THE FUTURE OF MATERIALS FOR LOW LOSS ELECTRONICS

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This report was prepared by:



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TABLE OF CONTENTS

1
5
6
6
13
13
14
19
21
23 23
25
25
25
27
28
29
34 35
40
40 41
41

Interconnect Materials	
Interconnect Materials	
Spin Based Interconnects	42
Superconductor Based Interconnects	
Magneto-optic devices	
Antiferromagnetic deviceS	
Two dimensional materials	43
Organic and Molecular spintronic materials	
Growth of nanocarbon and molecular thin films	45
Carbon based molecules	45
Spintronics on flexible substrates and sensors	46
UK capabilitieS	50
UK Community recommendationS	50
	50
CONCLUSIONS, RECOMMENDATIONS AND KEY MESSAGES	
CONCLUSIONS, RECOMMENDATIONS AND KEY MESSAGES	52 54
CONCLUSIONS, RECOMMENDATIONS AND KEY MESSAGES APPENDICES	52
CONCLUSIONS, RECOMMENDATIONS AND KEY MESSAGES APPENDICES	
CONCLUSIONS, RECOMMENDATIONS AND KEY MESSAGES. APPENDICES APPENDIX I: WORKSHOP DETAILS Workshop Methodology Workshop Design	
CONCLUSIONS, RECOMMENDATIONS AND KEY MESSAGES. APPENDICES APPENDIX I: WORKSHOP DETAILS Workshop Methodology Workshop Design Workshops Description.	
CONCLUSIONS, RECOMMENDATIONS AND KEY MESSAGES. APPENDICES APPENDIX I: WORKSHOP DETAILS Workshop Methodology Workshop Design Workshops Description. Indicative Workshop Agenda.	
CONCLUSIONS, RECOMMENDATIONS AND KEY MESSAGES. APPENDICES APPENDIX I: WORKSHOP DETAILS Workshop Methodology Workshop Design Workshops Description Indicative Workshop Agenda Dates of Workshops	
CONCLUSIONS, RECOMMENDATIONS AND KEY MESSAGES. APPENDICES APPENDIX I: WORKSHOP DETAILS Workshop Methodology Workshop Design Workshops Description Indicative Workshop Agenda Dates of Workshops	
CONCLUSIONS, RECOMMENDATIONS AND KEY MESSAGES. APPENDICES APPENDIX I: WORKSHOP DETAILS Workshop Methodology Workshop Design Workshops Description. Indicative Workshop Agenda. Dates of Workshops Royce Scientific co-ordinators IfM Facilitators	52 54 54 54 54 54 54 55 56 56 56

EXECUTIVE SUMMARY 1

- 2 In the context of the UK's ambitious target to bring all greenhouse gas emissions to net-zero
- 3 by 2050 the development and adoption of more energy-efficient electronic systems are an
- important enabler for the UK to achieve this goal. 4
- 5 The Henry Royce Institute (UK's national institute for materials research & innovation)
- 6 supported by the Institute of Physics, brought together over 50 UK academic and industrial

7 experts from different research, fabrication, equipment supply and user fields in a community 8 consultation of nine workshops to explore different materials and methods that are required

- for the future of such low-loss electronics. 9
- The consultation focused on three main areas identified as of the highest impact: 10
- 11 Materials for Power Electronics
- Materials for CMOS 12

