

# MATERIALS FOR THE ENERGY TRANSITION

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EXECUTIVE SUMMARY | JUNE 2020

*This document is part of the ongoing roadmapping to engage the academic and industrial materials research communities in exploring solutions to the grand challenge of “Materials for the Energy Transition”.  
The project has been enabled by:*

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## Introduction

### The Challenge: Materials for the Energy Transition

Following release of the Committee on Climate Change (CCC) 2019 Report<sup>1</sup>, the UK is committed to a new greenhouse gas emissions target: net-zero emissions by 2050.

The Executive Summary of the **2019 Committee on Climate Change Report** states:

***“Delivery must progress with far greater urgency.***

- ***2040 is too late for the phase-out of petrol and diesel cars and vans, and current plans for delivering this are too vague.***
- ***Over ten years after the Climate Change Act was passed, there is still no serious plan for decarbonising UK heating systems and no large-scale trials have begun for either heat pumps or hydrogen.***
- ***Carbon capture (usage) and storage, which is crucial to the delivery of zero GHG emissions and strategically important to the UK economy, is yet to get started. While global progress has also been slow, there are now 43 large-scale projects operating or under development around the world, but none in the UK.***
- ***However, falling costs for key technologies mean that the future will be different from the past: renewable power (e.g. solar, wind) is now as cheap as or cheaper than fossil fuels in most parts of the world.”***

In response, the Henry Royce Institute (Royce), in collaboration with the Institute of Physics (IOP), has engaged with academic and industrial materials research communities to explore solutions to the grand challenge of **“Materials for the Energy Transition”**. Through roadmapping workshops and associated community-led activities, energy technologies were identified where materials research can make a significant impact on greenhouse gas emissions.

The key drivers for this work have been (1) the pathways to net-zero emissions suggested in the CCC report, and (2) Royce-supported community workshops undertaken in 2019 to identify areas where investment in UK materials science can generate impact and contribute to the UK’s energy transition. These included the “Atoms to Devices” workshop in Leeds (May 2019); the “Operando and In Situ Characterisation of Energy Materials” workshop at the Diamond Light Source in Harwell (July 2019); and, the “Multi-Modal Characterisation of Energy Materials” workshop in Cambridge (November 2019).

As a consequence, the following four areas were identified where materials science is critical to enabling a step-change in greenhouse gas reduction:

1. Materials for photovoltaic systems
2. Materials for low-carbon methods of hydrogen generation
3. Materials for decarbonisation of heating and cooling
  - I. Thermoelectric energy conversion materials
  - II. Caloric energy conversion materials
4. Materials for low-loss electronics

<sup>1</sup> Committee on Climate Change Report: Net-Zero, January 2019, <https://www.theccc.org.uk/publication/net-zero-the-uks-contribution-to-stopping-global-warming/>

The outcomes of these roadmapping exercises are:

- (1) this **executive summary** report, highlighting the main findings of the four roadmapping activities;
- (2) four **materials development roadmaps** towards net-zero emissions for 2050. These will be published for research communities, funding bodies, government, policy-makers and industry leaders, in autumn 2020.

The four roadmaps generated are intended to be living documents, and Royce will engage with research communities to review regularly and develop further roadmaps as new materials systems and technologies emerge. Between March and June 2020, over 220 participants contributed to the creation of these four roadmaps from the UK academic and industrial materials communities. We would like to thank all who have participated in these activities through the roadmapping workshops, interviews, surveys and research summaries.

Oversight of community activities was through the “Materials for the Energy Transition” Steering Group: Professor Neil Alford, (Imperial College London), Professor Manish Chhowalla (University of Cambridge), Professor Richard Curry (University of Manchester), Professor Edmund Linfield (University of Leeds)

Programme management, reporting and community engagement were undertaken by Royce and IOP: Mia Belfield (Royce), Ellie Copeland (IOP), Anne Crean (IOP), Isobel Hogg (IOP), David Knowles (Royce), Amy Nommeots-Nomm (Royce), Suman-Lata Sahonta (Royce), Katharina Zeissler (Royce)

Roadmapping activities were coordinated by IfM: Nicky Athanassopoulou, Diana Khripko, Imoh Ilevbare, Arsalan Ghani, Andi Jones, Rob Munro

Technical oversight of roadmaps was undertaken by Oscar Cespedes (University of Leeds), Oliver Fenwick (Queen Mary University of London), Robert Hoye (Imperial College London), Xavier Moya (University of Cambridge), Ifan Stephens (Imperial College London), Sam Stranks (University of Cambridge)

## Materials Roadmaps

In 2020, the Henry Royce Institute has explored, with the respective research communities, the various materials challenges, targets, and timescales required to support the achievement of net-zero greenhouse emissions by 2050 in the four research areas below. In this activity, Royce has collaborated with the Institute of Physics (IOP) to set out the programme of work and ensure community-wide feedback and engagement. Skills and expertise from the Institute for Manufacturing (IfM) were brought into the programme to ensure a robust roadmapping methodology, to undertake a series of online roadmapping workshops, and to support community discussions. These roadmaps form the basis for bringing scientific research communities, industry and government together to address immediate and long-term requirements for the development of a suite of energy materials to replace fossil fuel-based energy technologies.

Roadmaps in this activity were developed in the following four technology areas (although the CCC report and related materials community engagement emphasises that these four areas are components of a broad ecosystem of materials technologies, which together can contribute to the UK's goals to deliver net-zero by 2050).

1. Materials for photovoltaic systems
2. Materials for low-carbon methods of hydrogen generation
3. Materials for decarbonisation of heating and cooling
  - I. Thermoelectric energy conversion materials
  - II. Caloric energy conversion materials
4. Materials for low-loss electronics

As of June 2020, the community-developed roadmaps for each of the above research areas are being prepared as technical reports, for publication in autumn 2020.

## Roadmap Objectives

The main objectives of the four materials roadmaps are as follows:

- To understand the current state-of-art for each topic
- To define the most significant technical challenges for each area that are providing barriers to impact on net zero targets
- To define the anticipated future challenges for each area in contributing to net zero targets
- To identify solutions to these challenges that can make step-changes in delivery of technologies to contribute to net zero targets
- To identify the desired performance targets of such solutions

## Methodology

The methodology adopted was based on wide-ranging engagement with research communities to define the roadmap objectives and expectations, to design and customise the strategic framework for the roadmapping; to develop questionnaires for the research communities involved, and to modify workshop process steps to ensure participation of the entire research community. The workshops brought together academic and industrial experts in the four respective technology areas, and involved both offline and online data collection phases. The offline phases were used for data collection from individual participants and publicly-available research sources, followed by data consolidation and, where necessary and appropriate, prioritisation. The online workshops were used for data review, analysis and deeper exploration of essential issues. The quality and reliability of the process was maintained by a Steering Committee involving roadmapping facilitators and technical leads from each of the four research communities.

