Welcome to the Materials for the Energy Transition Roadmapping Webinar

IOP Institute of Physics

HENRY ROYCE INSTITUTE
Dame Julia King
Baroness Brown of Cambridge
Materials:
Unlocking the Energy Transition

Baroness Brown of Cambridge DBE
FRS FREng
Chair,
Henry Royce Institute
Vice-Chair,
UK Committee on Climate Change
Climate Change Act 2008

CHAPTER 27

CONTENTS

PART 1

CARBON TARGETS AND BUDGETING:

The target for 2050
1 The target for 2050
2 Amendment of 2050 target or baseline year
3 Consultation on order amending 2050 target or baseline year

Carbon budgets
4 Carbon budgets
5 Level of carbon budgets
6 Amendment of target percentages
7 Consultation on order setting or amending target percentages
8 Setting of carbon budgets for budgetary periods
9 Consultation on carbon budgets
10 Matters to be taken into account in connection with carbon budgets

Limit on use of carbon units
11 Limit on use of carbon units

Indicative annual targets
12 Duty to provide indicative annual targets for net UK carbon account

Proposals and policies for meeting carbon budgets
13 Duty to prepare proposals and policies for meeting carbon budgets
14 Duty to report on proposals and policies for meeting carbon budgets
15 Duty to have regard to need for UK domestic action on climate change

UK Climate Change Act 2008
Net Zero 2019
Achieving an 80% reduction

- Energy efficiency
- Electrification
- Electric vehicles
- Growth in zero carbon power generation
- Carbon Capture, Utilisation and Storage
- Wood in construction
- Limited implementation of BECCS
- Afforestation 27,000 hectares per annum
- Remaining emissions:
  - Industry
  - Agriculture
  - Aviation
  - Heavy transport
  - Heat in buildings
From 80% to 100%
Towards Net Zero

Microporous composite for hydrogen
Encapsulation Courtesy V Ting et al.
Bristol University

- **Electricity**: 95% low carbon power, including hydrogen
- **Buildings**: 90% low carbon heating including hydrogen
- **Transport**: all cars and vans electric; HGVs electric or hydrogen
- **Industry**: CCS, hydrogen and electrification
- **Waste**: 70% recycling, zero biodegradable waste to landfill
- **Shipping**: efficiency and alternative fuels: hydrogen and ammonia
- **Aviation**: further technical improvements and synthetic fuels
- **Agriculture and land use**: improved livestock breeding and diets; 20% reduction in beef, lamb and dairy, increased yields, 30,000 hectares per annum afforestation; 55% peatland restoration, increased energy crops
- **CO₂ removal**
The scale of change: in the next 30 years

- Electricity system x2 to x4
- Offshore wind 10 GW to 75 - 100GW
- Hydrogen production 27TWh to 370TWh
- CCS 0 to 180 Mt CO₂
- Afforestation 10,000 to 50,000 hectares pa
- 30 million buildings converted to low carbon heat
- Zero carbon cars 250,000 to 35 million
- Major changes in land use
- 50% reduction in meat and dairy consumption
Materials: unlocking Net Zero

- **Hydrogen**: production, storage, transport, embrittlement...
- **Buildings**: low carbon construction, insulation, fuel cells, heatpumps, novel heating and cooling...
- **Energy efficiency**: lightweighting, electrical efficiency, ultra-efficient electronics...
- **Industry**: zero emissions processes, low carbon steelmaking...
- **Waste and resources availability**: circular economy, 100% recyclable plastics, new approaches to recycling, Nd, Ag, Li, Co, Ir...
- **Transport**: light weighting, efficiency, electrification, synthetic fuels...
- **Power**: increased efficiency, bigger turbine blades, more efficient photovoltaics, better energy storage...
Thank you
Introduction to Materials for the Energy Transition

Prof. Neil Alford

Imperial College London
Motivations

In 2019 the UK became the first major economy to pass an emissions law of net-zero by 2050

Data taken from: The estimated territorial greenhouse gas emission by source category in 2018
Material Opportunities

To address net zero 2050 challenge we have defined 4 key topics:

• The Future of Materials in Photovoltaic Systems
• Low-Carbon Methods of Hydrogen Generation
• Decarbonisation of Heating and Cooling
• Low Loss Electronics

Figure adapted from: S. B. Reese, T. Remo, J. Green, A. Zakutayev, 'How Much Will Gallium Oxide Power Electronics Cost?' Joule, Volume 3, Issue 4, 2019, Pages 903-907
Topic 1: The Future of Materials in Photovoltaic Systems

PV’s energy potential is over 100 times greater than the UK’s electricity usage per year. Currently PV supplies 4.1%\(^2\) of UK demand.

To meet net-zero we need to increase the number of solar cells by an order of magnitude at least.

Can materials innovation create devices which:

- Generate >50% more power per panel
- Utilise light from more of the solar spectrum
- Work in lower light levels e.g. indoor spaces
- Enable carbon neutral buildings
- Power electric vehicles and aerospace applications

\(^1\) Based upon the kWh/kWp per year photovoltaic power potential data from: https://solargis.com/maps-and-gis-data/download/united-kingdom.
Topic 2: Low-Carbon Methods of Hydrogen Generation

Fuel cells can generate electricity with no greenhouse gas emissions, however, they rely upon hydrogen.

Currently, around 95%\(^1\) of the world’s hydrogen is generated by steam reforming of natural gas and other fossil fuel sources at high temperature.

Can new materials enable:

- Green hydrogen production scalable to the TW level?
- More efficient hydrogen production?
- Longer lasting devices for hydrogen production?
- Uptake of hydrogen through alternative chemical carriers? e.g. ammonia

\(^1\)“Hydrogen in a low carbon economy”, Committee on Climate Change, November 2018.
Topic 3: Decarbonisation of Heating and Cooling

37% of the UK’s greenhouse gas emissions arise due to heating and cooling\(^1\).

