The role of materials chemistry in meeting the UK's net zero commitments

RSC Materials Chemistry Division workshop report

February 2021

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Background

Civilization employs thousands of energy intensive processes, taking place around the globe on an ever-increasing scale. Materials are at the centre of these processes, and materials chemistry will play an important role in reducing emissions of atmospheric carbon dioxide (CO_2) by supporting a transition to new low-carbon technologies.

The UK Government has set out a target of net zero emissions by 2050. Pathways for decarbonisation have been set out by bodies such as the UK's **Climate Change Committee**, and investments by the UK Government set out to achieve emissions reductions that will reduce our reliance on fossil fuels; for example, through the adoption of electric vehicles and home insulation. But technology innovations are needed – to bring forward the hydrogen economy, deploy negative emissions technologies, and reduce the lifecycle carbon impact of all technologies – as well as the infrastructure that will be needed to achieve net zero in other sectors.

The Royal Society of Chemistry's Materials Chemistry Division brought together experts from across the scientific community based in industry, academia and research institutes, to explore the role of materials chemistry in meeting the UK's net zero ambitions. This report is a summary of those discussions, highlighting opportunities for future research, emerging technologies that may play a role in moving to a net zero economy, as well as some of the barriers and potential enablers to this transition.

Key findings

Action is needed now

We need to deploy low and zero emissions technologies at scale by 2030 to achieve net zero by 2050. This requires a step change in the pace of technology development and deployment, underpinned by government investment and policies to incentivise the accelerated adoption of low emissions technologies.

Energy is an enabler for emissions reductions in other sectors

Energy supply is the main driver of carbon emissions in industry, as well as in the recycling processes essential to achieve a circular economy and reduce waste. We need to dramatically reduce emissions at all stages. This includes decarbonising the sources of power used in manufacturing, increasing the energy efficiency of manufacturing processes and transportation, and reducing the energy required for recycling or disposal of materials and products at end of life.

Circularity is vital

New technologies to reduce emissions will rely on raw materials, and increase pressure on supply in some cases (for example the lithium needed for lithium-ion batteries). We need to ensure that we manufacture efficiently and keep materials in circulation for as long as possible, to reduce pressure on our natural resources. Similarly, processes to recycle waste should not result in increased CO_2 emissions relative to new virgin materials. Circularity and carbon reduction must go hand in hand.

Applied and discovery science will both play a role – and collaboration is key

There are promising avenues of research across all areas of chemistry, including materials for energy generation and storage, construction, and carbon capture, utilisation and storage (CCUS), as well as manufacturing processes that use electrochemistry and new catalysts to reduce energy demand. An important theme is the need to collaborate across disciplines and sectors. Chemists need to collaborate with engineers, as well as experts in life cycle analysis, chemical engineering, design, and policy (among others), to support technology deployment and adoption.

To reduce environmental impact, we must be able to measure it

Life cycle assessment (LCA) is essential in developing technologies that are low carbon throughout their lifespan. This is an area where the UK faces a skills gap.