In total, 26 workshops sessions were held across the four technology areas between March 2020 and June 2020. These revealed several materials sub-topics of particular interest for contribution towards the net-zero targets, as well as highlighting important fundamental research and commercial technology enablers that need to be established. These outputs significantly aided research communities' understanding of the future direction of energy materials research, towards the achievement UK's net-zero emission targets by 2050. Summaries of the ongoing workstrands are provided in the sections below, with the publication of full technical reports planned for autumn of 2020.

## 1. Materials for Photovoltaic Systems

The UK has the third largest solar generating capacity (13.1 GW) in Europe after Germany (45.3 GW) and Italy (20.1 GW)<sup>2</sup>. Up 54 GW of installed solar PV may be needed by 2035 in order to meet net-zero targets, with further growth towards 2050. Along with a range of other renewable and sustainable energy technologies, solar power is anticipated to play a vital role in meeting the UK's priorities of fully-decarbonising buildings, transport, electricity, industry and agriculture<sup>3</sup>. This trend is not unique to the UK; global PV capacity is predicted to reach over 1 TW by 2023, and it is estimated that solar power may provide 70 % of the world's total energy by 2050<sup>4</sup>.

Roadmapping workshops and discussion groups were held to explore the three questions below:

- How can existing and new PV materials develop over the next 30 years to accelerate PV deployment, and achieve carbon neutrality by 2050?
- What are the materials challenges for established and emerging PV materials?
- Which materials are needed for applications that will enable new markets?

### ROADMAPPING OUTCOMES

The **current state-of-art** solar technologies on the market are well-established crystalline silicon solar cells and cadmium telluride-based (CdSeTe/CdTe) thin film solar cells. Due to their low-cost manufacture and global market saturation, established technologies will remain important for the UK's future solar market beyond 2050.

#### Established PV Materials

The module efficiency of **silicon solar cells** can be increased, and their levelised cost of energy ( LCOE) reduced to accelerate their deployment, by addressing the following **key challenges and research needs**:

- Extension of device lifetime to 40 years and achieving improved and stable charge-carrier lifetimes by eliminating light- and temperature-induced degradation
- Reduction of the thermal budget by developing lower-temperature cell processes
- Development of novel methods of *in operando* characterisation for real-time monitoring
- Tailoring silicon cells for high-efficiency structures, e.g. as bottom cells in tandems with perovskites
- Development of bifacial silicon solar cells to increase light collection
- Development of low-cost metallisation, i.e. elimination of silver
- Recycling of modules and recovering high value components

After silicon, cadmium telluride-based photovoltaic systems are the second commonest current approach for low capital-intensity solar cells. The **key challenges and research needs** for this technology are:

- Development to increase single-junction cell efficiencies to 25 %, and development of bifacial and tandem devices reaching 32 % efficiency
- Improvement in carrier lifetimes through Group V doping and improved surface passivation
- Manipulation of defect states and improved defect reduction strategies to enhance device performance

<sup>2</sup> EurObserv'ER: <https://www.eurobserv-er.org/online-database/#>

<sup>3</sup> The Solar Commission: A bright future: opportunities for UK innovation in solar energy - July 2019: <https://www.regen.co.uk/wp-content/uploads/The-Solar-Commission-web.pdf>

<sup>4</sup> Climate Change Committee, Net-Zero Report 2019: <https://www.theccc.org.uk/wp-content/uploads/2019/05/Net-Zero-The-UKs-contribution-to-stopping-global-warming.pdf>

The key challenges and research needs across all **established commercial PV** systems are:

- Identification of the causes and mitigation of potential induced degradation
- Reduction of cover glass soiling which reduces solar power output by 10 % in the UK
- Improvement of AC/DC conversion efficiencies for solar inverters
- 

### **New PV Materials Technologies and Applications**

New materials in PV systems were classified into three categories:

- I. Perovskites and perovskite-inspired materials
- II. Organics and dye-sensitised solar cell materials
- III. Emerging and established inorganic materials and emerging thin films

Different materials systems and device design concepts that are applicable at utility level, including rooftops and/or niche applications, were identified within each of these three materials categories. In the following list, the main challenges and research needs for some of the new materials technologies and device design concepts are explained.

A. **Multi-junction technologies** (perovskite-silicon and all-thin film tandem cells) for large-scale solar generation modules. They may also be used for a range of smaller-scale applications. There is a need to develop:

- 1) **all-thin film tandems**, which have the potential for much lower capital costs, as well as
- 2) **triple-junction tandems**, which can achieve significantly higher efficiencies.

A desired UK solar-powered future includes 35 % efficient perovskite-silicon tandem modules with 40 year lifetime and £4/MWh LCOE. For thin-film tandems, a scenario allowing for shorter device lifetimes than 40 years is possible if module replacement schemes are implemented, whilst still maintaining low LCOEs. There is potential for these PV technologies to have up to 50 % generation capacity in 2030, together with growing Si-based deployment.

The main challenges and research needs are:

- Stabilised bandgaps for thin film tandem structures
- Sustainable manufacturing routes, e.g. the use of non-toxic source materials
- Sustainable and inexpensive transparent conducting oxides, metallisation and packaging. This includes replacing silver and gold contacts with cheaper materials, e.g. copper or carbon

B. **Single-junction perovskites** are an approach for efficient future applications such as building-integrated photovoltaics (BIPV) e.g. solar cell windows, indoor PV for generating power from artificial lights. BIPV is of importance to net-zero goals since it will contribute to CO<sub>2</sub>-neutral buildings with solar power for domestic uses, envisioning that the BIPV will last over the duration of the building. BIPV can be used as roof-tiles, windows, façades, car-porches, industrial/agricultural buildings, greenhouses or in automotive applications.

Single-junction perovskites are also of interest for utility-scale PV applications such as solar-powered heating for the home. They can be used in high-efficiency solar cell modules with low capital-intensity and low light inputs. They also can be integrated with other technologies, such as for solar fuel generation, ammonia generation, and solar water-splitting.

General challenges and research needs for single-junction perovskites are:

- Sustainable and inexpensive transparent conducting oxides
- Research into the passivation of perovskite films and improving the stability against environmental and operational degradation. This requires a focus on both the fundamental science (theory and characterisation), and module engineering (scale-up)
- Focus on module design and achieving high efficiency in large-scale solar modules

The main challenges and research needs specific to BIPV integration are:

- Scale-up and solar module manufacturing, along with transportability to building site
- Sustainable and inexpensive transparent conducting oxides with high light transmittance (as close as possible to 100 %) with low sheet resistance
- Understanding how environmental changes affect solar cell performance (e.g. dirt, cleaning).

