to enable sustainable materials innovation and ultimately drive economic sustainability. This year we have seen efforts focusing on the target of the hydrogen economy, in line with the government's renewable energy and 'net zero' targets. Our ISG meeting at the end of 2020 brought together research and industry partners, along with CPI and Innovate UK, to begin to address the challenges and opportunities for materials chemistry in this area. The

event was adapted to a virtual format and brought together key players in the innovation space to focus on a particular topic within materials chemistry. This highlighted a great deal in terms of identifying opportunities for our partners and in how we can effectively come together to address specific goals.

Over the coming year, we expect the materials industry to continue to play a vital role in the transition to a more sustainable energy system. We can expect to see advances in energy storage and batteries, which will be fundamental not only in the electric transport revolution, but also for wider adoption of renewable energy in the economy. In addition, there will likely be many 'post-COVID' opportunities in relation to sustainable growth and rebalancing the economy in line with government priorities. KCMC will have a crucial role in connecting universities with industry to address these strategies, ensuring these projects align with our partners' goals and in the wider context of net zero. We will also continue to improve our ability to connect challenges in the High Value Manufacturing Catapult with the capabilities of our partners. Improving this connection will help to make the most of these opportunities. We look forward to continuing to work with our partners in academia and industry to address the exciting opportunities in materials chemistry in the UK.

We would like to recognise a change in staff at our partner university, the University of Southampton. Professor Gill Reid will leave her role as Head of the Department of Chemistry after being elected President of the Royal Society of Chemistry. We thank Gill for her support over the years and congratulate her on her eminent new role. We welcome Professor Jonathan Essex, as Gill's successor. Jonathan also brings his expertise in computational chemistry to KCMC and we look forward to working with him.

KCMC at a Glance


**£43.9
million**
Cumulative
research
income


5
New
case studies


5
Partner
research
institutions


6
CPI Innovation
Integrator supports
for KCMC
spin-outs


487
Industry
engagements


61%
New companies
that are SMEs


**£12.7
million**
Industry
income


135
First time
company
introductions

Building on the developments and achievements of the past year, there are many exciting opportunities to come for KCMC. Several new partnerships have been secured, including a Memorandum of Understanding with the Henry Royce Institute, which will help to drive advanced materials innovation. Good links have also been built within the cross-Catapult hydrogen economy arena, paving the way for innovation and development. In addition, KCMC has growing links with CPI Enterprises, helping to bring in innovation from start-ups and spin-outs, broadening its network of industry connections.

Over the past year, several exciting case studies have been completed, as well as an exciting project with NSG Pilkington, linking in with the net zero agenda. These projects highlight the impressive outputs that have been achieved despite the challenging circumstances of 2020. KCMC has also provided opportunities for its university partners to develop joint proposals with CPI, benefitting both organisations. KCMC will be looking to support more opportunities like these.

Perspectives on the Evolution of Materials Innovation

Why are Computational Modelling and Data Science Important to Future Materials Innovation?

By Dr Sheetal Handa, Materials Science Advisor & Associate Director bp-ICAM

Digital science, for example modelling and data analytics, is playing an increasingly important role in many industries. As we begin to tackle enormous challenges that will require innovation in materials, such as the transition to low carbon, I believe these digital approaches will be absolutely critical.

Throughout my career I have used computational molecular modelling to understand the behaviour, shape and compositional properties of molecules. With rapid developments in computational infrastructure, as well as algorithms and software, the opportunities to understand materials at molecular and macro-scales, as well as being able to predict shape and behaviour, are immense. Successfully linking computational techniques across these scales will allow us to understand a material at an atomic or molecular level and then accurately predict its real-world properties. This represents a huge challenge but one that would be game-changing for the industry once integrated.

The use of digital twins, or in silico modelling and testing, could allow scientists to design materials with desired properties, screen them using computational methods and test how they behave on a larger scale. In addition, processes designed and modelled accurately in silico could increase efficiency and optimisation throughout the materials discovery and development process. As these tools continue to advance, the way we use data will

become increasingly important. Modelling allows you to reduce the time needed for discovery and development, but, in my opinion, will never be a substitute for experimentation. Models are only as good as the data that generates them, and the optimal data and predictive ability of a model is dependent on experimental design and testing. This means we must ensure that we are using the vast quantities of data available to us effectively and linking it to experimentation in a virtuous circle. With the right data and the right computational tools, digital approaches have the potential to dramatically enhance the way we design materials.

At bp, we understand that effectively incorporating digital approaches is going to be transformative within the industry. Through the bp International Centre for Advanced Materials (bp-ICAM) partnership, we support the development of modelling techniques as well as the incorporation of modelling within interdisciplinary projects to help to drive the research. I believe an interdisciplinary approach is, and will continue to be, fundamental. Whilst technology may progress to the point where it is easy and practical for a chemist to use without support from other scientists or modellers, the biggest progress will be made at the interface between different disciplines. With a collaborative approach providing expert insight, we can ensure we get the maximum benefit from these promising digital tools.

Looking to the future of this field, a major challenge will be exploring how we can connect modelling across time and length scales, from an atomistic level to a process level. Achieving this will have significant implications for materials chemistry. Another development that may impact the industry in the medium to long term is the development of quantum computing. There are many uncertainties surrounding this technology and how applicable and usable it will be, but developments in both hardware and software are sure to open new avenues for what is possible. There is also interesting potential to use digital techniques such as machine learning for knowledge management and to inform decision-making. The challenges ahead will require innovative solutions and using computational modelling and data science collaboratively will help us to overcome them.



Computational Systems Chemistry – an Academic Perspective

By Professor Jeremy Frey, University of Southampton

The University of Southampton's Computational Systems Chemistry Section has a uniquely broad skill base in computational technologies and applications.

Research activities cover multiple length scales, timescales, and methods founded on strong activity in the development of new theories and computational techniques. The unifying theme is exploring interacting systems; larger scale behaviour of the whole system arises from complex interactions of individual smaller components, an area where the University can offer unique capabilities and insights. Investigations range from properties of nanoscale material, simulation of proteins, drugs, and biological membranes, through to atmospheric chemistry. Our activities are underpinned by the University's 25,000+ core supercomputer, which is amongst the largest in any UK university.