Going beyond carbon neutral

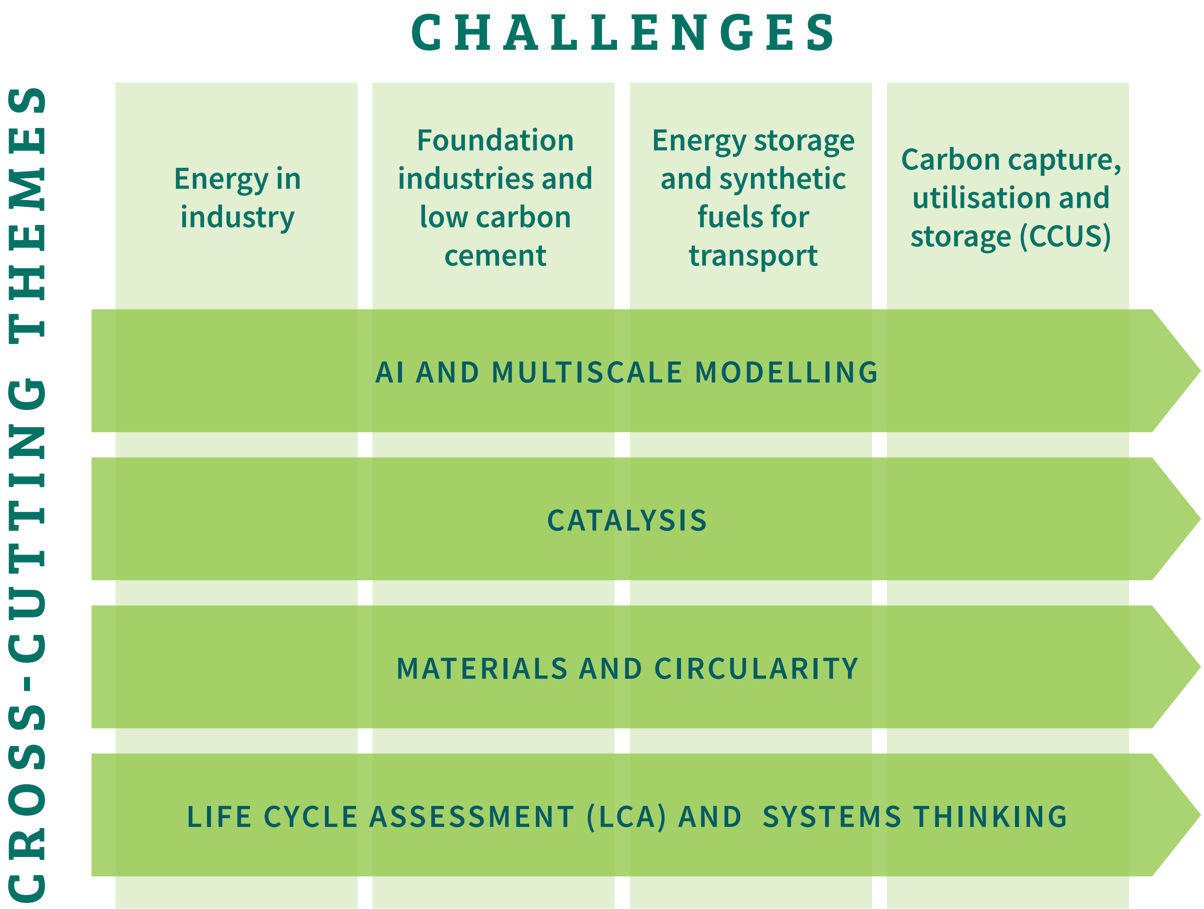
Emissions scenarios to 2050 require the use and widespread deployment of negative emissions technologies to keep global temperature rise below 1.5°C. An important example is carbon capture, utilisation and storage (CCUS). This is a set of technologies that take CO_2 out of the environment. Most CCUS technologies are at low Technology Readiness Levels in terms of efficiency, cost and scale, and a step change is needed to enable their widespread deployment. This requires funding as well as support for greater access to testing and pilot facilities.

Challenges and research priorities for the chemical sciences

The workshop identified a number of challenges and research priorities for the chemical sciences, particularly materials chemistry, in achieving net zero. These ranged from specific application areas to cross-cutting topics and design considerations.

This is not an exhaustive list, and materials chemistry underpins many other areas in sustainability not covered during the workshops, from renewable energy to sustainable plastics.

The four challenge areas and cross-cutting themes discussed at the workshops are depicted in the infographic below:



Challenge areas

Energy in industry

Energy is an enabler in all industries, as well as the recycling process essential to achieve a circular economy and reduce waste. Decarbonising the energy sources used by industry – not only in manufacturing, but also in transportation, recycling and disposal – will have a major impact on those industries' carbon footprint.