C. **Mobile PV applications** are essential for use in autonomous vehicles, aerospace, telecommunications, and space applications such as satellites. New materials can be deposited on flexible substrates, which can be more easily integrated with automotive and satellite systems that require high power densities.

The main challenges and research needs are:

- Radiation tolerance of PV materials needs to be understood, with high device reliability over a defined duty cycle
- Further development of stability and performance of relevant materials (including multi-junctions), including perovskites, organics, and III-V photovoltaic materials
- Development of inexpensive transparent conducting oxides

D. **Standalone PV applications** are required for indoor solar power or for autonomous small devices (e.g. Internet of Things).

The main challenges and research needs are:

- Sustainable and inexpensive transparent conducting oxides
- Manufacturing of materials using low-toxicity solvents
- Scale-up of device area
- Encapsulation of indoor devices, for example for flexible devices
- Development of optical structures to improve the management of light into the device
- Materials include: organic photovoltaic materials, dye-sensitised solar cells, perovskites, and emerging inorganic materials

**Key challenges in emerging PV**, especially to facilitate translation of lab-based research into commercial scaling up to terawatt-scale, and to capitalise on UK-developed and UK-led technologies, are:

- Stability and reliability of the PV materials and device material layers
- Development of encapsulation and packaging materials (both cell and edge sealants)
- Development of new types of transparent conducting oxides that are composed of abundant, low-cost elements
- Full life-cycle assessment to determine sustainability of new materials
- Capital and variable costs of scalability and manufacturability

The following **research and technology developments** were identified for the different PV technologies:

- Central testing facilities for industrial scale-up, including high-level outdoor and accelerated indoor environmental testing, operational lifetime testing, and testing of adhesive and lamination strength to ensure the safety of the BIPV
- Dedicated UK-based cell processing laboratory facilities to tailor and innovate silicon devices, e.g. perovskites tandems
- Broad training in technical skills, facility operation, research skills (e.g. doctoral training in photovoltaics) are needed to build up the UK's pipeline and number of skilled people in the field
- Consortia bringing academia, industry, asset managers, Innovate UK and international world leaders in solar technologies (e.g. First Solar, NREL and Fraunhofer ISE) are needed to exploit potential for growth of emerging solar markets in UK

The following **commercial enablers** were identified for the different PV technologies:

- Regulation for carbon-neutral buildings in order to encourage BIPV uptake on greater than 10 % of new-builds
- Large-scale manufacturing technologies need to be developed, using inexpensive raw materials and sustainable processing routes, e.g. development of non-toxic solvents for processing
- A techno-economic analysis of large scale manufacturing for CdSeTe/CdTe is required
- Support for SMEs in the solar power sector e.g. funding and investment opportunities, academic-industry programmes

## Conclusions

The above priorities, targets and enablers have been identified by the research community to help achieve a range of PV solutions, from enabling over 50 GW grid-scale solar capacity, to development of zero-carbon buildings, and solar power-integrated automotive applications. These capitalise on the UK's strong base in early-stage research in PV, and focus on linking this with downstream industry scale-up and commercial translation opportunities. Stronger links between low and medium TRL levels can enable the UK to take advantage of materials technologies for niche applications, which in turn will allow access to new PV markets and secondary supply chains.

## 2. Materials for Low-Carbon Methods of Hydrogen Generation

Around 25 % of the UK's greenhouse gas emissions are generated through the energy supply, which is still largely based on coal, oil and gas. Hydrogen is available as an alternative energy vector, and can significantly contribute to UK's net-zero goals as part of a fossil-fuel-free energy economy<sup>5</sup>. However currently 95 % of global hydrogen production is generated using fossil fuels<sup>6</sup>. Sustainable methods of hydrogen production that can replace fossil fuel-based methods are available, and have demonstrated high efficiencies. Further development of these petrochemical-free methods of hydrogen generation are critical to the UK's transition to net-zero by 2050.

There are broadly four methods of producing hydrogen:

1. From fossil fuels using reforming of natural gas and steam, thermal methods, or biomass gasification
2. By electrolysis that separates hydrogen from water using electricity in an electrolysis cell
3. Through biological methods, which predominantly use microbes to convert biomass to hydrogen
4. Through "solar to fuels" pathways, that use sunlight to split water into hydrogen and oxygen.

Essential technology developments for the hydrogen production processes above are (1) ability to reactivate and re-use catalytic materials, (2) a sustainable and stable resource supply, as well as (3) end-of-life recycling options.

Roadmapping workshops and discussion groups were held to explore the questions below:

- How can we enable hydrogen production technologies to be scalable to terawatt levels through improved materials?
- What are the key fundamental and technological breakthroughs that would enable hydrogen production technologies to go beyond the efficiency and durability of current methods?
- Are other viable hydrogen generation options available (e.g. from waste biomass)? How do these compare to steam reforming and electrolysis in terms of efficiencies, yields and scalability?
- Are there routes to improving efficiencies, reducing temperatures, and capturing carbon, from the steam reforming process so that its impact on greenhouse gas emissions can be minimised?
- How can improved materials enable the utilisation of hydrogen through other chemical carriers (e.g. ammonia)?
- What are the relevant targets that the materials and materials-systems need to demonstrate?

### ROADMAPPING OUTCOMES

The **priority materials topics** identified for enabling low-carbon methods of hydrogen generation towards 2050, are the following:

- Discovery of catalysts and other materials that enable sustainable thermochemical synthesis of chemical feedstocks at low temperatures and pressures
- Development of improved electrode and electrolyte materials for high temperature electrolytic production of hydrogen and other valuable chemicals
- Improvement in the performance of catalysts and membranes in alkaline electrolyzers
- Component development, e.g. durable and conductive alkaline membranes
- Discovery of catalysts, electrodes and electrolytes yielding high activity and selectivity for carbon dioxide and nitrogen reduction

<sup>5</sup> HM Government. 2017 The Clean Growth Strategy See: [https://www.gov.uk/government/uploads/system/uploads/attachment\\_data/file/651916/BEIS\\_The\\_Clean\\_Growth\\_online\\_12.10.17.pdf](https://www.gov.uk/government/uploads/system/uploads/attachment_data/file/651916/BEIS_The_Clean_Growth_online_12.10.17.pdf) (accessed 23 November 2017).