Caloric materials and thermoelectric materials can create carbon-free heating and cooling alternatives.

1. How do we improve the performance of thermoelectric materials?
2. Can thermoelectrics compete on efficiency with other technologies?
3. How do we improve the performance of caloric materials?
4. Can calorics replace current gas-based heating and cooling technologies?

Topic 4: Low Loss Electronics

40% of primary energy consumption is electricity, 30% of all electrical energy passes through power electronics – to reach 80% in the next decade\(^1\). 3-5% of global electricity used by computing\(^2\). Predicted to increase up to 21% by 2030, 8000 TWh\(^3\)

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Timeline of Roadmapping Process

- Idea conceived: September 2019
- Collaborated with the IOP: October 2019
- Online launch of key findings: 15th June 2020
- Publication of Roadmaps: September 2020
- 272 Responses: Community Survey (Feb-March 2020)
- Online Workshops: March-June 2020
- Community refinement: July-August 2020

IfM - Institute of Physics
Roadmap Contributors

>170 Participants in 26 Workshops
From 48 Organisations
>500 delegates for today's launch
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 unleash potential

• Legislate the uptake and implementation of low-carbon technology

• Researched materials should be resource abundant, scalable and recyclable

• People: Training, PhD programme, PDRA support etc.
Impact for the UK

Meet our 2050 net-zero target

New jobs and filling the skills gap

Energy security
# Webinar Agenda

<table>
<thead>
<tr>
<th>Time</th>
<th>Session</th>
<th>Speakers</th>
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| 9:50 - 10:20 | Plenary Session, Chair: Professor Manish Chhowalla | Professor Clare Grey, University of Cambridge, UK  
Professor Jenny Nelson, Imperial College London, UK  
Professor Nora de Leeuw, University of Leeds, UK  
Professor Stuart Parkin, Max Planck, Halle, Germany |
| 10:20-10:30 | Q&A                                        |                                                                          |
|            | 10 minute break                            |                                                                          |
Plenary Speakers

Professor Clare Grey
University of Cambridge

Professor Jenny Nelson
Imperial College London

Professor Nora de Leeuw
University of Leeds

Professor Stuart Parkin
Max Planck, Halle
Professor Clare Grey

University of Cambridge
The Role of Batteries in a Sustainable World

Clare P. Grey
Why is this important?

- Electrification of transport. Cheaper, safer and longer lasting batteries are critical for widespread adoption.

Reducing carbon emissions… reducing pollution

- Storage on the grid is vital if we are to increase the use of renewables.
- Current batteries are generally only suitable for short term back-up and frequency regulation, or on micro-grids.

Sustainability of resources

I. Gyuk, A. Nourai and C. Shafer, 2009
We are reaching the theoretical limits and (radically) new approaches are required

Tesla projects that battery costs will drop to $100/KWh (down to approx. $160/KWh in 2019)

Critical need to increase battery longevity and monitor state of health (SoH):
  • cost,
  • sustainability,
  • safety
  • second-hand use etc.

Pushing the limit has safety consequences
Energy Storage and Sustainability

![The 90 natural elements that make up everything](image1)

The approx. 45 giga-factories being built will need approx. 840,000 tonnes/yr of lithium, 193,000 tonnes/yr of cobalt, and 480,000 tonnes of nickel chemical. [https://stockhead.com.au/resources/there-are-now-45-battery-mega-factories-driving-demand-for-lithium-cobalt-and-graphite/](https://stockhead.com.au/resources/there-are-now-45-battery-mega-factories-driving-demand-for-lithium-cobalt-and-graphite/)

But as we move towards high Ni cathodes in Evs Ni is now becoming an issue..

![Cobalt Production in metric tons](image2)

Source: US Geological Survey

Ways to Reduce Cost

- Cheaper materials
- Increase energy density (capacity x voltage)
- Increase capacity
- Thicker electrodes – reduce amount of separator, current collector, packaging etc.
- Increase longevity (calendar life and cycle no. – often require different chemistries)
- 2nd hand market for batteries
  - Insurance
  - Pricing
  - Guaranteeing longevity

Life Cycle Analysis

- Today’s battery assembly process requires 400 kWh of energy to make batteries that deliver 1 kWh of energy, releasing 75kg of CO₂.

To relate external stimuli and stresses (high temperature, charging rates) to physical and chemical processes that cause degradation of performance inside the battery, and to develop solutions to this through materials and systems design.

Lead: Clare P Grey

Partner universities: Cambridge, Glasgow, Imperial College, Liverpool, Manchester, Newcastle, Southampton, Strathclyde, University College Warwick + 10 industry partners

Materials – NMC-811 + graphite
Increasing energy density:

3.75 Li + Si -> Li_{3.75}Si vs. Li + 6C -> LiC₆

<table>
<thead>
<tr>
<th></th>
<th>Carbon</th>
<th>Silicon</th>
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<tbody>
<tr>
<td>Gravimetric Capacity (mAh/g)</td>
<td>372</td>
<td>3572</td>
</tr>
<tr>
<td>Volumetric Capacity (mAh/cm³)</td>
<td>843</td>
<td>8322</td>
</tr>
</tbody>
</table>

Strategies: New electrolyte additives
Limit capacity used
Graphite (graphene) – silicon composites

Alison Michan et al. JACS, 2016
Some current directions in the battery field

Moving Beyond Li?