Chemistry's role will be vital in:

- achieving new and more effective catalysts to reduce the energy input required in manufacturing materials such as plastics, bulk chemicals, fertilisers and pharmaceuticals
- improving circularity and the recycling of materials with high embedded emissions, including those produced in the foundation industries (defined below), ensuring that the recycling processes are less CO_2-intensive than using virgin raw materials
- measuring and improving emissions intensity at all stages of manufacturing, to understand bottlenecks and quick wins
- considering low CO_2 ways to manufacture new technologies at the outset (avoid 'baking in' inefficiency)
- improving energy efficiency; for example, by development of low friction materials
- reducing the embedded carbon in renewable energy technologies such as photovoltaics and batteries

Foundation industries and low carbon cement

Foundation industries (including cement, paper, glass, ceramics, metals and bulk chemicals) are worth £52 billion annually to the UK economy, but are also responsible for 10% of the UK's carbon emissions. One of the most important, but also most carbon-intensive, foundation industries is the production of cement.

Cement and concrete are vital materials used across the globe in large quantities, providing housing and critical infrastructure for the majority of the world's population. Worldwide, it is estimated that cement production has a **higher carbon** footprint than any country in the world, except the USA and China. Almost all the world's cement is produced as Portland cement; a mixture of limestone and clay which undergoes calcination in a high temperature kiln before being ground and mixed with gypsum and other mineral components.

Around 90% of the CO_2 emissions of Portland cement are from the production process, particularly the high temperature calcination reaction, which is usually powered by coal combustion, and involves the direct release of CO_2 as the limestone decomposes.

While it is possible to move to **low carbon fuel sources** in cement production (such as biomass or hydrogen), achieving net zero with traditional cement products will be extremely challenging, since around 70% of the CO_2 emissions in cement production are from limestone decomposition.

Concrete provides highly desirable properties and is hard to replace – particularly in the construction industry, where high investment and proven alternatives would be needed to move away from a low cost, reliable material that has been in use for centuries. Safety considerations are paramount in the construction industry, so alternatives will need rigorous testing and validation.

Chemists and engineers are developing a range of lower carbon cement materials that work for specific situations, allowing for lower impact and more efficient use in construction. For widespread adoption, the cost of replacement materials must be low. Another promising avenue is to develop materials with enhanced properties, eg high strength, for early adoption in niche application areas. In the short term, a critical review of the CO_2 emissions in novel cement production is needed, to guide our understanding of which types of cement are most promising for achieving net zero emissions.

Alternative materials and approaches include:

- alkali-activated materials for potential replacement of certain Portland cements
- graphene and nanocellulose additives that can produce desirable properties – this is particularly important for more niche applications in industry and is currently an active area in the study of cements
- recycling the used materials as raw materials for the production, and developing methods to pre-condition used materials to make them suitable for reuse
- polymer materials with equivalent durability to existing construction materials. These materials are already in use for gas and water pipes, and will be important for a future hydrogen economy

Effective regulation (especially in areas like construction where safety concerns are paramount), as well as policies to incentivise the transition to low carbon alternatives, are needed to overcome barriers to change, particularly in industries like cement and steel which have long investment cycles and expensive capital requirements. Structural and safety properties of any replacement material will need to be well characterised, understood and validated to enable widespread adoption in construction.

Collaboration across disciplines, particularly with engineering, is required, as the carbon saving opportunities are likely to require a combination of chemistry innovation and implementation.

Energy storage and synthetic fuels for transport

Around a third of **UK emissions in 2019** were from transport. In order to reduce emissions to zero, the UK Government has a target to increase take up of electric vehicles, with the planned phase out of new petrol and diesel car sales brought forward to 2030.

The £240 million Faraday Challenge and **Faraday Institution** aim to accelerate research in batteries for electric vehicles to realise this vision, which will require research in fundamental and applied materials chemistry as well as addressing engineering and manufacturing challenges.