Materials chemistry applications have included the use of linear-scaling density functional methods (ONETEP software) to studying the electronic and structural properties of a variety of nanostructures (e.g., tuning luminescent semiconductor nanorods), solar energy conversion materials and batteries and polymer design methodologies. Computational and Machine Learning

driven prediction of crystal structures in a design-synthesis-model loop is a rapidly developing area for the Section in collaboration with expertise in robotic and automated synthesis. Life sciences applications use similar fundamental approaches and cover the spectrum, from understanding biochemical pathways, through drug development to drug binding studies and drug transport.

We have a strong track record in developing and applying simulation-based methods to the drug development process, predicting drug binding geometries and affinities, and modelling drug transport. We are combining quantum and classical mechanical simulations through to differential equation modelling of biochemical pathways to understand better the role of calcium signalling and its effect on certain metabolic diseases. Similar developments in linear-scaling density functional methods (ONETEP software) are applied to calculating protein-ligand binding affinities.

These areas of computational chemistry are complemented by increasing the involvement of data science and machine learning technologies to bring the growing methods of AI into chemistry in ways accessible to the modern research laboratory.



Dr Rick Anderson
Head of Hartree Centre
Chemistry and Materials
at STFC

A recent development in digital support for materials chemistry and design is the commissioning of the latest Joint Academic Data science Endeavour (JADE 2) platform. Building on the success of the JADE National Tier 2 facility, the new platform is the largest GPU-based system in the UK, at more than double the size of its predecessor, which is also hosted at the STFC Hartree Centre. The academic consortium, led by the University of Oxford and the Alan Turing Institute, includes 19 research-intensive universities. In addition to being the national facility for AI research, the benchmarking of JADE 2's molecular dynamics software shows that its architecture represents a major new opportunity to accelerate computational chemistry research. JADE 2 is available to businesses through the Hartree Centre via a platform-as-a-service model or through collaborative projects.



Digital R&D

By Dr Steve McBride, Matthew Reeves and Alfredo Ramos

KCMC academic partners are driving multidisciplinary approaches to combine computer science, machine learning, AI and automation with materials chemistry and advanced materials research. This is exemplified by the University of Liverpool's Doctoral Training Centre in Next Generation Materials Chemistry led by Prof Matt Rosseinsky, to deliver data enabled science and training of future research leaders with unique skill sets at the discipline interfaces. Industrial recognition as to the power of digital tools is driving their adoption and utilisation across a range of challenges, from accelerated materials discovery to deriving relationships between materials processing, formulation and long-term application performance.

The University of Liverpool is world-leading in autonomous robots for materials chemistry research and development, designed to assist researchers by performing repetitive work and rapid screening, freeing them to analyse interesting data and formulate new hypotheses and research directions. In a recent trial, the autonomous robot at the University of Liverpool completed 688 experiments in 8 days optimising a 10 variable experimental space. The work is based on developments from Prof Andy Cooper's group and now being deployed on a wide range of challenges, while increasing access through the Materials Innovation Factory and the recently awarded EPSRC Strategic Equipment Grant to further develop capability and opportunities for wider academic and industry partners.

KTN, in partnership with Innovate UK, is working to establish communities of chemical, formulation and material companies and solution/service providers of digital technology. There is a clear need to accelerate

the adoption of digital tools in both the R&D and manufacturing arenas to boost productivity, increase the rate of innovation and bring new products to market. In addition, the motivation for digital adoption has become more acute in recent months, due to the disruption of traditional lab/factory activities and to physical distancing measures introduced in 2020. Industry adoption of digital tools towards digitally-integrating end-to-end innovation, product development, supply chain and manufacturing pipeline will increase resilience, and competitiveness of the sector. This will help the UK economy to grow and meet future challenges in mobility, energy, achieving net zero and sustainable manufacturing.

CPI is working at the forefront of the application of digital technologies, to help accelerate product development, lower cost and reduce time to market in our industry. Materials innovation is a particular focus with applications in predictive modelling for design of complex formulations and materials, design and simulation of manufacturing processes using multiscale modelling, and digitally connected process analytical technologies (PAT). This is the start of a journey as our industry partners find increasing applications for digital techniques across the board in materials innovation, often working with our research institution partners on the leading edge of defining what is possible. This will drive future competitive advantage, thereby shaping where CPI can most effectively support technology translation to market application.



Dr Steve McBride
Knowledge Transfer Manager,
KCMC



Dr Matthew Reeves
Knowledge Transfer Manager,
KTN



Alfredo Ramos
Managing Director of
CPI Enterprises

CPI is working at the forefront of digital technology application to accelerate product development, lower costs and reduce time to market.

The Future of Carbon Dioxide

To meet net zero emissions goals, we must address the considerable mismatch between the amount of CO₂ we produce and the amount we use. Leveraging the UK's world class capabilities in materials chemistry to develop effective carbon capture and utilisation technology will help us create a more sustainable and circular carbon economy.

The National Interdisciplinary Centre for Circular Chemical Economy (NIC3E) is an academic partnership, bringing together both university and industry partners to 'close the carbon loop'. As part of the partnership, we at the University of Liverpool's Rosseinsky and Cowan research groups are interested in developing sustainable fuels and studying the catalysts that are needed to make them. Our work focuses on two different transformation routes; the chemical recycling of waste polymers and

the electrochemical conversion of CO₂. With the net zero target in mind, we are also particularly interested in more general ways in which we can utilise CO₂ as it is produced. Developing effective and viable technology for carbon utilisation will help to support a circular carbon economy, driving progress towards net zero goals.

Connectivity throughout the supply chain is also vital in developing effective carbon utilisation and recycling solutions that will be adopted by the industry. By working with KCMC, we gain access to a broad network of partners to support the work of NIC3E. Through such collaborations, we can begin to bring together the broad range of approaches needed to transform the future of carbon use.

Leveraging the UK's world class capabilities in materials chemistry to develop effective carbon capture and utilisation technology will help us create a more sustainable and circular carbon economy.

Professor Alex Cowan
University of Liverpool



Industry Steering Group Meeting 2020

Growing the Hydrogen Economy

KCMC's Industry Steering Group (ISG) meeting was hosted virtually this year and centred on the emergence of the hydrogen economy in the UK. The event brought together key stakeholders in both industry and government to begin to address the needs and opportunities for materials chemistry in developing the hydrogen economy.