<sup>6</sup> 'Options for producing low-carbon hydrogen at scale, Policy briefing', The Royal Society, January 2018

- Development of more efficient and more stable photoelectrode materials for photocatalytic water splitting
- Reduction or elimination of precious metals from catalysts in proton exchange membrane (PEM) electrolyzers
- Development of the fundamental understanding of reaction mechanisms
- Improvement of stability and conductivity of electrode materials in PEM electrolyzers

The following **research and technology enablers** were identified:

- Early-stage testing facilities of new materials for prototype devices at the single fuel cell-level, using device geometries intermediate between those available in academic institutions and those available in full commercial electrolyser stacks
- Methods to improve the recyclability and reactivation of existing or new materials
- Community-wide bench-marking and testing standards must be developed to accelerate scale-up
- Ultra-sensitive analytical techniques, to observe and track reaction intermediates, desired reaction products as well as undesired side products, including corrosion products, over the broad range of timescales of typical electrochemical reactions
- Advanced *in operando* and *ex situ* microscopy and spectroscopy techniques that are strongly integrated with benchmark performance tests, to establish the characteristics of materials that are responsible for superior functionality
- Integrated experimental and computational programmes where simulation tools both guide materials discovery and aid interrogation and interpretation of experimental data.

For commercialisation the following **commercial enablers** were identified:

- Capability and funding to manufacture materials, catalysts, and systems on a commercial scale with high throughput e.g. establishment of scale-up and pilot facilities
- Improvement in the cost of electrode materials in PEM electrolyzers
- Access to venture capital and investment in order to support early-stage research and development materials discovery.
- A business case that differentiates the benefits of producing hydrogen through electrolysis using renewable power sources (green hydrogen) from hydrogen produced from fossil fuels (blue hydrogen)
- Identification of niche markets and industrial processes for the electrolytic production of hydrogen and other related fuels and chemicals. Capacity rather than availability is important for the growth of the new sector
- British industrial champion(s) to establish consortia to drive forward the commercialisation of new technologies, as well as to establish hotspots of concentrated industry to integrate with these new technologies
- Well-resourced collaboration and funding opportunities within the UK between academia, industry, and research institutions in order to accelerate routes to commercialise new materials systems
- Strong collaboration with international partners and integration into international supply chains
- Participation in international research funding programmes (e.g. Horizon Europe's forthcoming Sunergy programme)
- Improved and new training opportunities to fill the hydrogen skills gap, which is large in the UK, including technical training for new types of chemical plants, PhD and postdoctoral opportunities (e.g. doctoral training in hydrogen technologies)
- Regulatory, political and/or tax incentives, e.g. carbon tax, to support a wide roll-out of renewable energies enabling 100 % green hydrogen generation by both decentralised and centralised means, for distributed and non-distributed generation and across different scales

## **Conclusions**

The above priorities, targets and enablers have been identified by the research community to help to achieve efficient, durable and sustainable hydrogen production, which is scalable to the terawatt level for the UK and globally, with a net-zero carbon footprint. The UK has a globally-leading position in low TRL early-stage materials research in this area, however this is not currently exploited towards the deployment of hydrogen as a viable energy source at scale. Further co-ordinated and targeted support will help the UK's ambition for net-zero by building a robust efficient, durable, and sustainable hydrogen industry. Harnessing the UK's early-stage research base in development of catalysts for petrochemical-free hydrogen production will provide the UK with economic potential for exporting technology, as well as develop new UK markets.

### 3. Materials for Decarbonisation of Heating and Cooling

37 % of the UK's greenhouse gas emissions are through the use of natural gas for providing heating and hot water in 84 % of UK homes.<sup>7</sup> The electrification of home heating will significantly reduce the UK's greenhouse gas emissions, and will reduce reliance on the UK gas grid. In this context, there is increasing interest in using air-source heat pump systems in the UK to replace natural gas with a carbon-free means of providing domestic water and heating/air-conditioning. It is predicted that by 2040, around 3.6 GW of heat pumps will be installed in the UK, requiring 11 TWh per year of electricity demand, but offsetting 50 TWh per year of natural gas demand.<sup>8</sup>

Given that currently-used heat transfer materials (e.g. refrigerants such as hydrofluorocarbons, HFCs) contribute strongly to the increase in greenhouse gas emissions, heat exchange systems that use **thermoelectric materials** and **caloric energy conversion materials** are being investigated as alternatives to vapour compression technology. Advantages over vapour compression-based heat exchange materials are a lack of moving parts, small size, and tunable device geometries. Both thermoelectric and caloric materials systems have a strong academic research base in the UK and have been exploited commercially. They offer the UK a broad range of opportunities in emerging new technology markets for a range of low-power heat exchange applications.

#### ROADMAPPING OUTCOMES

The topic of decarbonisation of heating and cooling technologies was run in two workstreams, comprising thermoelectric materials and caloric energy conversion materials.

##### I. Thermoelectric energy conversion materials

These materials make use of temperature differences to generate electricity, and are used in various low-power applications to harvest any heat generated in a system and convert this into electricity for other uses i.e. for refrigeration, air-conditioning and heat pumps. Additional to their applications built environment heat exchange systems, thermoelectric materials can be used to shift energy draw from automotive engines to other electronic components within the car. They will play a part in future cogeneration domestic heating systems and large-scale power plants, as well as in conversion pathways within integrated solar thermal energy generation systems.

The main challenge of this technology is their low efficiency, described by the thermoelectric figure of merit, ZT. A ZT value greater than 3 is required to replace traditional heating and refrigeration technologies such as vapour compression of HFCs. The highest ZT values currently available are around 2, although there is no upper limit to the theoretical ZT of thermoelectric materials. This enables thermoelectric generators to occupy niche application where efficiency and cost offered by heat exchange applications based on HFCs are less important than reliability, light weight, and small size. Nevertheless, numerous materials with potential for high ZT thermoelectric applications are reported in the literature each year. This suggests that with further research optimizing efficiencies thermoelectric materials could compete with, and perhaps replace, vapour compression-based heat pumps in the future.

The UK has an established academic base in thermoelectric research for a range of device applications. To develop a UK roadmap for thermoelectric materials, 17 participants attended four workshops with representatives from 13 different academic institutions, and one company specialising in manufacture of thermoelectric generators. Answers to the following questions were discussed:

<sup>7</sup> Dodds, McDowall, Energy Policy 60 (2013) 305–316, DOI: <http://dx.doi.org/10.1016/j.enpol.2013.05.030>

<sup>8</sup> National Grid Report: Future Energy Scenarios, 2016. URL: <http://fes.nationalgrid.com/media/1363/fes-interactive-version-final.pdf>

- Which materials systems show the most promise for viable energy-saving applications towards net-zero emissions by 2050, and what is the current state of the art?
- What are the current materials challenges that limit deployment of these materials?
- What performance can be achieved with current materials, and what could be achieved by 2025, and by 2050?
- How can improvements be made in the characterisation of these materials?
- How can improvements be made in provision of advanced facilities required for industrial scale-up and commercial testing?