Na ion batteries:
- Replace Cu current collectors by Al
- Higher abundance of Na
- Almost a drop-in technology
- But energy density is lower than for Li-ion

Mg ion batteries:
- Mg batteries – higher capacity due to 2+ charge?
- But: Electrolyte that allows Mg stripping/plating and desolvation and insertion into cathode challenging
- Mobility in non-sulfide containing cathodes is very sluggish at best


Beyond Conventional Li-ion

Cheaper, More Abundant Materials:

\[ 2Li + S \rightarrow Li_2S \]

Cheap and high energy density
- But soluble polysulfides cross over to the negative electrode

Lithium Sulfur Batteries

Lithium Air Batteries

The Highest Energy Density?

\[ 2Li + O_2 \rightarrow Li_2O_2 \]

Cheap and very high (gravimetric) energy density
- But far from commercial due to problems with electrolyte degradation, large overpotentials, protection of Li metal etc.


But steady progress: e.g., Redox Mediators and Water


DBBQ + H2O Tao Liu.. N. Garcia-Araez, CPG. JACS 2018

LiOH vs. Li$_2$O$_2$ chemistry?

RM

\[ Q_{\text{red}} + \text{Li}^+ + e^- = \text{LiQ}^- \]
\[ \text{LiQ}^- + \text{O}_{2\text{air}} = \text{LiQO}_{2\text{air}} \]


\[ Q_{\text{red}} + \text{Li}^+ + e^- + xH_2O = \text{LiQ}^-\text{-}(nH_2O)_{\text{red}} \]
\[ \text{LiQ}^-\text{-}(xH_2O)_{\text{air}} + \text{O}_{2\text{air}} = \text{LiQO}_x\text{-}(nH_2O)_{\text{air}} \]

DDQB: 2,5-di-tert-butyl-1,4-benzoquinone
The ultimate in safety? All-solid-state batteries

Many Challenges:
Conductivity of solid electrolyte; transport of (Li) to active materials
No conductor is stable against Li metal
Dendrites can still push through grain boundaries in ceramics
Volume changes, cracking and mechanical issues
Energy density

Polymer batteries are sometimes (now) being called solids state batteries!

Membranes needed for Li-S and Li air

Scalable batteries: Redox Flow

Lifetime cost  
Scalability  
Power/Energy density  
Safety

Vanadium ions  
Zinc-bromine  
Organic molecules  
Aqueous systems?

But cost is still no lower than for LIBs

Decouple the materials from the electrochemistry

Investigations of quinones: Lower cost but faster degradation

Towards a more sustainable battery chemistry: Battery Degradation and Increased Lifetime

We need to understand how chemical and mechanical processes that occur over extremely wide length and time scales.

- We need to be able to control materials under harsh non-equilibrium conditions.
- We need to develop ways to understand and control interface processes.
Where possible studies should be performed In-situ:

Development of *in-situ* methods to probe Li dynamics cathodes

Safety and Li dendrite formation

Metastable Si electrode phases

Solving the structures of amorphous anode materials

Sn Anode: PDF and $^{23}$Na NMR

Hard carbon: $^{23}$Na NMR

Josh Stratford, Phoebe Allan
New Chemistries: Designing Materials For High Rate Applications

\[ \text{Nb}_{18} \text{W}_6 \text{O}_{55} \]
Block structure

Bronze-like structure of \( \text{Nb}_{18} \text{W}_{16} \text{O}_{93} \)

Conclusions

• The battery market is growing so fast that there is, I hope, room for many different chemistries – but growth should be sustainable..
• But the challenges are huge..
• In particular we need to:
  – Control non-equilibrium processes and metastable materials and systems
  – Learn how to mitigate degradation
  – Reduce cost
• Batteries should be designed upfront to be recycled

Materials for the energy transition: Photovoltaics

Jenny Nelson
Imperial College London

jenny.nelson@imperial.ac.uk
Rapid growth in installed capacity .. but PV only supplies ~3%
Net Zero:
UK capacity needs to grow from 13.5 GWp to >200 GWp by 2050

How can we enable faster growth?
New technology, incentives or regulation?
Factors influencing the growth of PV power

• Variability of resource
  • Mismatch of supply and demand raises costs
  • Impacts reduced via electricity storage, distribution, use in transport or fuels production

• Cost of technology
  • Module efficiency
  • Balance of systems
  • System design and integration
  • Cost of production: choice of materials and process

• Regulatory
  • Regulation and policies
  • Finance, incentives and pricing
  • Testing and standards
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Issues for materials science

Materials for PV:

- Semiconductors and electrodes
  - Design
  - Manufacture / Processing
  - Optoelectronic properties
  - Defect chemistry
  - Stability (chemical, thermal, mechanical)
  - Contact selection

- Functional coatings
  - Optical (transparency, ageing)
  - Encapsulation

Rest: Interconnects, metals, substrates, coatings, control systems
Factors influencing the growth of PV power

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- Regulatory
  - Regulation and policies
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Issues for materials science

Materials for related technologies:
- Battery electrodes and electrolytes
- Transmission and distribution
- Catalysts, electrolysers
- Heat management and harvesting

Materials for PV:

Semiconductors and electrodes
- Design
- Manufacture / Processing
- Optoelectronic properties
- Defect chemistry
- Stability (chemical, thermal, mechanical)
- Contact selection

Functional coatings
- Optical (transparency, ageing)
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Rest: Interconnects, metals, substrates, coatings, control systems
Improving energy yield of Si Module lifetime Light harvesting (bifacial cells, optical coatings) Thinner cells

Crystalline Silicon
Improving energy yield of Si
Module lifetime
Light harvesting (bifacial cells, optical coatings)
Thinner cells

“Silicon + X”
e.g. Si / high gap tandem
Si + spectral conversion

Crystalline Silicon
Silicon + X

e.g. Si / high gap tandem
Si + spectral conversion

“Silicon + X”

High efficiency designs
Multijunctions
Multijunctions + concentration
Novel multi-gap concepts

Improving energy yield of Si
Module lifetime
Light harvesting (bifacial cells, optical coatings)
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Low cost, low energy production
Solution processible semiconductors (molecular, perovskite, nanoparticle)
Improving energy yield of Si
Module lifetime
Light harvesting (bifacial cells, optical coatings)
Thinner cells