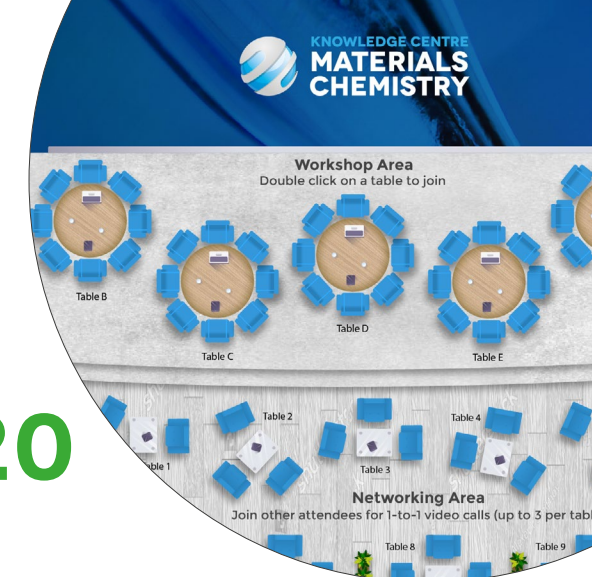
As an industry, we have a timely opportunity to contribute to a greener energy landscape whilst driving innovation in materials science. The focus on the hydrogen economy has been sharpened by increasing concern around climate change and the government's goals. In addition, the COVID-19 crisis has added emphasis to the need for change, further increasing demand for greener energy.

At the event, we heard from several of our partners about their individual approaches to the challenge. There are several main areas of opportunity for materials innovation within the hydrogen economy, including catalytic systems for generation and use of hydrogen, materials for storage and transportation of hydrogen, and safety at scale. Further, there are opportunities to use hydrogen as a feedstock in a future zero-carbon chemical industry. Developing all these aspects will draw on diverse innovations in materials chemistry. KCMC and its partners will have a fundamental role in realising this potential, establishing a more sustainable energy landscape and driving innovations that will help to shape the future of the industry.

In 2021 the Henry Royce Institute, one of the key partners in this area, is leading a targeted review of the research and innovation opportunities and challenges for materials, across the end-to-end hydrogen value chain. The findings will be used to inform policymakers and help funders to shape future programmes.

This study covers all applications of materials in hydrogen economy: from hydrogen production and compression; through storage, distribution and dispensing; to end use in transport, heat, energy system integration, chemicals and foundation industries. The activity builds on the community roadmap developed for research on green hydrogen production. The review is sponsored by the EPSRC.

**HENRY
ROYCE
INSTITUTE**



KCMC Metrics

From growing connections with SMEs to facilitating new networks for our partners, KCMC has continued to progress in the UK's dynamic innovation environment. By looking at the metrics from the 2019/2020 and 2020/2021 financial years we can gain insight into how KCMC has adapted and contributed to industry growth and success.

CONNECT

KCMC enables industry connections – engaging with a variety of company types across a wide range of sectors. When compared to previous years, industry engagements over the past two financial years have remained more or less stable. In the 2019-21 period, the industry sector with the greatest engagement was 'Chemicals and Materials' (Figure 2), representing 67% of all industry engagements. This is slightly up on 2018/19, where this sector represented 62% of all engagements and it continues to be a significant and stable portion of KCMC's engagements, highlighting the consistency in KCMC's broad drivers.

Industry engagements across another eight sectors were also significant. The top four industry sector groupings outside of 'Chemicals and Materials' were 'Energy and Environment', 'combined MedTech and Pharma', 'Food, Agriculture and FMCG' and 'Aerospace and Defence' at 8, 8, 4 and 4% respectively (Figure 2). This wide range of sectors supports the multi-disciplinary and multi-sector focus of KCMC and the materials industry as a whole, wherein major themes, such as sustainability and the circular economy, are represented not by a single sector, but rather a combination. This reflects on the broad impact potential of materials chemistry innovation.

Looking at company type, of the 47 industry engagements over this period, UK SMEs represented the highest percentage at 38%, a slight decrease from the previous year's 39%. However, UK corporations and foreign-owned/multi-national companies were also well represented over this period, with industry engagements at 34% and 29% respectively (Figure 1). Crucially, these engagements included 135 first-time introductions of companies to KCMC, of which the great majority were either UK SMEs (61%) or multinational UK subsidiaries (24%). This represents an increased amount of first-time company introductions per year (67) compared to the prior year 2019 (57).

This stability in engagement is impressive given the difficulties and challenges associated with the 2020/21 year, considering local, national and global COVID-19 restrictions. But three years into KCMC's new positioning within its host organisation, CPI, and the wider High Value Manufacturing Catapult, it is evident that the fruits of this collaboration are being seen more clearly. Connections are being strengthened and KCMC is effectively engaging with different companies across many sectors to promote innovation and success.

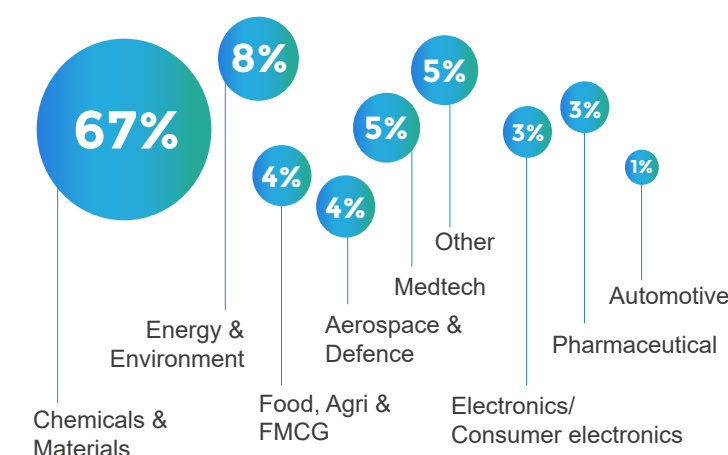
Figure 1:

Industry Engagement by Company Type 2019-2021



Figure 2:

Industry Engagement By Sector 2019-2021



FACILITATE

A main focus of KCMC is facilitating new connections for the multi-sector and multi-levelled materials network. Along with the 135 first-time company KCMC introductions, a total of 317 engagements delivered new connections between researchers and industry across KCMC partners in the 2019-21 period.

KCMC's referrals outside of its Research Institution (RI) partners represented approximately 27% of its total engagements over this period. This is significantly up on the 22% recorded in 2018/19. Referrals outside of its RI partners include 'business-to-business', and wider network connections, such as KTN, which have been broadly consistent with the prior year (6% and 3% of total engagements respectively). But the highest percentage of these referrals are 'business to Catapult', primarily through CPI (now 18% of total engagements and 70% of referrals made).