In line with the main aim of decarbonisation of heating and cooling applications, focus was placed on materials and material systems for temperatures < 230 °C.

The **current state-of-the-art** material is bismuth telluride,  $\text{Bi}_2\text{Te}_3$ , which is used devices. It has the following limitations:

- Abundance – tellurium is a scarce element
- Performance – the current figure of merit, ZT, at ambient temperature is around 1.

**New materials** discovery is key to making step-changes to reach the 2050 targets. Those materials identified that have the potential to reach the 2050 targets (with a ZT of around 3, equivalent to around 20 % conversion efficiency and can compete with HFC-based technologies) are as follows:

#### **Ceramic Thermoelectrics:**

- Chalcogenides;  $\text{Mg}_3\text{Sb}_2/\text{MgAgSb}$  and Zintl phases; clathrates; skutterudites; nanostructured Si-based materials; half-Heuslers; topological and Weyl-based materials; silicides including SiGe

#### **Emerging Materials:**

- 2D materials; organic materials including small molecules and polymers and carbon nanotubes; composites between organic and inorganic materials; mixed-alloy materials; halide perovskites; metal-organic framework materials; conformable and flexible thermoelectric and periphery materials; printable thermoelectric materials; molecular junctions

In order for these materials to reach their potential, the following **research and technology developments** were identified:

#### **A. Materials Discovery and Optimisation**

Ability to measure the Seebeck coefficient efficiently, together with electrical and thermal conductivity, and standardisation of the characterisation of these factors

##### **Ceramic Thermoelectric Materials:**

- Accelerated materials discovery and engineering of new mixed-alloy thermoelectric materials
- Better understanding of the relationship between material structure and transport properties
- Development of tools to calculate and simulate accurate electronic and thermal transport in highly disordered nano-structured materials on the micron length-scale
- Research into hierarchical nano-structure designs to reduce thermal conductivity and to improve power factors
- Modulation doping to create high mobility regions
- Methods of decoupling (1) the relationship between thermal and electrical conductivity, and (2) the relationship between electrical conductivity and the Seebeck coefficient in thermoelectric materials  
Potential solutions utilise multi-band materials or phase transitions
- Development of materials with resonant energy levels or topological states to device-level

##### **Emerging Thermoelectric Materials:**

- Development of materials with morphologies that are suitable for scalable processing methods
- Development of materials that match environmental standards for commercial deployment e.g. toxic heavy metals such as lead should be avoided
- Interface materials research to achieve high electrical and high thermal conductivity
- Development of modelling of the stability and reliability of interfaces, together with access to characterisation tools
- Improved accuracy in density-of-states modelling for new materials
- Computational tools to simulate morphology, disorder and interfaces, and stability
- Computational tools to predict non-Wiedemann-Franz materials
- Predictive modelling to guide synthesis of new molecules and materials, in particular to inform on trends in properties upon structural modification
- Identification and development of new dopants for organic materials
- Synthetic chemistry expertise to aid in the exploration of new organic materials for thermoelectric devices
- Development of methods to self-assemble monolayers on electrodes and surfaces, which are defect-free on the atomic scale

#### **B. Integration into Devices**

- Preservation of optimal morphology and performance during scale-up
- Better understanding of the electrode interface chemistry in working devices
- In the specific case of molecular junction devices, the development of larger-scale structures, in which electrode materials and molecules are combined to optimise thermoelectric performance
- Development of nano-fabrication techniques for creation of atomically precise structures

#### **C. Scale-up**

- Development of growth and processing techniques at scale, enabling the move from thin films or small nanostructures to bulk production
- Development of process technologies for synthesis of complex molecules and materials at scale

The following **commercial enablers** were identified:

- Engagement with Centre for Process Innovation (CPI), and related Research and Technology organisations, to provide commercial scale testing
- A dedicated accelerated materials discovery programme
- Advanced characterisation facilities dedicated to scale-up and *in operando* testing, to speed up the development of new materials
- Funding opportunities for interdisciplinary partnerships between chemists, physicists, and engineers to deliver integrated device systems
- State-of-the-art nano-fabrication facilities to explore commercial potential of molecular devices
- Improved collaboration and engagement with industry to focus research on the needs and requirements of the end users, and to address the knowledge gap between fundamental materials research and commercial device development
- Establishment of a collaborative community of modelling experts and engineers for device innovation, to tackle the gap between small scale materials production and large-scale applications

These developments could collectively help to achieve:

- Significant improvements in the efficiency of thermoelectric devices, which will allow a greater market share
- A step-change in ZT values to >5, allowing thermoelectric technologies to compete on efficiency with incumbent technologies

## II. Caloric energy conversion materials

Caloric energy conversion (calorics) is a field in solid-state physics which provides an alternative for refrigeration, air conditioning and heating. These materials have the potential to provide high energy efficiency, compactness and environmentally-friendly operation. The technologies within calorics fall under four broad areas defined by the mode of energy conversion within the material:

1. electrocalorics (conversion is mediated by polarisation)
2. magnetocalorics (conversion is mediated by magnetisation)
3. barocalorics (conversion is mediated by compression)
4. elastocalorics (conversion is mediated by stretching)

The potential impact of calorics to UK heating and cooling is a 50 % reduction in energy consumption, saving about £15 bn if one considers only cooling; this is coupled with use of refrigerants that are not harmful to the environment. To develop a UK roadmap for calorics, 13 participants attended 6 workshops with representatives from 5 academic institutions, and one company.

The four caloric effects were explored individually within the context of their room temperature application, i.e. for refrigeration, air-conditioning and heat pumps. During the roadmapping workshops, expert contributors had two key objectives:

- 1) Agree the most critical weakness(es) or challenge(s) in development and application of caloric materials and associated devices in heating or cooling
- 2) Provide a strategic outlook that answered the following:
  - a. What are the key strands of materials-level, device-level and system-level research and development necessary to overcome the most critical challenge(s)?
  - b. What resources and capabilities are crucial to facilitating the necessary research and development, and to generally progress the field of calorics towards making an impact on UK decarbonisation targets by 2050?

**Key materials research and developments** identified include:

Electrocaloric materials:

The most **critical challenges** identified are:

- Extension of the operational temperature range as current  $\Delta T$ s are just within useful operational range
- Reduction of the electric fields required to achieve higher  $\Delta T$ s
- Improvement of electrical breakdown and thermal diffusivity structures in ferroelectric oxides
- Exploration of low spontaneous polarisation nylons in ferroelectric polymers
- Exploration of ferroelectricity in organics
- Basic research into ferroelectric liquid crystals to maximise spontaneous polarisation, polar nematics, and tunability of phase transitions, in order to identify candidate materials for devices and scale-up

Magnetocaloric materials:

The most **critical challenges** identified are:

- Improvement in the thermal response under magnetic fields is needed
- Reduction of cracking during production, and cracking due to fatigue during cycling.