“PV + X”
Integration e.g.
Electric / thermal
PV / fuels
PV / storage

“Silicon + X”
e.g. Si / high gap tandem
Si + spectral conversion

High efficiency designs
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Multijunctions + concentration
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Low cost, low energy production
Solution processible semiconductors
(molecular, perovskite, nanoparticle)
Example: Silicon + perovskite tandem for high efficiency

“Silicon + X”
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High efficiency designs
Multijunctions
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Example: Silicon + perovskite tandem for high efficiency

“Silicon + X”
e.g. Si / high gap tandem
Si + spectral conversion

Perovskite-on-Si tandem can increase efficiency without high fabrication costs of III-V multijunctions

High efficiency designs
Multijunctions
Multijunctions + concentration
Novel multi-gap concepts

• Materials issues
  • Perovskite defect control, Pb content
  • Si surface compatibility with perovskite
  • Design optimisation (thicknesses, e.g.)
  • Transparent conducting electrodes, interlayers
  • ‘Green’ manufacturing processes

Oxford PV
Example: Flexible lightweight solar cells for mobile power

Low cost, low energy production
Solution processible semiconductors
(molecular, perovskite, nanoparticle)
Non-traditional markets for mobile power such as IoT, indoor power, remote sensing, satellite power, are growing rapidly.

Different demands in terms of spectral response, operating conditions, lifetime, power/weight and production cost.

Example: Flexible lightweight solar cells for mobile power

Low cost, low energy production
Solution processible semiconductors (molecular, perovskite, nanoparticle)
Example: Flexible lightweight solar cells for mobile power

Non-traditional markets for mobile power such as IoT, indoor power, remote sensing, satellite power, are growing rapidly.

Different demands in terms of spectral response, operating conditions, lifetime, power/weight and production cost.

- Materials issues
  - Optimisation of semiconductor for light source (spectrum, intensity, diffusivity)
  - Lightweight, flexible, robust device
  - Radiation hardness, temperature response, lifetime
  - Integrated design and product fab
  - Non-toxic components and manufacture

Low cost, low energy production
Solution processible semiconductors (molecular, perovskite, nanoparticle)
Thank you
Professor Nora de Leeuw

University of Leeds
Computation has role to play in designing and/or improving sustainable energy materials

Following concept of *Materials Genome Initiative*

Examples:
Iron sulfide (photo)catalysts
Nature-inspired iron sulfides for CO$_2$ conversion to fuels and chemicals

Origin of Life

Synthetic and Model Greigite

Enzyme reactive sites

Ferredoxin
# Importance of pH in electrochemical reaction

<table>
<thead>
<tr>
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<th>pH = 4.5</th>
<th>pH = 6.5</th>
<th>pH = 10.5</th>
<th>H$_2$O</th>
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<tbody>
<tr>
<td>Fe$_3$S$_4$</td>
<td><img src="image1.png" alt="Image" /></td>
<td><img src="image2.png" alt="Image" /></td>
<td><img src="image3.png" alt="Image" /></td>
<td><img src="image4.png" alt="Image" /></td>
</tr>
<tr>
<td>(001)</td>
<td>$E_B = 0.00$ eV</td>
<td>$E_B = -0.36$ eV</td>
<td>$E_B = 1.24$ eV</td>
<td>$E_{B[n=10]} = -0.65$ eV</td>
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<td><img src="image5.png" alt="Image" /></td>
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<td><img src="image7.png" alt="Image" /></td>
<td><img src="image8.png" alt="Image" /></td>
</tr>
<tr>
<td>(111)</td>
<td>$E_B = -0.62$ eV</td>
<td>$E_B = -1.63$ eV</td>
<td>$E_B = -0.46$ eV</td>
<td>$E_{B[n=10]} = -0.73$ eV</td>
</tr>
</tbody>
</table>
The Mechanism

\[
\begin{align*}
H_2CO_3(aq) + 2 \cdot H_2O & \rightarrow \text{HCOO}^* + H_2O \rightarrow \text{HCOOH} + 2 \cdot \text{OH}^* \\
H_2CO_3 + 6 \cdot H_2O & \rightarrow \text{COOH}^* + 5 \cdot H_2O \rightarrow \ldots \rightarrow \text{H}_3\text{COH} + 6 \cdot \text{OH}^*
\end{align*}
\]

- **One** initial reactant: C(OH)O₂
- **Two** possible sites for intermediates: Feₐ & Feₐ
- Dissociation and Migration processes
- More than 170 intermediates characterised
The Products

**pH 4.5**
- Formation of C-C bonds
- Implies preference of **alkaline** over acidic hydrothermal vents
- Circumstantial evidence for greigite acting as a **primordial catalyst** to the modern Acetyl-CoA pathway

**pH 6.5**

**pH 10.5**

$^1$H-NMR Analysis
Iron pyrite FeS$_2$ for photocatalysis

Unique properties

▪ Earth-abundant, non-toxic
▪ Suitable band gap for efficient visible light absorption (~0.95 eV)
▪ Large photon absorption coefficient of $10^5$ cm$^{-1}$ (two orders of magnitude higher than that of crystalline silicon)
▪ High carrier mobility

Limitations

▪ Photo-electrochemical cell efficiency ~3%
▪ Small open-circuit voltage ($V_{OC}$) of ~0.2 eV

Potential

▪ Theoretical $V_{OC}$ limit is 0.71 eV
The presence of orthorhombic marcasite inclusions in pyrite is generally believed to be detrimental for its photochemical performance.

**An early experiment (1980):** reported the band gap of marcasite to be $0.34 \text{ eV}$ from temperature dependent (53-370 K) electrical resistivity measurements.