Following KCMC's hosting transfer from the KTN to CPI in 2017, there has been a steady increase in these referrals from KCMC across the Catapult network. This has continued throughout the 2019/20 and 2020/21 periods (Figure 3).

Despite the growth and stability in these broader metrics, there has been some variability in quarterly connection facilitations as a result of COVID-19 and the restrictions in place. The initiated engagement numbers were very high in January-March of 2020 (77), with a slight drop in numbers in April-June (53), followed by the lowest quarter, July-September (31), where the impact of the pandemic was most felt. However, these numbers have already rebounded in the last quarter of 2020 – with 51 from October-December – and are set to stabilise or even increase in 2021.

The way contacts and connections are typically made is through networking opportunities at events – i.e., seminars and conferences. While COVID-19 has impacted this method of networking, it has coincided with a time in which KCMC's existing network is strong. This existing network across the Catapults, through CPI and other partners, is continuing to facilitate networking, despite an overall change in the way these new businesses are introduced.

Figure 3:

KCMC Referrals Outside RI Partners 2020-2021



DELIVER

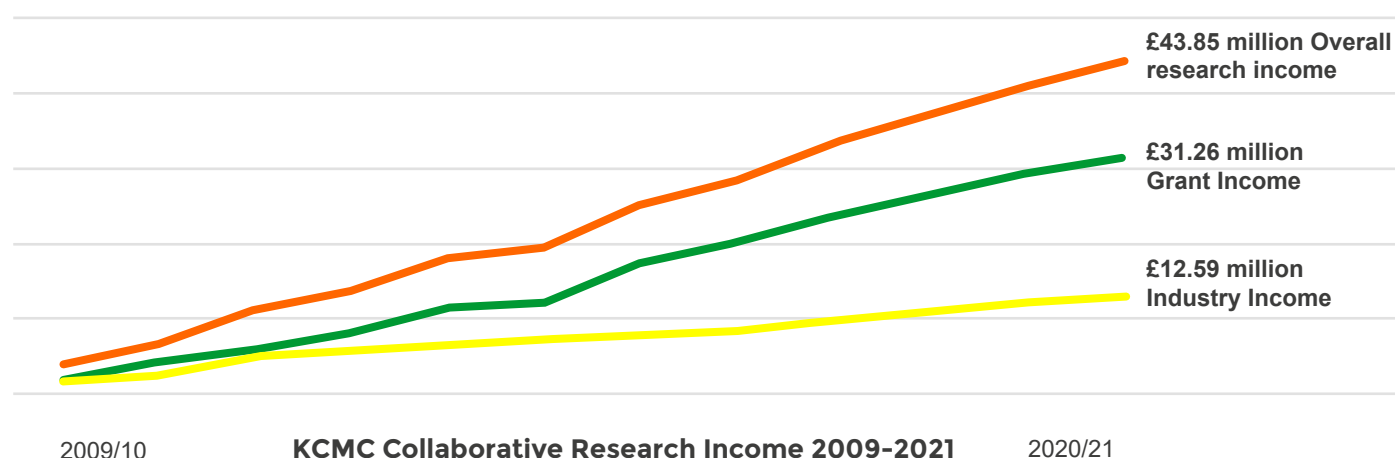
KCMC continues to deliver successful research collaborations between industry and research institution partners, illustrated by its collaborative research income. The 2019/20 year was very strong in terms of financial growth, with a cumulative growth of £4.20 million in research income over this period. In fact, there was an approximate 15% cumulative growth in the 2019/20 period when compared with 2018/19. £1.41 million of this growth originated from industry income, up from the £0.8 million contracted in 2018/19.

The 2020/21 period reversed this trend, with COVID-19 impacting the industry as a whole, as well as the availability of grants. Despite the slowdown, there was still a £2.8 million cumulative growth, and with KCMC's engagement numbers increasing in the last quarter of 2020, this growth is expected to pick back up as we move further into 2021.

Overall, KCMC is continuing on its strong trajectory and continuing to deliver significant research income. Since its founding in 2009, the total delivered across the KCMC partnership is now cumulatively £43.7 million, including £12.7 million in industry funding.

Figure 4:

KCMC Collaborative Research Income 2009-2020



Growing engagement and a science-driven technology pipeline

In 2019-21, the highest proportion of KCMC's industry engagements were from UK SMEs at 183 engagements, consistent with the past four years' results. A significant number of these are with University spin-outs, at 58 or 32% of UK SME engagements in the past two years. This represents a significant increase over the two previous reporting periods (21% for 2019 and 23% for 2017/18 respectively as a % of total UK SME engagements).

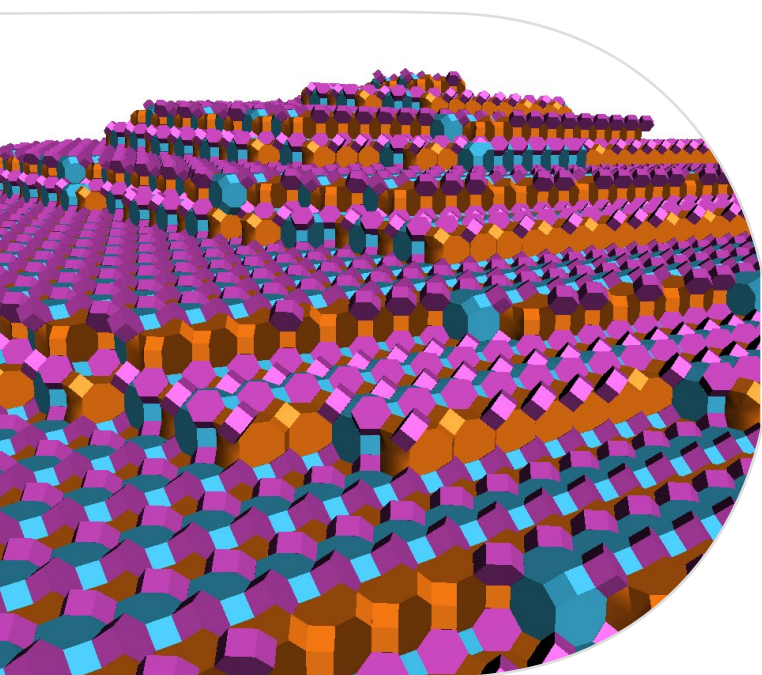
With a significant proportion of SME engagements coming from University spin-outs, the Catapult model provides these new businesses with a unique opportunity to bridge the gap between research and industry. Building on this connection with KCMC, and CPI more broadly, can help enable new ideas and innovations to become marketable products. This is clearly shown in the data from the past four years, where engagements with SME

University spin-outs leading to referrals to CPI have grown from 4% in 2017/18 to 10% in 2020/21. Even more strikingly, referrals to CPI of UK SME spin-outs from KCMC partners have grown from 1% to 6% (% refers to % of total UK SME engagements).