- Exploration of composite magnetocaloric materials to increase thermal response and increase temperature
- Understanding and reduction of hysteresis to reduce the required driving magnetic fields

Barocaloric materials:

The most **critical challenges** are:

- Reduction in hysteresis in caloric materials is needed, in order to reduce the driving pressures required to produce the caloric effect
- Improvements must be made in thermal conductivity, in order to reduce cycle time
- Exploring the use of hybrid materials to bypass hysteresis
- Developing materials with increased thermal conductivity which exhibit large  $\Delta S$  and  $\Delta T$ , and can work below 300 bar

Elastocaloric materials:

The most **critical challenges** are:

- Reduction in hysteresis, mechanical breakdown, and fatigue in elastocaloric material is required, as these factors limit device lifetime the current lifetime of  $10^5$  cycles needs to be extended to  $10^{10}$  cycles
- Developing precipitates for metals and functional groups of polymers, to reduce driving stresses required for device operation

Research to discover new caloric materials featured prominently across all of the four caloric effects.

Key **device research and development areas** were identified for each of the caloric effects which must be developed in parallel to the materials:

All materials systems:

- Heat transfer and energy recovery, including understanding of how to thermally connect/couple the regenerator fluids/coolants to the caloric material

Electrostatic materials:

- Research into the electronics to drive the systems/materials, e.g. the use of inductive circuitry and stitching techniques to recycle the charge

Magnetocaloric, barocaloric, and elastocaloric materials:

- Development of heat switches that are heat leak free, fast, have large ON/OFF ratios, and can operate under high driving fields
- Lifetime analysis on accelerated timescales to show robust performance of all components

The following **research and technology enablers** were identified:

- Investment in and development of partnerships and collaborative systems across academia and industry within the UK to address challenges more efficiently and effectively within and across the range of caloric effects
- Investment in fundamental research into materials discovery and development, to overcome some of the key challenges described above
- Funding for researchers and engineers skilled in materials engineering, materials discovery and systems engineering, characterisation, computational materials modelling, and thermal modelling
- Synchrotron and neutron-scattering opportunities targetted towards applications development

- Partnerships between academia and industry specialised in air-conditioning, refrigeration and manufacturing, to explore incorporation of caloric materials into existing applications space
- A cohesive network of leading academics and stakeholders across the UK, under which all caloric strands unite to address common challenges in assessing performance, scale-up and device architecture, and advanced testing

The following **commercial enablers** were identified:

- Standardisation of safety and performance measures across communities
- Investment in demonstration of prototypes and scale-up technology to improve cost-efficiencies of components and devices
- Investment in new UK manufacturing capability and support of current manufacturing for caloric devices (e.g. high-quality multi-layer capacitor structure manufacturing, which is critical to electrocalorics)

## **Conclusions**

The roadmapping workshops and community activities have shown that both thermoelectric materials and caloric materials can enable step-change reductions in energy consumption towards supporting the UK's net-zero goals, as well as creating new product markets and secondary supply chains. This is through exploring pathways towards accelerated deployment of thermoelectric and caloric energy conversion devices for refrigeration, air conditioning and heating, that are non-polluting, compact, efficient, and can be manufactured using sustainable methods.

#### 4. Materials for Low Loss Electronics

The world market in electronics is worth £602 billion with a predicted growth rate of 2.3 % over the next five years.<sup>9</sup> Furthermore, approximately 30 % of all electrical energy generated utilises power electronics, with the global market estimated at £135 billion, with a growth rate of 10 % per year.<sup>10</sup> However, UK revenue in the electronics sector was reported in 2019 to be only £1.9 billion,<sup>11</sup> emphasizing the need to stimulate manufacturing and policies in this critically important sector. But, this comes at a price. Digital technologies consume about 5 % of the world's energy, a figure which is expected to reach 21 % by 2030.<sup>12</sup>

A challenge for the UK is how to grow its economy, whilst satisfying the ever-increasing demands and expectations of consumers, and meeting the UK government's net-zero greenhouse gas emissions by 2050. Research and Innovation is needed into the development of **materials for low loss electronics**, which provided a focus for this community consultation.

Three broad categories were identified for consultation: (1) Materials for power electronics; (2) Materials for CMOS; and, (3) Materials for 'beyond CMOS device architectures' (*'More than Moore'*).

1. **Materials for Power Electronics** – underpinning local energy generation, distribution, and future transport. This topic focuses on exploiting emergent SiC and GaN technologies; developing next-generation materials (e.g. 3C-SiC, Al(Ga)N, and Ga<sub>2</sub>O<sub>3</sub>); and, addressing recycling, the scarcity of source materials, and, the whole-life energy costs of manufacture in the electronics sector.
2. **Materials for CMOS** – advancing society's digital connectivity and mobility, and supporting remote operation of ever more complex devices for monitoring of the environment, health and security. This topic focuses on integrating new materials into CMOS devices to demonstrate new concepts (e.g. 'tunnel', 'negative capacitance' and 'piezoelectric' field effect transistors), thereby reducing the operating voltage and energy consumption of CMOS. It also considers monolithic integration of different materials to enhance significantly device functionality (e.g. delivering compact, low-power, radio-frequency (rf) sources).
3. **More than Moore** – accelerating performance and energy efficiency of computing for the future. This topic addresses the development of new paradigms for computing and information processing. It goes beyond traditional CMOS 'von Neumann' computing (e.g. through developing neuromorphic computing architectures), and is underpinned by new materials, (e.g. spintronic, topological and organic materials), and new device concepts (e.g. chargeless computation and collective switching).

All are underpinned and enabled by fundamental research into **New Materials**.

To develop UK roadmaps in each topic, 50 participants participated in nine workshops with representatives from 20 different academic institutions, 10 companies, and UK national facilities (NPL and STFC-RAL). The industrial participation included representation from those working in wafer fabrication and equipment manufacture, as well as end users from the Electronics and Defence Sectors. The **main questions** that were investigated through the process were:

- Which materials systems and frameworks show the most promise for viable energy-saving or increased performance without increasing energy consumption, and can contribute towards net-zero emissions by 2050?