**Recent Theoretical Calculations:** however, predict that marcasite should have a band gap of $0.8-1.2 \text{ eV}$.

**A Recent Experiment (2016):** using diffuse reflectance spectroscopy measurements on natural marcasite samples reported the band gap to be $0.83 \pm 0.02 \text{ eV}$.
Chopped light voltammetry curves of FeS$_2$ films

- Mixed phase = $4.30 \text{ mA/cm}^2$
- Mixed phase = $1.98 \text{ mA/cm}^2$
- Pure pyrite = $0.14 \text{ mA/cm}^2$
Band alignment: marcasite & pyrite

**Vacuum Level**

- **Marcasite**
  - $E_g = 1.17$ eV
  - $\Delta E_{CBM} = 0.64$ eV

- **Pyrite**
  - $E_g = 0.96$ eV
  - $\Delta E_{VBM} = 0.43$ eV

**Conduction Band**

**Valence Band**
Acknowledgements

- **Dr Alberto Roldan** – UCL PDRA, now Lecturer at Cardiff University

- **Dr Nathan Hollingsworth** – UCL PDRA, now senior scientist at Infineum

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- **Longfei Wu, Dr Jan-Philipp Hoffman**
  TU Eindhoven, The Netherlands
Professor Stuart Parkin
Max Planck
Halle
Low Energy Electronics
Beyond charge currents: spin and ion currents for future data storage and computing technologies

Stuart Parkin
Max-Planck Institute for Microstructure Physics
Halle (Saale)

Martin Luther University
Halle-Wittenberg

stuart.parkin@mpi-halle.mpg.de
The end of charge-based computing!

Beyond charge $\rightarrow$ spin, ions
2D $\rightarrow$ 3D

Neuromorphic Computing

Quantum Computing

CMOS: electrons 40 years

$\$1000 Buys: Computations per second
Spintronics – from materials and phenomena to applications

Parkin & Yang, Nature Nanotechnology (March 2015)
Spintronic technologies evolution

HDD GMR/MTJ read heads

- Oscillatory interlayer coupling
- Co/Cu
- Interface spin-dependent coupling
- Dusting layers

1988-1991

GMR Spin Engineering
- Oscillatory interlayer coupling
- Co/Cu
- Interface spin-dependent coupling
- Dusting layers

1995 MTJ proposal

1996 1 Kbit array
- High MR
- Low RA
- 0.25 μm
- 2.3 ns R/W

1997 Spin-valve recording heads (mass-production)

1999 16 Mbit demonstrator
- (180nm CMOS)
- Field switched

2001 Giant TMR using MgO

2005 Magnetic Tunnel Junction recording heads (mass production)

2015 Slow-down of increased HDD capacity

2019 Samsung announces shipment of high-performance foundry 28nm CMOS STT e-MRAM
Magnetic Racetrack Memory

- Bits = Domains in the tracks

- A novel *three-dimensional* storage-class memory

- The capacity of a hard disk drive

*Parkin, US patents 6834005, 6898132 (2004)*

*Parkin et al., Science 320, 190 (2008)*

*Parkin, Scientific American (2009)*
Memory on Racetrack!
4+ stages

Computers and the Brain are Dramatically Different

Separates memory and processor
Sequential, centralized processing
Ever increasing clock rates, high active power
Huge passive power
Programmed system, hard-wired, fault-prone
Algorithms and analytics

Integrates memory and processor
Parallel, distributed processing
Event-driven, low active power
Does “nothing” better, low passive power
Learning system, reconfigurable, fault-tolerant
Substrate and pattern recognition
Cognitive computing needs new materials, novel devices, innately 3D

**Neuromorphic (or cognitive) computing**
- Mammalian brains all have a similar structure
  - **Neurons** (computing elements), each connected via ~10,000 synapses
  - **Synapses** weaken and strengthen according to rules e.g. spike timing dependent plasticity (STDP)
  - Large devices (micron size) that operate slowly (100 msec)
  - Very low power – $10^6$ x less energy per computing operation than CMOS
- Many possible approaches to building artificial brains
  - **Charge based**
    - Mostly based on resistive switching concepts
    - Electrical breakdown of oxides, nitrides to form atomic scale filaments
    - Leakage currents → high energy
    - Capacitive charging of electrical wires → high energy
  - **Spin based**
    - Currents of spins or magnons
    - All proposed concepts to-date consume too much energy
  - **Ion based**
    - Nature uses ionic currents and liquids

Jiang et al. (unpublished)
Innately 3D memory-storage and logic devices

Racetrack Memory

10 to 100 times the storage capacity of conventional solid state memory → displace flash memory and hard disk drives

Chiral magnetic, topological nano-objects

Cognitive Devices emulating synaptic functions in a solid state device → Million times more energy efficient than charge based computers
Thank you
# Webinar Agenda

<table>
<thead>
<tr>
<th>Time</th>
<th>Session</th>
<th>Speaker/Institution</th>
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</table>
| 9:50 - 10:20 | Plenary Session Chair: Professor Manish Chhowalla | Professor Clare Grey, University of Cambridge, UK  
Professor Jenny Nelson, Imperial College London, UK  
Professor Nora de Leeuw, University of Leeds, UK  
Professor Stuart Parkin, Max Planck, Halle, Germany |
| 10:20 - 10:30 | Q&A                          |                                                      |
| 10 minute break |                              |                                                      |
Plenary Speaker Q&A

Dame Julia King
Baroness Brown of Cambridge

Professor Clare Grey
University of Cambridge

Professor Jenny Nelson
Imperial College London

Professor Nora de Leeuw
University of Leeds

Professor Stuart Parkin
Max Planck, Halle
# Webinar Agenda: Session 2

<table>
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<td>11:40-11:45</td>
<td>Close of Session: Prof. Neil Alford</td>
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</table>
Motivations