Currently, energy storage for electric vehicles is dominated by lithium battery technology, Li-ion (lithium-ion) batteries in particular. Research challenges include increasing the efficiency, energy density, lifetime, safety and charging speed of these batteries. There are also challenges in recycling batteries, particularly in reducing the cost and labour intensity of extracting and recycling critical or scarce elements from the spent batteries. In parallel, researchers are developing alternatives to Li-ion batteries to mitigate pressures on the supply of critical elements such as lithium and cobalt.

There is an opportunity to increase focus in the UK on super capacitor research for high speed charging, eg metal oxides on graphene. Supercapacitors could also represent a potential alternative to Li-ion batteries, particularly in applications where rapid charging is required.

Another potential avenue in reducing emissions from transport is to consider low carbon synthetic fuels, either in applications where electrification is unfeasible at present (eg aviation, shipping), or to act as a bridge to newer net zero technologies which are not widely available yet. Synthetic fuels such as dimethyl ether (synthesised from captured CO_2), can be used in modified internal combustion engines, enabling an overall net reduction in emissions compared to a petrol vehicle.

Carbon capture, utilisation and storage (CCUS)

Negative emissions technologies form part of most models for meeting the target set out in the Paris Agreement and in assessments of **pathways to net zero set out by the Government**.

Many CCUS technologies currently exist; however, most are at low technology readiness level (TRL) in terms of efficiency, cost or scale. A targeted approach is needed to drive up the TRL of these technologies and bring down the cost, as well as economic incentives to spur adoption of CCUS technologies. More investment is needed in these technologies, specifically with bigger grants that connect lower TRL to mid TRL research. Economic incentives can come from many places through direct subsidy, carbon taxes, or the creation of new industries and opportunities using captured carbon.

The process of CCUS

CCUS requires: the capture of CO_2 from the air; where necessary its transportation to a storage or conversion facility; conversion of CO_2 to useful products or its geological storage.

The following examples highlight how materials chemistry can address challenges at all stages of the CUS process shown below.

Capture (direct air capture, point source capture)

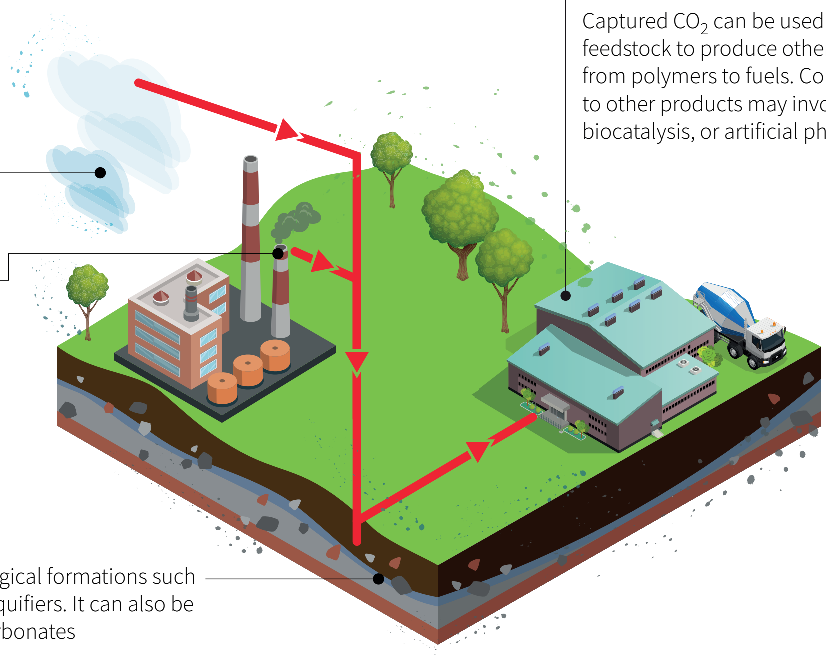
- improved CO_2 sorbents and reactive capture media. This includes sorbents with increased CO_2 selectivity for concentrated point sources, as well as dilute streams of CO_2 or those with impurities
- access to industrial environments and testing facilities for CCUS technologies, with sufficient funding to support pilot and scale up projects