31

- 13 Materials for 'beyond CMOS device architectures' ('More than Moore').
- 14 Key findings include the needs for:
- 15 Investment to support UK prototyping/pilot-plant scaling of devices from research to 16 wafer-scale fabrication and manufacture, including validation and testing; this 17 provides a supply chain to test and translate new ideas.
- 18 > Investment in a network of state-of-the-art 'fab-of-the-future' centres, accessible to 19 the whole UK, encompassing the design, growth and fabrication of new materials. 20 This would be supported by UK Centres in Materials Replacement & Recycling, High-21 frequency Devices, and High-throughput Testing, each underpinned by world-class 22 scientists and engineers, with dedicated specialist technical staffing
- > Development of techniques to effectively and efficiently embed new materials into 23 24 high performance, energy efficient devices, including interfacing with the external environment. 25
- 26 Establishment of big data and machine learning (AI) approaches to materials 27 discovery (Materials 4.0) and advancing the understanding of interfacial properties 28 (Interface 4.0), supported by accessible materials databases, and simulation and 29 modelling development across the length scales - from atoms to devices.
- 30 Investment to support the development of new computing architectures, and next generation wide-bandgap semiconductors for power electronics.
- 32 > Funding approaches to support UK-wide collaborations between academia and 33 Industry.
- Investments and incentives for industry to undertake research, and lead and develop 34 exploitation strategies. 35
- > Influencing policy, including setting power consumption targets, supporting the 36 37 circular economy through end of life considerations, and removing reliance on scarce 38 materials

39 It is proposed that these will be critical factors in establishing an environment where the UK

40 takes a leading position and becomes the place for investment for the future development

- 41 of *low-loss electronics*.
- 42

43 Over the next three months these findings will be developed into targeted business cases
44 for funding approaches to support UK-wide collaborations between academia and
45 Industry.

46

47 INDUSTRY AND MARKET

48 Today, an estimated 40% of natural resources are converted to electrical energy. This is expected to grow to 60% by 2040¹. The way we generate and use electricity will have a 49 huge impact on greenhouse gas emissions. How we use and more importantly how efficient 50 we use electricity to achieve desired outcomes, such as performing a computational task or 51 52 propelling an electric car will shape our path to net zero and will impact the UK economy. The resulting world market in electronics is worth £602 billion with a predicted growth rate 53 54 of 2.3% over the next five years². It is also notable that approximately 30% of all electrical 55 energy generated utilises power electronics, with the global market estimated at £135 billion, 56 and a growth rate of 10 % per year³. However, in 2019 UK revenue in the electronics sector was reported to be only £1.9 billion⁴, emphasizing the need to stimulate manufacturing and 57 58 policies in this critically important sector. But this comes at a price. Digital technologies 59 consume about 5% of the world's energy, a figure which is expected to reach 21 % by 2030⁵. 60

To reduce the carbon footprint of digital technologies, improving performance beyond current fundamental limits is critical. But even greater than this is developing new kinds of devices, for all aspects of low-loss advanced computing and power conversion. These new devices, which are needed in all things related to Big Data, in IoT, AI, a smart grid, and electric and autonomous vehicles, impact hugely on achieving a green, high quality way of life. The discovery and development of eco-friendly materials lies at the very heart of this area.

69 PROBLEM STATEMENT

The consultation on materials and frameworks for sustainable, low loss electronics is intended to identify ways to enable the UK to meet its goal of net-zero greenhouse gas emissions by 2050. By bringing together academic experts from different materials research fields, the workshops aimed to review the state of the art and set realistic performance targets for materials leading up to the 2050 goal. The workshops fed into a low loss electronics roadmap on sustainable low loss electronics to help the UK to meet its net-zero goal, and is focused on the following high-level questions:

77

¹ ECPE_Position_Paper_Energy_Efficiency.pdf

² IBIS World Industry report C2524-GL Global Semiconductor & Electronic Parts Manufacturing – C. Mieles (January 2020)

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

⁴ IBISWorld Industry Report C26.110 Electronic Component Manufacturing in the UK –Samuel Kotze (January 2019)

⁵ N. Jones, The information factories, Nature 561, 163 (2018)

- Which materials systems and frameworks show the most promise for viable energysaving applications towards net-zero emissions by 2050, and what is the current state of the art?
- 81 2. What are the current materials challenges that limit the deployment of these82 materials?
- 83 3. What performance could be achieved with current materials, and what could be achieved by 2030, and by 2050?
- 4. What should be the key standards and metrics for the performance of materials and devices?
- 5. How can improvements be made in the characterisation of these materials?
- 6. What are the best action plans to integrate a wide range of strategies into highlydeveloped and widely used technologies?
- 90
 7. How can improvements be made in the provision of advanced facilities required for
 91 industry scale-up and commercial testing, in comparison to the availability of suitable
 92 lab-scale tools?
- 93

97

Furthermore, a key strategy to enable the manufacturing of materials and devices at
 commercial scale must be the consideration of circular economy thinking and more
 specifically recycling of materials embedded in devices at the end of life.