In 2019 the UK became the first major economy to pass an emissions law of net-zero by 2050

Data taken from Estimated territorial greenhouse gas emission by source category in 2018
Material Opportunities

To address net zero 2050 challenge we have defined 4 key topics:

• The Future of Materials in Photovoltaic Systems
• Low-Carbon Methods of Hydrogen Generation
• Decarbonisation of Heating and Cooling
• Low Loss Electronics

Figure adapted from: S. B. Reese, T. Remo, J. Green, A. Zakutayev, 'How Much Will Gallium Oxide Power Electronics Cost?' Joule, Volume 3, Issue 4, 2019, Pages 903-907
Timeline of Roadmapping Process

- Idea conceived: September 2019
- Collaborated with the IOP: October 2019
- Online launch of key findings: 15th June 2020
- Publication of Roadmaps: September 2020
- Community refinement: July-August 2020
- Community Survey: Feb-March 2020
- Online Workshops: March-June 2020
- 272 Responses
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Imperial College London

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Dr Oliver Fenwick
Queen Mary University of London

Calorics
Dr Xavier Moya
Cambridge University

Low Loss Electronics
Prof. Edmund Linfield
Leeds University
Photovoltaics

Dr Robert Hoye

Imperial College London
Photovoltaics: Motivation

- UK PV deployment needs to increase from 13.5 GW today\(^1\) to >200 GW by 2050 to fulfil net-zero targets\(^2\)
- UK has a very challenging environment for commercialising new PV technologies, despite active academic and start-up environment
- *What is the future of PV materials research to achieve carbon neutrality by 2050, and also enable the UK to gain a competitive advantage in emerging markets?*

\(^1\) The Solar Commission (2019)
Photovoltaics: Road Mapping Scope

Future of photovoltaic materials research from now to 2050

Consultation with 14 academic institutions/national laboratories and 10 companies

Industry challenges in existing and emerging PV

Utility-scale

Emerging markets

IOP Institute of Physics
Photovoltaics: Key Research Challenges

• Understanding and overcoming loss processes limiting absorber efficiency and stability

• Scaling up new technology and prototyping at the module level

• Extending device lifetime of current commercial technology from 25 years (now) to 40 years (by 2050) for terrestrial applications

• Development of electrodes (transparent and opaque) and metallization that are not reliant on expensive or rare elements
Photovoltaics: Key Opportunities Identified

• Low capital-intensity solar cells with extended stability – multi-junction devices especially promising

• CO₂ neutral buildings – BIPV can be used as roof-tiles, windows, façades, car-porches, greenhouses

• Lightweight, flexible PV to work under lower light levels and power electric vehicles/be used for aerospace applications

• Enablers of other renewable technologies – e.g.: solar fuel generation, generating ammonia, solar water splitting
Photovoltaics: Requirements

- Dedicated funding for PV absorber and contact material development
- Central facilities for device metrology and degradation testing
- Catapults and pilot facilities
- Consortia to bring together the key stakeholders: people in R&D (academics, SMEs), manufacturers, funders (e.g.: InnovateUK), end-user industries (asset managers, architects, consumer goods marketing specialists, satellite and automotive industries)
- CDTs and training networks
### Roadmapping Session Speakers

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Materials for production of hydrogen and related fuels and chemicals

Dr Ifan Stephens

Imperial College London
Hydrogen Production: Motivation

UK Greenhouse gas emissions\(^1\)

- Land, land use change and forestry
- International shipping bunkers
- Public
- Industrial processes
- Waste management
- International aviation
- Agriculture
- Residential
- Business
- Energy supply
- Transport

![Graph showing UK Greenhouse gas emissions](image1)

UK hydrogen demand\(^2\)

![Graph showing UK hydrogen demand](image2)

Global hydrogen demand\(^3\)

![Graph showing Global hydrogen demand](image3)


Hydrogen Production: Materials

Discussion focused upon the development of new catalysts, membranes and electrode materials

Consultation with 20 academic institutions/national laboratories and 6 companies
Hydrogen Production: Key opportunities

- **Proton exchange membrane electrolysers**
  - Decrease or eliminate precious metals from catalysts
  - Improve cost, stability and conductivity of electrode materials

- **Alkaline electrolysers**
  - Improve membrane stability and conductivity
  - Improve catalyst activity

- **Solid oxide electrolysers**
  - Improved electrode and electrolyte materials

- **Direct photocatalytic water splitting**
  - More efficient and stable photoelectrode materials

- **Thermochemical synthesis of chemical feedstocks**
  - Catalysts and other material for low pressures and temperatures

- **Electrochemical reduction of carbon dioxide and nitrogen**
  - Discover catalysts, electrodes and electrolytes yielding high activity, and selectivity

Proton exchange membrane electrolyser, with inset showing oxide nanoparticles, to catalyse oxygen evolution at electrode
Hydrogen Production: Requirements

• State-of-the-art facilities

• World-class scientists and engineers

• Integration of academia and industry across the UK

• Strong integration into international partnerships, research programmes and value chains

• Routes and facilities for the testing of new materials at single cell level
  • Intermediate between the laboratory scale testing in academia and full electrolyser stacks used in industry
Hydrogen Production: Opportunities

• UK has leading companies in¹:
  • Electrolysers and fuel cells (ITM Power and Ceres Power)
  • Catalysts and other materials for hydrogen production (Johnson Matthey)

• Harnessing the UK’s enormous potential for renewable electricity¹:
  • 29-96 GW of onshore wind
  • 145-615 GW of solar power
  • 92-245 GW of offshore wind

• Enable decarbonisation of²:
  • Vehicles (especially heavy duty)
  • Heat
  • Production of steel, methanol and ammonia

• Become Europe’s leading exporter of hydrogen¹

Roadmapping Session Speakers

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Dr Robert Hoye
Imperial College London

Hydrogen Production
Dr Ifan Stephens
Imperial College London

Thermoelectrics
Dr Oliver Fenwick
Queen Mary University of London

Calorics
Dr Xavier Moya
Cambridge University

Low Loss Electronics
Prof. Edmund Linfield
Leeds University
Thermoelectrics

Dr Oliver Fenwick

Queen Mary, University of London
Thermoelectrics: Motivation

Temperature gradient ↔ Electrical power

• About 2/3 of primary energy is currently wasted as heat; emitted at different heat source temperatures.