Utilisation

- selective and sustainable catalysts for CO_2 conversion, supported by computational models to predict best performance
- electrocatalysis
- microbial CO_2 conversion and bio-based systems for CO_2 conversion. For example, systems to convert CO_2 to propane are in development but these are currently small scale
- manufacturing polymers from CO_2
- catalytic conversion of CO_2 to fuel as a means of storage, for example dimethyl ether (DME)
- conversion of CO_2 to elemental carbon for use in batteries, as activated carbon, or in MOFs

Storage

- approaches to using mineralisation and metal carbonates including biomineralisation or calcium carbonate precipitation
- storage solutions will be needed alongside utilisation to ensure that CCUS technologies are carbon negative, ie that they lead to an overall reduction in atmospheric CO_2



Capture

Direct air capture (DAC) collects CO_2 from the air, a more dilute source

Point source capture (PSC) collects CO_2 from a concentrated source, for example the flue of power station or industrial facility. CCUS facilities can be integrated with point-source capture to minimise transportation distance

Utilisation

Captured CO_2 can be used as a feedstock to produce other products, from polymers to fuels. Converting CO_2 to other products may involve catalysis, biocatalysis, or artificial photosynthesis.

Storage

CO_2 is stored underground in geological formations such as oil fields, coal seams, or saline aquifiers. It can also be stored in mineral form, as metal carbonates

Cross-cutting themes

AI and multiscale modelling

Designing new systems and assessing their environmental impact can be supported by new computational technologies including multiscale modelling and data science, allowing modelling of properties and synthetic pathways, to identify the most promising approaches.

Modelling approaches to predict properties and synthetic routes are already well advanced for molecular modelling and widely used (for example, retrosynthesis modelling of small molecules has been used for many years by synthetic chemists and in the pharmaceutical industry). With advances in computational power and AI in recent years, similar tools for materials could be widely available within four to five years.

These tools could ultimately be used to calculate the cost of materials synthesis (including CO_2 impact and atom efficiency).

Beyond modelling the synthesis of materials, multiscale modelling – looking at all the length scales in one – is the ideal. An example application would be to design a polymer that degrades in a predictable manner and has a predictable set of physical properties for specific applications. This kind of predictive modelling provides connectivity between the atomic and system length scales, potentially also providing information on how it will function throughout its lifespan. This will be a major opportunity for the future.

The RSC's **Digital Futures** report explores the use of data and digital for scientific discovery in more detail.

Catalysis

Catalysis plays a part across a wide range of technologies essential for decarbonisation, including:

- production of hydrogen through electrocatalytic water splitting
- CO_2 conversion and utilisation
- reducing the energy cost of industry by opening up low energy reaction pathways in synthesis

Catalysis is important right across the discipline of chemistry, and expertise from beyond materials chemistry will play a role, including fundamental organic and inorganic chemistry, and reaction mechanisms, alongside catalytic strategies borrowed from biology.

Many approaches to catalysis employ scarce elements such as palladium, rhodium and ruthenium. Research is ongoing to develop sustainable catalysts based on more earth-abundant elements, and to explore the use of organic compounds and biological approaches such as enzyme catalysis in these processes.

While catalysis research is an area of strength for the UK, participants advocated for a more joined-up approach across UK and greater investment; for example, into an institute or centre that can bring these new technologies to market more quickly.

Materials and circularity

The climate impact of a product depends on both the processes used to make it and that of the raw materials. Reducing the impact of materials on a product or technology includes the use of low carbon feedstocks, improvements to production efficiency to reduce wastage, and making the final products more reusable and recyclable to reduce reliance on virgin raw materials. Alongside this, we need to consider the impact on available resources, particularly critical or scarce elements. Finally, disassembly and recycling should be embedded in manufacturing design, backed up by regulation and standards.