By introducing these SMEs to CPI, this is resulting in more connectivity across KCMC and its partners, therefore enabling a better and accelerated translation of innovations. Over the past two years, 11 spin-outs from KCMC partner universities have been introduced to CPI; in many cases initially working with the investment support unit of CPI (CPI Enterprises) and then leading to project working and in one recent case an Innovate UK grant. The role of CPI Enterprises is highlighted on page 25 of this report.

One of the services already available to these university spin-outs is CPI's Innovation Integrator®, which provides SMEs with further access to CPI's innovation expertise. Overall, this network provides SMEs with the ability to better translate innovations from the bench to commercial applications, supporting the R&D landscape of the UK as a whole.

Partner Updates



CrystalGrower Visualiser of Screw Dislocation in Nanoporous Catalyst, University of Manchester



Professor Mike Anderson
University of Manchester

Work to complete the Christabel Pankhurst Institute for health technology research and innovation took place throughout 2020, and the institute formally opened in January 2021. This Institute is a unique partnership between the University of Manchester, NHS, business and local government, and will form an important part of the Greater Manchester health innovation ecosystem, working together to translate world-leading research into new products and services.

In a major milestone, researchers have begun to move into the Henry Royce Institute's flagship Royce Hub Building on campus at the University of Manchester. Royce has also launched the Sustainable Materials Innovation Hub. This major investment was part-funded by the European Regional Development Fund and aims to work with SMEs across Greater Manchester to create sustainable solutions for plastics use. In addition, the University is in the final stages of creating the Manchester Engineering Campus Development (MECD). The ambitious MECD project will establish the single largest home for engineering in any UK university and will offer world class research and teaching facilities, leading the way in terms of innovation in technology and working practices.

In the Department of Chemistry, Professor Mike Anderson has developed software that is capable of simulating the growth of crystals. This tool permits the rapid simulation of crystal surface maps generated by scanning probe microscopies in combination with overall crystal habit. This Monte Carlo and visualisation software, CrystalGrower, is able to simultaneously simulate both crystal habit and nanoscale surface topography. This is achieved for generic crystal forms under non-equilibrium conditions, with the ability to add growth modifiers and to incorporate dislocations and defects. The original concept has been described in *Nature*, 2017, 544, 456–459 and *Chem. Sci.*, 2021, 12, 1126–1146. CrystalGrower Ltd has recently spun out from the University of Manchester with initial investment from BASF to work on future IP. Commercial licences of the software are available as well as free licences to academia.



Throughout 2020, the STFC Hartree Centre has been stepping up to support businesses through the COVID-19 pandemic, with many keen to explore the benefits of digital-first approaches to design and manufacture, which enable us to be productive from home. The continuation of the highly successful Bridging for Innovators programme, as part of the Industrial Strategy Challenge Fund, has benefitted several companies engaged with KCMC. The Hartree Centre has been involved in several COVID-19 related projects, providing our supercomputing power to assist in the global computational drug discovery efforts of the folding@home project, and exploring an AI chatbot to help inform hospital staff about COVID-19 and keep abreast of the latest information. Hartree Centre Research Software Engineers are also working with other UKRI scientists to develop a robust, low-cost ventilator to help patients in low- and middle-income countries suffering from severe respiratory problems due to COVID-19.

There have been new additions to our infrastructure, with our Scafell Pike industry-accessible supercomputer receiving an upgrade with extra processing capability optimised for AI and Molecular Dynamics workloads. In addition, in 2020 the UK's largest AI supercomputer, JADE-2, was made available for industrial access, also with benchmarks showing strong performance in certain computational chemistry applications.

In September 2020, the Hartree Centre achieved ISO9001 accreditation, recognising our commitment to quality and professional delivery in everything we do, and we are now looking forward with great optimism to the next stage of our development and working with even more businesses to help them prosper.



This year has seen the new chemistry undergraduate teaching laboratories and the electrochemistry research labs operational with further improvements to the chemistry buildings completed. Construction has started on the new chemical engineering teaching laboratories within the Chemistry building complex, which will be ready in January 2022. An MSc in Advanced Chemical Engineering has started, with a graduation this year, and the first group of undergraduate students (BEng and MEng) will start their degrees in September 2021.

In a change of responsibilities within the School of Chemistry, Professor Jon Essex has taken on the role of Head of School from Professor Gill Reid. We would like to thank Gill for her part in establishing Southampton as a Partner in KCMC and congratulate her on her success in becoming President-elect of the Royal Society of Chemistry. Thanks also to Darren Bradshaw for his work as co-PI with Andrew Hector and welcome to Robert Raja who is the new Head of the Functional Inorganic, Materials and Supramolecular Chemistry Section and will be replacing Darren as co-PI.

The quality of research within the School has also been recognised, with major grants awarded in the areas of flexible hybrid thermoelectric materials; the development of the next generation p-type transparent conductors; the use of highly integrated computational modelling and experimental approach for the next generation of ammonia synthesis and new interstitial palladium nanoparticles for directed catalysis.

Southampton remains at the forefront of battery development as partners in several Faraday Battery Challenge projects, from next generation electrode manufacture, Lithium-Sulphur technology accelerator to advanced meta-materials for sodium-ion battery anodes. There has also been a successful EPSRC grant application on Correlative Raman, SEM and EDX for operando electrochemistry research.



The University of Bolton maintains an applied focus, with fire materials research continuing to help the industry develop safer fire retardant products. Advanced techniques for fibre spinning are being deployed in biomedical applications, such as synthetic tendons and highly engineered vascular implants, and auxetic materials are being developed for potential use in hip replacements with improved structure and mechanical properties closer to bone. The university is also active in environmental science, offering a BSc programme and leading research into dielectrophoresis-assisted adsorption technology for removal of biological, organic and inorganic pollutants from water.