Figure taken from: https://flowcharts.llnl.gov/
Thermoelectrics: Motivation

• More effective waste heat harvesting is an important technology for contributing to the energy transition to zero carbon by 2050.

• Key technologies:
  • Heat engines for low grade waste heat
  • Thermal storage
  • Long distance heat transmission
  • Thermophotovoltaics
  • Thermoelectrics

• Thermoelectric generators directly convert waste heat into useful electricity.

Thermoelectrics: Background

Heat-to-electricity conversion efficiency:

\[ \eta = \frac{T_h - T_c}{T_h} \frac{\sqrt{1 + ZT} - 1}{\sqrt{1 + ZT} + T_c/T_h} \]

\[ \eta(ZT = 3) \approx 20\% \]

Automotive
Nanostructured thermoelectric generator

Improvement in fuel efficiency
2-10% (ZT≈0.5-1)


Peltier cooling
Refrigerant-free, no moving parts.

Industrial heat recovery

Vining, Nat. Mat. 8, 83 (2009)

Carnot efficiency
Thermodynamic limit
ZT=\infty

ZT=20, unlikely
ZT=4, ambitious
ZT=2, plausible eventually
ZT=0.7, available today

Coal/Rankine
Solar/Brayton
Nuclear/Brayton+Rankine
Solar/Stirling
Nuclear/Rankine
Solar/Rankine

Geothermal/Org. Rankine

Cement/Org. Rankine

Heat source temperature (K)
Efficiency (%)
Thermoelectrics: Materials

• Figure of merit: $ZT = \frac{S^2 \sigma T}{\kappa}$
  - $S$ – Seebeck coefficient
  - $\sigma$ – electrical conductivity
  - $\kappa$ – thermal conductivity

• No known theoretical limits of $ZT$, but difficult materials challenge.

• Road Mapping for different classes of thermoelectric materials with 10 academic institutions/national laboratories and 3 companies

Thermoelectrics: Roadmapping Scope

Thermoelectrics materials research from now to 2050

Consultation with 10 academic institutions/national laboratories and 3 companies

<table>
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<tr>
<th>Applications</th>
<th>Materials technologies</th>
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<tr>
<td>Chalco-genides</td>
<td>Si/ Silicides</td>
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<td>Skutterudites</td>
<td>Zintl/Half-Heusler</td>
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<td>2D Materials</td>
<td>Organic SCs</td>
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<td>Hybrid</td>
<td>Topological</td>
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Established Materials

Emerging materials

IOP Institute of Physics
Thermoelectrics: Key Opportunities

• Largely a materials challenge

• **Near term applications** – Can be addressed with established materials with proven performance (Bi₂Te₃, PbTe, SnSe, Si)

• **Classes of emerging, new thermoelectric materials with new physics**
  - Rapid performance improvement, particularly for low temperatures in Heusler alloys, organics, organic-inorganic hybrids
  - Emerging quantum/topological thermoelectric materials
  - Opportunities for overcoming limits difficult to overcome in conventional materials – Potential for ZT > 3

• **Addressing issues of materials abundance**
Thermoelectrics: Requirements

- Exploration of structure-property relationships
- Better understanding of charge and heat transport across nanoscale interfaces – Decoupling of electrical and thermal conductivity
- Need for accurate measurements of thermoelectric properties
- Device prototyping: Architectures for different applications, electrical & thermal contact resistances; operational reliability
- Scale-up: Materials abundance, cost, scalable processing, life cycle analysis
- Need for close co-operation between academic exploration of different materials classes and industrial prototyping and scale up
Thermoelectrics: Opportunities

• Establishing thermoelectric converters as a broadly applicable technology for efficient waste heat harvesting across a range of low temperature and high temperature applications.

• Significant improvements in the energy efficiency of key industrial, residential as well as transportation processes.

• A step-change in ZT could deliver a huge market expansion.

• Business opportunities for UK materials companies, device manufacturers as well as end users (automotive, refrigeration, chemical industries, ...)

IOP Institute of Physics
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Calorics

Dr Xavier Moya

University of Cambridge
Calorics: Motivation

• 17% of UK CO₂ emissions are from space heating and cooling of buildings

• Most are from burning natural gas and compressing volatile greenhouse gases

• Reaching the 2050 net-zero carbon target will require energy-efficient heat pumps that operate without gases

• Caloric materials can provide a solution for zero-carbon heating and cooling

BEIS December 2018 Report
Clean Growth – Transforming Heat
Calorics: How does a heat pump work?