Chemistry's role includes:

- building in recyclability to materials, devices and products at all scales. This could include polymers that can be easily broken down into reusable monomers, as well as designing modularity in materials and devices to enable easy disassembly
- considering the sustainability of the starting materials, moving away from critical raw materials (CRMs) towards more abundant materials. An example of the latter is the development of rare earth-free magnets for use in wind turbines
- improving efficiency and reducing the cost of CRM recovery and recycling
- separation processes to overcome the challenges in recycling complex mixtures, additives, and composite materials

Life cycle assessment and systems thinking

Assessing technology options and making sustainable choices depends on our being able to measure the total environmental impact of different options and approaches.

Life cycle assessment (LCA) is a critical tool in assessing the impact of a process, product or approach on a whole system basis – incorporating the carbon impact of manufacture, in use, and at end of life.

Despite the importance of LCA, workshop participants noted that there is a skills gap in the UK in this field. Government should support the training of more experts trained in life cycle assessment, and should emphasise the learning of these principles across the education system and as part of existing training curricula in universities.

There are research opportunities too, in developing improved LCA methodologies, as well as predictive modelling tools enabling scientists to predict the properties and environmental impact of a new material from the atomic to the device level and up to the level of the entire system.

Beyond new materials, chemists also need an understanding of the challenges associated with scaling up, and to consider these at the discovery stage with long-term sustainability in mind.

Conclusions

Achieving net zero carbon emissions in the UK will require a combination of existing technologies at scale, as well as rapid development of new technologies in hard-to-decarbonise sectors. Alongside this, support and incentives to invest and develop will be needed to achieve the kinds of reduction necessary to reduce emissions and limit dangerous climate change.

Materials chemistry will play a key role in driving these new technologies forward, and this report summarises just a few of these areas. We hope that these findings will be useful to a broad audience in understanding the important role of materials chemistry, and the broader chemical sciences, working in partnership with other disciplines. We also hope that the report will inspire materials chemists, both current and future, to celebrate the contribution that materials chemistry will make in tackling climate change and securing a sustainable future.

About the RSC Materials Chemistry Division

The RSC Materials Chemistry Division supports the study and dissemination of materials chemistry in all its forms. We support networking and community building among materials chemists across academic and industrial research, advance scientific knowledge through conferences, events and scientific activities, and act as an advocate for the field of Materials Chemistry to the scientific community, influential audiences and society as a whole.

We organise scientific activities and workshops to:

- bring together communities of experts and create new collaborations
- highlight research challenges and opportunities for materials chemistry
- promote the role of the division in advancing the science of materials chemistry

Our previous report, **Sustainable Plastics – the role of chemistry**, is available online.

For more information about the Royal Society of Chemistry Materials Chemistry Division please **visit the website**.

About this report

This report is a summary of two workshops held in summer 2020, organised by the Royal Society of Chemistry, with participants from the institutions listed below. This activity forms part of ongoing work by the Royal Society of Chemistry and its Divisions to develop a technical and future looking viewpoint on topics in chemistry research and innovation.

It does not represent an official position of the Royal Society of Chemistry or the institutions listed, and neither the RSC nor the organisations listed can be held responsible for the accuracy or completeness of the report's contents.

Please contact **science@rsc.org** with any questions about this report.

Workshop participants were drawn from the following institutions

Aalto University	SABIC
Bolam Materials Research Ltd	Swansea University
BP	Tata Institute of Fundamental Research
Carl Zeiss Microscopy	TNO (Netherlands Organisation for Applied Scientific Research)
CDT Ltd	UKRI EPSRC
Chemviron	Universidad de Magallanes
Dayalbagh Educational Institute	Universiti Sains Malaysia
Diamond Light Source	University College London
EDF Energy	University of Bradford
Henry Royce Institute	University of Brighton
Heriot-Watt University	University of Bristol
IISER Kolkata	University of Liverpool
Imperial College London	University of Manchester
Kingston University	University of Nottingham
Newcastle University	University of Pisa
NSG Pilkington Glass	University of Sheffield
Open University	University of Southampton
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