The University of Liverpool has broad and diverse materials chemistry research interests with current innovation priorities including materials for hydrogen production, sustainable fuels and chemicals, novel battery materials, transparent conducting coatings, thermo-regulating paints, infection control, sustainable packaging and advancing the state of the art in solid state NMR. The university is world leading in autonomous and digital approaches to materials chemistry research, deploying them with industry partners to solve complex formulation and materials discovery challenges. Committed to developing long term and impactful relationships with industry, the chemistry department runs the annual IChEM meeting to share research highlights with present and future industrial partners.

Several spinout companies have been formed, Cage Capture Ltd exploiting the unique attributes of porous organic cages for pollution management, Meta Additive Ltd developing functional inks for additive manufacturing of metals and ceramics and a JV initiated with Scott Bader in polymer chemistry through Polymer Mimetix. During 2020, the university's unique on-line learning tool ChemTube3D reached in excess of 5.5 million users, benefitting chemistry students across the globe and providing an invaluable open access chemistry learning resource throughout the global coronavirus pandemic.

In 2020 the university also welcomed Professor John Bower as Regius Chair of Chemistry, his research focussing on organic synthesis catalysis. As we move in 2021, we look forward to new partnerships including the National Interdisciplinary Circular Chemical Economy Centre, Battery2030+, prosperity partnership with Unilever and through robotic laboratory capabilities at the Materials Innovation Factory.



Mobile robotic chemist at University of Liverpool's MIF

The Role of Materials Innovation in Achieving a More Sustainable Future

The cars we drive, the buildings we live and work in, our clothes, medicines and digital devices are all products of manmade materials – they are all around us. Making materials, supplying products and disposing of them are all major sources of waste and pollution, as well as contributors of roughly 15% to global CO₂ emissions. Since many of these materials are essential to life – focused on health and basic living needs – we cannot simply stop making them, but instead must bring fresh innovation to the materials sector in order to achieve a sustainable future.

Materials development has always been driven by a desire to create 'better' – better being both performance and sustainability, albeit with the relevant priorities oscillating between these themes. Sustainability, in the form of best practice technology, has been a legal requirement in the UK since 1848 and the principle of BATNEEC 'Best Available Technology Not Entailing

Excessive Cost' has been the framework for western economies since 1984. So, has anything changed?

As climate change and its impacts have become more obvious, citizens are increasingly demanding change from governments, with industry having to respond to these needs through changes to policy and investment priorities. Whilst enhanced product performance was the primary driver for innovation hitherto, over the next 30 years we can be certain that sustainability will be driving innovation for materials manufacture, application, and especially new process innovation. Most of CPI's customers tell me that they have not experienced such a degree of change in their lifetime. As such, there is a need for a national strategy and a framework that puts UK-based opportunities in an international context.

UK energy price competitiveness:

Historically high cost compared to EU competitors. However, there are now huge investments committed to 'green electricity' from the North Sea wind estate, grid infrastructure upgrades, and new initiatives in hydrogen and solar. This unprecedented level of re-investment will change the UK's ranking for energy input costs.

Protection from 'dirty' competition:

Legislating away unsustainable manufacturing practices that avoid offshoring and so-called 'dirty' competition. This is a live issue within government, implementing workable ways to count embodied carbon emissions in products.

New business and supply chain models:

With two drivers of change:

- Developing new business models for the circular economy
- Tying the digital revolution into the circular revolution so that we don't re-invent new business models twice over.

What price will the consumer pay for sustainability?

Consumers and governments demand innovation with minimal additional operating cost. Articulating the price for sustainability and exposing the true

cost of existing approaches will be key to successful market adoption of new technology.

Cost of risk capital:

The cost of global capital is extraordinarily low, where investors can quantify the risk in innovation. A UK legislative framework is required that allows for better quantification of risk for sustainability-based investment. There is a need for European companies to access risk capital at rates competitive with Asian and Chinese state-backed enterprises.

Crosscutting competitive advantage:

Enabling companies to read across from complementary market sectors. Historically conglomerate chemical companies operated this model, but globalisation has tended to focus companies into specialisation which makes it harder to spot adjacent market opportunities. We have a role as a 'materials' community to accomplish this activity.

Complex innovation landscape:

Companies will have to implement a larger number of costly technology innovations in a relatively short period of time. There is no one silver bullet for sustainability. Several process changes will be required, and this presents greater complexity for companies than they have seen in a generation.

The role of materials innovation... continued

Of these factors many are macroeconomic and require dialogue at a national level, but the last two are within our sector's control. We can build on existing work; BEIS, the Chemistry Council, and the other industry sector councils have strategies for the discrete materials technologies, so it's an issue of joining and synthesising cross-sector information.

Within the Catapult network we have been coordinating our activities for net zero with cross CPI/HVMC programmes and a partnership with the Energy Systems, and Offshore Renewable Energy Catapults to provide an end-to-end overview. We have cross-sector teams in the following areas:

- Circular economy – across HVMC and its members
- Energy generation, storage, distribution, and use – in collaboration with Energy Systems Catapult
- Hydrogen generation, storage, transport, and use – across HVMC and members
- Net zero transportation – across HVMC and its members
- New materials – across HVMC and its members

The aim is a common approach by these Research and Technology Organisations (RTOs). Our first deliverable is a report prepared for BEIS - on 'Enabling Conditions for NET Zero Manufacturing'. This is an ambitious comprehensive UK report with input and feedback from industry, including several members of KCMC. A prime recommendation of the report, which will be published later this spring, is to develop a net zero strategy for materials.

Projects under the banner of sustainability account for a major part of CPI's income. We have developed in-house tools for Life Cycle Assessment (LCA). Process engineers are naturally versed in the issues, as heat and mass balance are the first considerations of a process design, just requiring more knowledge of up and down stream processes. Teaming up with our colleagues via the HVMC has enabled us to extend this work across supply chains, from raw materials to applications in finished goods. An idea of the breadth of sustainable projects can be seen from these three customer case studies:

LiNa - the future of battery technology

LiNa Energy (LiNa), a Lancaster-based SME and spin-out from Lancaster University have invented a novel sodium-nickel-chloride (Na-Ni-Cl) battery technology as an alternative to the widespread, but resource limited, lithium-cobalt ion (Li-ion) battery. LiNa Energy worked with CPI to demonstrate low-cost scalability of the technology and proved the viability of this novel battery chemistry.