Temperature

Hot air

Field off

Field on

Cycle

Temperature

Cooling

Heating

Cold air

Phase 1

Phase 2

IOP Institute of Physics
Calorics: Roadmap Consultation

• Comprehensive integrated programme on development of caloric materials and devices

• 8 academic institutions

• 2 companies

• Research needed across technology readiness levels (TRLs)

• Develop fundamental and applied research in academia and industry
Calorics: Key challenges

- **Magnetocaloric** materials driven using magnetic field
  - Reduce cracking
  - Reduce driving field

- **Electrocaloric** materials driven using electric field
  - Improve fabrication of multilayers
  - Increase breakdown field

- **Elastocaloric** materials driven using stress
  - Reduce fatigue
  - Increase breakdown field

- **Barocaloric** materials driven using pressure
  - Reduce hysteretic losses
  - Reduce driving pressure
Calorics: Opportunities

• 150bn world market for heating (£50bn) and cooling (£100bn) of buildings

• £300bn market when including domestic and commercial refrigeration, with projected annual growth 5-10%

• Heat pumps based on caloric materials will:
  • Permit decarbonisation of heating and cooling
  • Provide energy independence
  • Enable world leadership on net zero-carbon heating and cooling

• Energy, environmental and job security
Roadmapping Session Speakers

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Dr Robert Hoye
Imperial College London

Hydrogen Production
Dr Ifan Stephens
Imperial College London

Thermoelectrics
Dr Oliver Fenwick
Queen Mary University of London

Calorics
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Cambridge University

Low Loss Electronics
Prof. Edmund Linfield
Leeds University
Low-loss Electronics

Professor Edmund Linfield

University of Leeds
Low Loss Electronics: Motivation

- The world market in electronics is worth £602bn with a predicted growth of 2.3% over the next five years.¹

- Yet UK revenue in 2019 was reported to be only £1.9bn, emphasising the need to grow the UK’s electronics sector.²

- Digital technologies consume about 5%³ of the world’s energy, and this is expected to reach 21% by 2030.⁴

- Approximately 30% of all electric power generated utilises power electronics. The global market is estimated at £135bn, growing at a rate of 10% per year.⁵

How do we stimulate the UK economy, meet consumer’s expectation, and yet achieve the UK government’s net-zero greenhouse gas emissions by 2050?

Low Loss Electronics: Roadmapping Consultation

- 50 participants from 20 academic institutions, 10 companies, one national laboratory, and one central facility were consulted

- Industrial interest represented by wafer fab, equipment manufacturers, and end users
Low Loss Electronics: Roadmapping Opportunities

- Power Electronics – the key technology to control flow of electrical energy from source to load
  - A pipeline for industrial exploitation from academic research to wafer scale up
  - Investment in UK’s ability to innovate and manufacture GaN and SiC devices
  - Materials for next generation power electronics, beyond GaN and SiC
  - Replacing scarce materials, recycling, and evaluating full energy cost of manufacturing.

Percentage power loss in wind generation for SiC and Si

![Graph showing power loss percentages for SiC and Si](image-url)
Low Loss Electronics: Roadmapping Opportunities

• CMOS – Monolithic integration to reduce energy:
  – Tunnel and negative capacitance field effect transistors
  – New channel materials such as 2D materials (e.g. graphene) and III-V semiconductors

Monolithic integration to add functionality:

  – Sensing, energy harvesting and low power radio-frequency (RF) devices
  – Photonics, magnetics, piezoelectrics, 2D materials, electronics and plasmonics

Figure adapted from: A. Chen, IEEE Design and Test, 36, 3 (2019)
Low Loss Electronics: Roadmapping Opportunities

‘More than Moore’ - beyond CMOS and beyond von Neumann computing

Beyond von Neumann
– In-memory computing
– Neuromorphic computing

Beyond CMOS
– Spintronic, topological and organic materials
– Chargeless computation, collective switching

A. Chen, IEEE Design and Test, 36, 3 (2019)
**Low Loss Electronics: Summary**

State-of-the-art facilities, and world-class scientists and engineers

- Big data and AI approaches to materials discovery (Materials 4.0)
- Simulation and Modelling
- Integration of Academia and Industry
- Routes for piloting new materials to wafer-scale fabrication and manufacture
- Centers for Materials Recycling, Testing, and Metrology

A transformative programme to address society’s increasing energy demands, and its carbon footprint

- Inward industrial investment into the electronics sector, capitalising on UK’s strengths in advanced materials
- Enable the UK to be an internationally-leading innovator in the device supply chain, providing sovereign capability
## Webinar Agenda: Session 2

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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 unleash potential
- Legislate the uptake and implementation of low-carbon technology
- Researched materials should be resource abundant, scalable and recyclable
- People: Training, PhD programme, PDRA support etc.
Impact for the UK

Meet our 2050 net-zero target

New jobs and filling the skills gap

Energy security
Q&A session

• If you’d like to ask a question please submit it in the question box:

Please submit in the following format:
‘To whom: Question Content’
e.g: ‘Prof. E Linfield : what is your favourite colour?’

Questions will be asked anonymously

• Please note: we may not be able to answer all the questions today, but a FAQs document on the road mapping session will be made available on the Royce website after the event
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Timeline of Roadmapping: Next Step

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- Collaborated with the IOP: October 2019
- Online launch of key findings: 15th June 2020
- Publication of Roadmaps: September 2020
- Online Workshops: March-June 2020
- Community Survey: Feb-March 2020
- Community refinement: July-August 2020
- 272 Responses
What happens next?

This week all participants will receive a link to the executive summaries

From July draft roadmaps will be available, on which we welcome community feedback

If you are not already involved with the roadmapping work but would like to be going forward please get in touch at: scienceandinnovation@iop.org

Or respond to the survey which will be sent to all participants after this event
Thank you

To the Materials for the Energy Transition community—especially the workshop attendees

Plenary speakers: Julia King, Clare Grey, Nora de Leeuw, Jenny Nelson, and Stuart Parkin

Steering group: Manish Chhowalla, Richard Curry, Edmund Linfield

Roadmapping Leads: Oscar Cespedes, Oliver Fenwick, Robert Hoye, Xavier Moya, Ifan Stephens, and Sam Stranks

The IfM: Nicky Athanassopoulou, Arsalan Ghani, Imoh Ilevbare, Andi Jones, Diana Khripko, Rob Munro

The Institute of Physics, and the Henry Royce Institute: Anne Crean, Ellie Copeland, Isobel Hogg, Mia Belfield, Amy Nommeots-Nomm, Lata Sahonta, Katharina Zeissler.
Thank you