<sup>9</sup> IBIS World Industry report C2524-GL Global Semiconductor & Electronic Parts Manufacturing – C. Miele (January 2020)

<sup>10</sup> S. B. Reese, How much will gallium oxide power electronics cost? Joule 3, 4, 903 (2019)

<sup>11</sup> IBISWorld Industry Report C26.110 Electronic Component Manufacturing in the UK – Samuel Kotze (January 2019)

<sup>9</sup> A.S.G. Andrae and T. Edler "On global electricity usage of communication technology trends to 2030", challenges, 6, 117 (2015), and 'Tsunami of data' could consume one fifth of global electricity by 2025,

<https://www.theguardian.com/environment/2017/dec/11/tsunami-of-data-could-consume-fifth-global-electricity-by-2025>

<sup>12</sup> N. Jones, The information factories, Nature 561, 163 (2018)

- What are the current materials and technology challenges that limit deployment of these materials?
- What performance targets could be reached by 2025, 2035, and by 2050?
- How can improvements be made in the characterisation and functionalisation of these materials?
- What are the best ways to integrate new materials and application concepts into highly developed and widely used technologies?
- What improvements can be made in the provision of advanced facilities required for industry scale-up and commercial testing?

## ROADMAPPING OUTCOMES

The narrative that follows is organised into **research and technology enablers, development and scale-up and materials for the energy transition**.

For **research and technology enablers**, requirements include:

- Materials Discovery and Development, supported by artificial intelligence (AI) and machine learning approaches; measurement and analysis; and, understanding of the characteristics and dynamics of materials and their interfaces.
- Simulation and Modelling, including ab-initio atomistic and empirical/phenomenological models to determine fundamental material parameters; underpin electronic and opto-electronic device designs; and, interpret and predict experiment.
- Benchmarking testing protocols and databases to compare with existing technologies and devices, including use of high-throughput testing, and scale-validated proxies, with new testing standards enabling translation from development laboratories to large scale pilot lines.
- Recyclability and recovery of materials, including identifying incentives, targets and life-cycle analysis when selecting materials and processing routes, and considering availability of scarce materials and the whole-life energy cost of manufacture and use.
- Collaboration to stimulate the exchange of ideas between academia, industry and research institutions (both within the UK and outside), including provision of incentives for industry to co-develop fundamental research programmes from the outset.

For **development and scale-up**, requirements include:

- Pilot line facilities to move device concepts from academia to industry accompanied by suitable industrial certification and demonstrations of scalability, thereby establishing an ecosystem and supply chain. Exemplars include integration of new materials with CMOS; scale-up of wide bandgap semiconductors and silicon photonics to wafer fab; and, large-scale integration of III-V semiconductors with silicon.
- Development of manufacturing technologies required for new materials integration, alongside and complementary to established techniques, including deposition (e.g. MBE, PLD, CVD), processing, patterning, annealing, and validation of quality, uniformity, and functionality.
- Centrally-managed facilities (e.g. Research Training Organisation) to support scale-up, fabrication, component development, testing, seeding of commercialisation, and incentivising and support of start-ups, with specialist staff, consolidated and dedicated equipment, and on-going funding for proving projects, and training of manufacturing and technical staff.
- Enabling Technologies and Skills to accelerate product development by understanding design processes and process control in 4<sup>th</sup> Industrial Revolution (4IR) manufacturing processes.

- Routes to market, provided through engagement with early adopters from industry, as well as engaging with multi-national end users and global foundries, and supporting the commercialisation of intellectual property arising from the UK research base.

**Materials** identified for the energy transition are:

- **Materials for Power Electronics** including SiC, 4H-SiC, 3C-SiC, GaN, Al(Ga)N, Ga<sub>2</sub>O<sub>3</sub>, BN and B(Al)N, and diamond. Key challenges include high quality, low defect, ≥8-inch wafer growth; dopant control; and, thermal management.
- **Materials for CMOS** to (a) demonstrate negative capacitance, tunneling, and piezoelectric field effect transistors to reduce operating voltages and increase energy efficiency; (b) incorporate alternative channel materials, such as 2D materials and III-V semiconductors; (c) increase energy efficiency through device integration with low loss and/or high thermal conductivity dielectric substrates such as Al<sub>2</sub>O<sub>3</sub>, MgO, diamond, SiC, high-resistive Si, polycrystalline AlN and thick GaN; and, (d) add functionality through incorporation of tunable materials such as piezoelectrics, antiferromagnetics, plasmonics and photonics, whilst maintaining CMOS compatibility.
- **Materials for ‘More than Moore’** to achieve high computational power with lower energy consumption using new computing architectures (e.g. neuromorphic architectures). Exemplars include (a) nano-oscillatory neural networks; (b) in-memory computing using memristive materials such as redox, phase change, and spin transfer torque materials; ionic synaptic transistors; and, metal-oxide bilayers; (c) edge computing; (d) probabilistic computing; (e) all optical or hybrid computing; (f) quantum computing, with low temperature compatible memory; (g) non-volatile logic operations and (h) chargeless computation utilising spin, the electrical dipole or orbital states in materials such as ferroelectrics, magnetic materials, light metals, semiconductors, 2D materials, organic and molecular materials, topological insulators, quantum wells, molecules and crystals. The key challenges are the identification of the right materials system for the specific targeted computing architecture; the optimisation of the active materials; and, conversion of input/output signals, such as charge current/light to spin current, and vice versa.

**The preliminary recommendations** for developing low-loss electronics include:

- Investment to support UK prototyping/pilot-plant scaling of devices from research to wafer-scale fabrication and manufacture, including validation and testing; this provides a supply chain to test and translate new ideas.
- Investment in a network of state-of-the-art ‘fab-of-the-future’ centres, accessible to the whole UK, encompassing the design, growth and fabrication of new materials. This would be supported by UK Centres in *Materials Replacement & Recycling*, and *High-frequency & High-throughput Testing*, each underpinned by world-class scientists and engineers, with dedicated specialist technical staffing
- Establishment of big data and machine learning (AI) approaches to materials discovery (Materials 4.0) and advancing the understanding of interfacial properties (Interface 4.0), supported by simulation and modelling development across the length scales – from atoms to devices
- Investment to support the development of new computing architectures, and next generation wide-bandgap semiconductors for power electronics
- Funding approaches to support UK-wide collaborations between academia and Industry
- Influencing policy, including setting power consumption targets, supporting the circular economy through end of life considerations, and removing reliance on scarce materials

**Conclusion**

The above priorities, targets and enablers have been identified by the research community to help to achieve more efficient electronics in the context of power electronics and computing. The UK has a strong position in fundamental materials research in this area, however this is not currently exploited towards devices. A crucial pathway towards achieving commercially viable products is a close collaboration between industry and academia at the onset of the materials discovery and optimisation.