LiNa Energy's battery has the potential to be a cheaper, safer, and more sustainable method of energy storage.

NPIC - innovative packaging

Liverpool City Region Combined Authority (LCR CA) is creating a Future Packaging Cluster, featuring the National Packaging Innovation Centre (NPIC), to be delivered in partnership with CPI and Unilever PLC. The centre will accelerate sustainable packaging development and play a key role in enabling transformational manufacturing, recycling technologies, packaging for emerging channels and smart supply chains. To drive innovation in packaging in the UK, the centre will:

- Provide access to industrially relevant capabilities and expertise for packaging innovation, development and demonstration,
- Facilitate collaboration across current and future packaging supply and value chains,
- Catalyse an ecosystem for growth and productivity through harnessing opportunities presented by disruptive and market-creating innovation and its commercialisation.

New drivers, such as clean growth, smart supply chains and empowered consumers, will shape the future of the growing global packaging market. With the right interventions, the UK could capture a significant share of this market, providing the UK packaging industry with access to new technology solutions and supporting the growth of packaging innovation capability.

SusWIND - sustainable wind turbines

The National Composites Centre (NCC) has launched SusWIND – an initiative to ensure the sustainability of future wind turbine technology. The project is part of the Sustainable Composites Partnership – a national initiative led by the NCC and CPI to develop the next generation of sustainable composite materials by turning research breakthroughs into industrial applications. By building a community of stakeholders and experts in the UK's composites industry and energy sectors, the project aims to create end-of-life value from the current generation turbine blades and embed circularity at the heart of future generations of turbines. To make that happen, the programme will solve the following challenges:

- Recycle: Demonstrating viable technologies for recycling the existing stock of wind turbine blades
- Sustain: Driving the use of more sustainable materials and manufacturing processes
- Design: Developing innovative new approaches based on circular economy principles

SusWIND will be delivered in partnership with the Offshore Renewable Energy Catapult, and has support from The Crown Estate, RenewableUK, Shell and BVG Associates. The commercial partners at time of launch are: Vestas, SSE Renewables, EDF Renewables and OGTC.



Dr Tom Taylor
Director of Future
Business, CPI



In my opinion the materials industry is at a real turning point. If CPI's portfolio of projects is a yardstick for the wider sector, it may signify a historical shift in materials innovation. Similar to the move from coal to oil, and the technology advancements and market opportunities that arose, the transition to net zero and sustainable materials has the potential to create much-needed improvements and opportunities within this sector.

Over the coming months we will be working with others to pull together a UK strategy for sustainable materials in a net zero economy and provide our sector with a little more confidence on innovation choices going forward.



Formeric Ltd

Formeric Ltd puts supercomputing into the hands of formulation scientist for the development of improved surfactant-based products.

With an annual global market predicted to grow from \$36 billion in 2017 to \$45 billion by 2022, surfactants are widely used in applications ranging from cleaning products in home and personal care settings, to controlled drug release systems, friction modifiers, and remediation of contaminated soils. A major driver for innovation is the need to support decarbonisation of the market by moving away from petrochemicals, and traditional plant-based feedstocks, towards sustainably sourced raw materials. These challenges can be met in part by the be met in part by deployment of predictive computer-aided formulation design and engineering approaches.

Whilst it is becoming increasingly recognised that access to high performance computing and sophisticated predictive simulation methods can shave months off time-to-market, it is a complex process and can be a daunting task without an in-house specialist and significant computational hardware.

Recently, the STFC has spun out a company offering easy access to cloud-based simulations of formulated products. Formeric Ltd builds upon over a decade of developments in the simulation of formulated products by the team at the Hartree Centre, allowing formulation scientists to evaluate the performance of candidates prior to commencing lab trials, without the need for prior computational knowledge. This approach can decrease the time to screen new molecules and their compatibility, increasing the likelihood of identifying the desired formulation. With this approach it is possible to screen a number of candidates in-silico in a fraction of the time taken for lab trials.

Cleaning products, cleaner fuels, and more sustainable crop protection products - these are just some of the widely varying consumer and industrial goods that could benefit from this capability. Company needs can all be very different, but they all have in common the need to understand the ingredients they use as quickly and efficiently as possible.

CPI Enterprises

In 2020, CPI Enterprises was formed to extend investment support to fast growing, high potential companies in the deep-tech space. Enterprises connects investors and entrepreneurs across the UK to stimulate impactful and capital-efficient investment into innovative technology companies. Enterprises' support is available to engage with potential investors, understand the fundraising process and position early stage companies to secure private investment to drive novel technology through to commercialisation. In addition, Enterprises is directly investing in early-stage technology companies, with a particular focus on pre-seed and seed funding rounds.

Enterprises is headed by Alfredo Ramos Plasencia and Hannah Wade, who lead a team of Investor Relationship Managers and Investment Analysts, helping companies access a range of investment opportunities including pre-seed, seed, series A and follow-on capital for scale up to accelerate their next stage of development. Direct investments from Enterprises come in the form of sweat equity and cash with a focus on pre-seed and seed investment rounds. The Enterprises Investment Committee is supported by high-calibre external advisors: Tim Cockcroft, CEO of N+1 Singer, a leading investment bank dedicated to advising and funding ambitious growth companies in the UK; Saar Shafir, CIO of Treisar Investments, investing in and supporting visionary teams with transformative

technologies and business models in the UK and Israel; and Andrew Schemmel, Director at Eisvogel Group, a specialist industrial investor investing in growing family or owner managed businesses across Europe, and with a particular focus on Industry 4.0 and the ageing population.

The formation of Enterprises builds on CPI's service offer, integrating industry-relevant expertise and assets, knowledge and application of innovation processes with investment support. Since formation, Enterprises has assisted over 60 early-stage technology companies, including KCMC partner university spin-outs, to develop investment prospects and to understand the investment environment.

Dr Ming Liu, CTO of Cage Capture Ltd, a University of Liverpool spin-out developing novel porous materials for pollution management, has worked with CPI Enterprises and said:

“Working with CPI has allowed Cage Capture Ltd to address technical challenges in the scale up of our technology and also to develop our business case as the company grows and works towards securing investment. CPI is uniquely placed to give such support to advanced materials innovation.”

Alfredo Ramos
Managing Director
of Enterprises, CPI



Hannah Wade
COO of CPI Enterprises



Dr Ming Liu
Co-Founder & CEO at
CageCapture Ltd



Industry relevant expertise and assets
Delivering product development, proof of concept, and scale-up services.