- 98 The main outputs from the consultation were organised into research and technology
 99 enablers, development and scale-up and materials for the energy transition.
- 100 The **Materials** identified for the energy transition are:
- Materials for Power Electronics underpinning local energy generation, distribution, and consumer use. This topic focuses on exploiting emergent SiC and GaN technologies; developing next-generation materials (e.g. 3C-SiC, Al(Ga)N, and Ga₂O₃); and, addressing recycling, the scarcity of source materials, and, the whole-life energy costs of manufacture in the electronics sector. Materials include 4H-SiC, 3C-SiC, GaN, Al(Ga)N, Ga₂O₃, BN and B(Al)N, and diamond. Key challenges include fabrication methods and device design and optimisation.
- 108 > Materials for CMOS – advancing society's digital connectivity and mobility, and 109 supporting the remote operation of ever more complex devices for monitoring of the environment, health and security. This topic focuses on integrating new materials 110 111 into CMOS devices to demonstrate new concepts (e.g. 'tunnel', 'negative 112 capacitance'), thereby reducing the operating voltage and energy consumption of 113 CMOS. It also considers integration of different materials to enhance significantly 114 device functionality (e.g. delivering compact, low-power, radio-frequency (rf) 115 sources and the incorporation of tuneable materials such as piezoelectrics, 116 antiferromagnetics, plasmonics and photonics, whilst maintaining CMOS 117 compatibility).
- 118

119 Materials for 'More than Moore' to achieve high computational power with lower 120 energy consumption using new computing architectures, accelerating performance 121 and energy efficiency of computing for the future. This topic addresses the 122 development of new paradigms for computing and information processing. It goes 123 beyond traditional CMOS 'von Neumann' computing (e.g. through developing 124 neuromorphic computing architectures), and is underpinned by new materials, (e.g. 125 spintronic, topological and organic materials), and new device concepts (e.g. 126 chargeless computation and collective switching). Exemplars include (a) nano-127 oscillatory neural networks; (b) in-memory computing using memristive materials 128 such as redox, phase change, and spin transfer torgue materials; ionic synaptic 129 transistors; and, metal-oxide bilayers; (c) edge computing; (d) probabilistic 130 computing; (e) all optical, optoelectronic or magneto-optic computing; (f) quantum 131 computing, with low temperature compatible memory; (g) non-volatile logic 132 operations and (h) chargeless computation utilising spin, the electrical dipole or 133 orbital states in materials such as ferroelectrics, magnetic materials, light metals, 134 semiconductors, 2D materials, organic and molecular materials, topological 135 insulators, quantum wells, molecules and crystals. The key challenges are the 136 identification of the right materials system for the specific targeted computing 137 architecture, and the optimisation of the active materials, and conversion of 138 input/output signals, such as charge current/light to spin current, and vice versa.

139 Reduction of electronic power consumption and elimination of losses which cause the 140 generation of parasitic heat are key for reducing energy demands of digital processes, and 141 can be achieved through developing advanced functional materials and novel 142 methodologies. In scope are the materials developments that reduce heat generation and 143 improve performance of dielectrics, and the design of new frameworks of operation which 144 use spintronics, photonics, metamaterials, negative capacitance, 2D materials, topological 145 insulators, superconducting electronics and neuromorphic computing. Themes not in scope are strategies involving quantum computing, communications networks, displays and 146 147 screen technologies.

The table below summarises the current and anticipated future status of the differentmaterials based on information available in the public domain.