## Overall Conclusion

Research communities have identified four key materials science and engineering topics that can make an impact on accelerating the UK's achievement of net-zero greenhouse gas emissions by 2050:

1. Materials for photovoltaic systems
2. Materials for low-carbon methods of hydrogen generation
3. Materials for decarbonisation of heating and cooling
  - I. Thermoelectric energy conversion materials
  - II. Caloric energy conversion materials
4. Materials for low-loss electronics

Workshops were held to explore challenges, targets, enablers, and timescales for advancement of the materials properties, device performance, and system-level integration required to achieve significant greenhouse gas reductions by 2035, with a view to achieving net-zero emissions by 2050.

The roadmapping workshops captured the commercial and technological challenges and targets essential for developing advanced energy materials technologies, and enabling the UK to pursue its ambitious goal of reducing greenhouse gas emission to net-zero by 2050. Below are summaries of the key messages made by the academic and industrial communities resulting from the roadmapping workshops.

### 1. Materials for photovoltaic systems

Photovoltaic (PV) energy generation has the potential to reach 50 % of the UK's total generation capacity by 2030, and provides a significant opportunity for addressing the UK's net-zero goals for energy generation. To ensure national energy security, enabling UK-based PV manufacturing is critical. Several routes to achieving this exist, but they require an ambitious rollout, including deployment of new tandem technologies. The UK has a world-leading position in PV innovation, where research in material sciences plays a significant role – there is broad academic and practice expertise in existing and emerging materials systems, as well as in device design concepts. There is, however, a need for translation of innovations into products, through proactive consortia that bring different ecosystem actors together. The innovation capability could be increased through the development of a new pool of talent through PhD-level training, as well as establishing innovative funding programmes to enable new technology scale-up. By establishing a centre for PV materials characterisation, device stability, and reliability testing, along with rapid prototyping of new products, the UK can become a world leader in the standardisation of PV device testing methods, e.g. indoor PV applications and accelerated device testing of new modules. To achieve this, better engagement between academics, industry and end-user industries is essential to ensure that product development efforts are focussed in areas where they are most needed.

### 2. Materials for low-carbon methods of hydrogen generation

There is a significant opportunity within the UK for investing in green hydrogen technologies owing to the UK having one of the largest renewable electricity generating capabilities in Western Europe. For the UK to capitalise on this opportunity, government support is required in terms of regulation frameworks and incentives for industry. Furthermore, due to the multidisciplinary nature of the field, integration of the different research activities and early engagement with industry are essential for accelerating commercialisation of technology. Hydrogen generation is a multidisciplinary area that requires a variety of skills and knowledge, from modelling and surface science, to process engineering, to large-scale operations. Agreement on community-wide benchmarking and testing protocols will allow synergistic technology developments across the broad range of academic groups and commercial entities involved.

### 3. Materials for decarbonisation of heating and cooling

### **i. Thermoelectrics**

The UK has a leading research base in thermoelectric materials. Yet commercial exploitation for a range of applications is proving to be an ongoing challenge within the UK despite the rapidly-growing global thermoelectrics market. In order to allow thermoelectrics to expand into non-niche areas, a step-change in the figure of merit, ZT, to values greater than 3 is needed to compete on efficiency with incumbent technologies. More advanced characterisation facilities are required to speed up the development of new materials, including state-of-the-art nano-fabrication facilities to explore the potential of molecular devices. Improved collaboration and engagement with industry is essential to enable targeted research that focusses on the needs and requirements of end-users bridging the knowledge gap between fundamental materials research and commercial device development. Niche application markets are ripe for exploitation, based on hybrid thermoelectric materials systems, where UK researchers have demonstrated clear value propositions. Upstream research to TRL 3 is underway across the UK. To capitalise on the UK's thermoelectric research base, and in order to promote commercial scale-up, the establishment of an accelerated materials discovery programme is necessary across a range of disciplines, including partnerships between chemists, modelling experts, physicists, synthetic chemists and engineers.

### **ii. Calorics**

The potential impact of calorics to UK heating and cooling is a 50 % reduction in energy consumption (saving up to £15 billion for cooling alone), and the use of refrigerants that do not contribute to the greenhouse effect. The key message in this technology area is the need for partnerships and collaboration networks across UK academia and industry, to address the challenges within and across the four caloric effects more efficiently and effectively. Investment is needed to enable fundamental research in materials discovery and development. Additional investment is needed in developing the UK's ability to manufacture high quality multilayers.

## **4. Materials for low-loss electronics**

There are significant opportunities for the UK in materials research and development for low loss electronics. Through instigating a transformative research programme encompassing UK academia and industry, it is possible to address society's increasing energy demands whilst reducing its carbon footprint. This will support inward industrial investment, capitalise on UK's strengths in advanced materials, and enable the UK to be an internationally-leading innovator in the device supply chain, providing sovereign capability.

Despite the fact that future mass-production of silicon CMOS will continue to be undertaken outside of the UK, strategic investments into UK prototyping and pilot plants, combined with high throughput device testing capabilities, will enable scale-up of devices from research to wafer-scale fabrication. Furthermore centres for growth, fabrication and characterisation are needed to develop new materials to the point of proof-of-principle. Supporting and implementing new material discovery approaches, e.g. machine learning (AI) approaches and simulation and modelling across different the length scales, was identified as a key enabler to accelerate material developments. A critical factor is also the establishment and maintenance of UK-wide collaborations between academia and industry that focus on materials development towards commercial applications. To achieve tangible outcomes by 2050, a clear collaborative dialogue between academia and industry needs to be established from the outset of the materials development. Finally, establishing policies that set power consumption targets, and support the circular economy through end of life considerations, will be a critical factor in establishing an environment where the UK takes a leading position and becomes the place for investment for future development of *low-loss electronics*.

### **Key findings common to all topics**

- The need for infrastructure to transfer technology from lab to prototype devices
- National facilities for device metrology and degradation testing
- National coordination of industrial and academic research programmes
- Targeted investment from UKRI to unlock potential
- Legislate the uptake and implementation of low-carbon technology
- Researched materials should be resource abundant, scalable and recyclable
- People: training including facility operation, PhD programmes, postdoctoral researcher support

This executive summary has provided an overview of the main outcomes of the roadmapping activities, and full technical reports on all four research topics will be published in autumn of 2020. The roadmaps are living documents, and Royce will support research communities to update and revisit roadmaps as new materials technologies and commercial enablers become established over coming years.

Materials science and engineering plays a key role in developing innovative and disruptive technologies, in particular in the energy sector, and in development of energy-efficient applications and processes. The UK is in an excellent position to take advantage of a strong fundamental research base in these areas, to enable a range of sustainable energy technologies for a carbon-free future.

To find out more about the ongoing roadmapping and to input your ideas please visit [www.royce.ac.uk/materials-for-the-energy-transition](http://www.royce.ac.uk/materials-for-the-energy-transition) or contact [scienceandinnovation@iop.org](mailto:scienceandinnovation@iop.org)