Expertise in securing funding and investment for companies

Enabling the right partnerships, connections, and funding routes at the right time.

Knowledge and application of innovation processes

Business services and consultancy to reduce risk and speed up time to market.

Case Study



Vitafoam

Ensuring fire safety of next-generation foams

Through industry networks that KCMC and KTN support, a collaboration between Vitafoam (Middleton, UK) and the UK's leading fire materials research group, led by Professor Baljinder Kandola at the University of Bolton, has been forged to develop next-generation fire-retardant polyurethane foams.

Vitafoam, founded in 1949, pioneered the manufacture and commercialisation of "Combustion Modified Foams" in the UK and maintains an industry-leading position for supply of foams to furniture, bedding and specialist applications. Enabled by an Innovate UK Knowledge Transfer

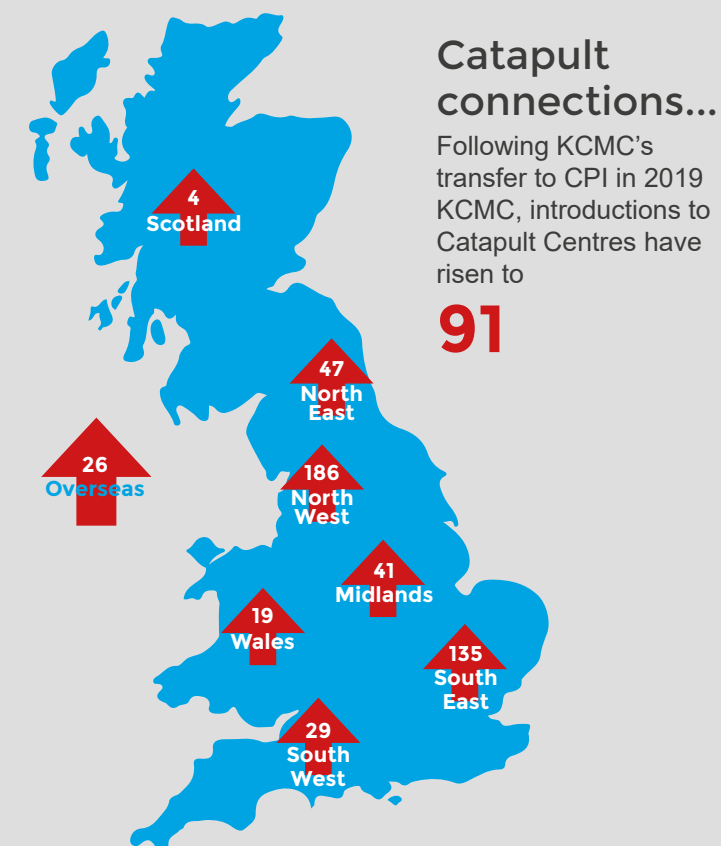
Partnership (KTP) awarded to the University of Bolton and Vitafoam, a product development strategy has been developed to mitigate potential chemical legislation under REACH that may impact the continued use of established flame retardants. The objective of the partnership is to safeguard the fire performance of future foam products through investigating alternative retardants and re-formulation.

KCMC has helped secure several KTPs with its research partners; the flexibility and industry-focussed assistance for companies that the KTP supports is an ideal mechanism for skills and knowledge transfer between academia and industry. Please get in touch if you would like to know more Info@materialschemistry@uk-cpi.com.

Image above provided courtesy of Vita Group

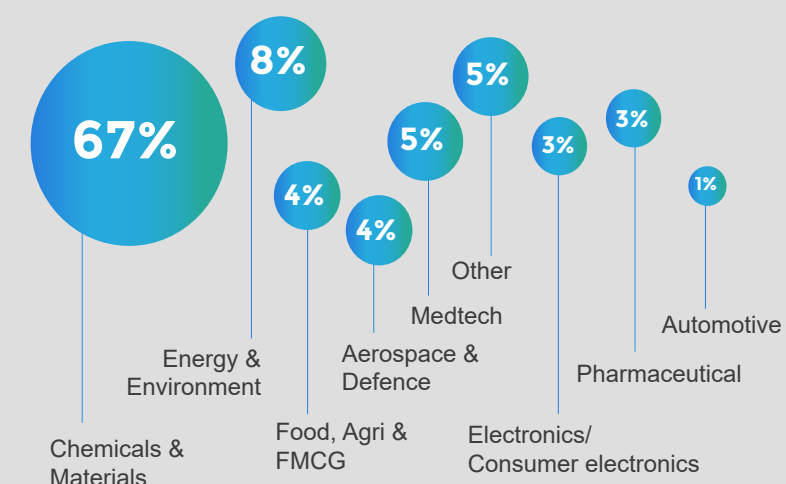
Connect

KCMC has made 487 business engagements across the UK and internationally



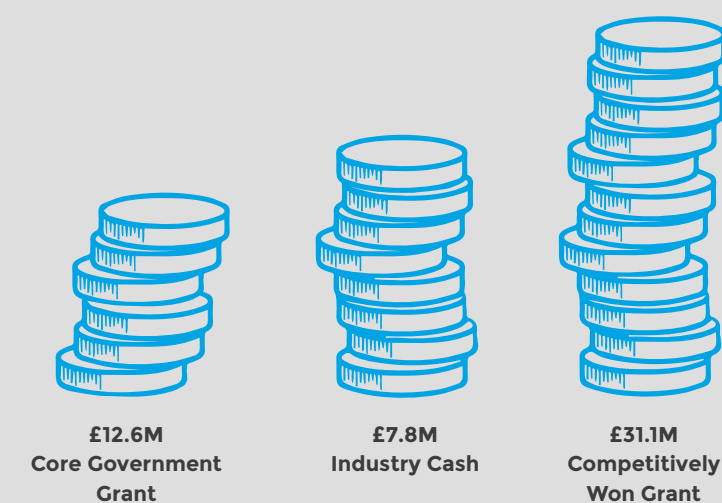
Facilitate

KCMC has facilitated projects within key Industry Sectors



Deliver

Leveraged £44m Collaborative Research Income from £8m Core Grant



Leadership Team



Professor Matt Rosseinsky
Professor of Inorganic Chemistry,
University of Liverpool



Professor Michael Turner
Professor of Materials Chemistry,
University of Manchester



Professor Baljinder Kandola
Professor of Materials Fire Science,
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