150

Category	Page in report	Material	2020- 2030	2030- 2040	2040- 2050+
	14	4H-SiC			
Wide band gap materials	14	3C-SiC			
materialo	15	GaN			
	16	Diamond			
Ultra-wide band	15	Gallium Oxide (Ga ₂ O ₃)			
gap materiale	16	Aluminium Nitride			
Other novel materials	16	BN and B(AI)N			

	Category	Page in	Materials	2020- 2030	2030- 2040	2040- 2050
		report	Heterogeneous material integration with CMOS			
	Enhancing current	21	e.g. Piezoelectrics, ferroelectrics, 2D Materials, III-V semiconductors			
	functionality to increase productivity	22	Materials for integration with Microelectromechanical systems (MEMS)			
tion	productivity	22	Monolithic integration of different device functionalities e.g. Si photonics ⁶			
Integra	Integration of new materials into CMOS to	23	New Tunnel FET concept development and integration with CMOS e.g. 2D materials, SOI, Ge, SiO ₂ , Ta ₂ O ₅ , Si-Ta ₂ O ₅			
MOS	reduce energy consumption	23	Materials for CMOS and negative capacitance e.g. ferroeletrics doped HfO ₂ , SiN			
Ö	Interconnecto	25	Cu			
	Interconnects	25	Silicides, carbon based materials			
	Substrate development	25/26	Low-loss dielectric substrates SiC, GaN, BN			
	for heat dissipation	25/26	Low-loss dielectric substrates Al ₂ O ₃ , MgO, diamond, SiC, high-resistivity Si			
	CMOS Based	28	Loihi, True North			
ohic		30	Joule heating oscillators (PrMnO ₃)			
uting	Nano-oscillator Networks	30	Magnetic based oscillators			
ompi		30	Volatile filamentation (Ta Q_2)			
20						
Probabilistic	Magnetic	31	Unstable magnetic tunnel junctions			
Edge		31	Semiconductor sensors, smart sensors, light			
computing	Sensors		sensors Antiferromagnetic materials as THz source and			
		43	sensor (CuMnAs, Mn ₂ Au, MnN, NiO, Mn(II)Au, CoO, RuO ₂)			
b	Optic	33	Si photonics			
utin	opilo	33	Photonic logic gates			
dmo	Optoelectronic		(Ge ₂ Sb ₂ Te+InP+Plasmonic nanostructure)			
с Б		33	Nanocavities (InGaAs, InGaAsP)			
Hybrid	Magneto-optic	42	GdFeCo, [Co/Pt]/Cu/GdFeCo, YIG:Co,Pt/Co/Gd, Mn ₂ Au)			
		36	Transition metal oxides – Resistive materials (Ta ₂ O ₅ , HfO ₂ , TiO ₂)			
		36	Phase change chalcogenides			
Iting		38	Magnetic tunnel junctions (e.g., W/CoFeB/MgO/CoFeB/W/Co/Ru/Co/Pt/Co/Pt] ₆)			
Compu	In memory computing	36	Ferroelectric (HfO (doped and undoped), HfO ₂ - ZrO ₂ , PbZr _x Ti _{1-x} O _x , (1-x)[Pb(Mg _{1/3} Nb _{2/3})O ₃] - x[PbTiO ₃], SrBi ₂ TaO ₃ , BiFeO ₃)			
neter	-	37	Piezoresistive (SMS, Heusler compounds, chalcogenides, oxides)			
aran		43	Antiferromagnetic (CuMnAs, MnN, NiO, Mn(II)Au, CoO, RuO ₂)			
der F		40	Heavy metals (Pt, W, Ta, Ir) (used in memory computing)			
ò	Spin Current Generation	40	Topological oxides (Bi ₂ O ₃ , SrIrO ₃ , SrTiO ₃ , LaAlO ₃)			
		40	Topological materials and superlattices (Bi _{1.5} Sb _{0.5} Te _{1.7} Se _{1.3} , Cr _x Bi ₂ Se ₃ , Bi ₂ Se ₃ , α-Sn)			

⁶ "Roadmap on silicon photonics" D. Thomson et al Journal of Optics, 18, 7 (2016)

	Category		Page		2020-	2030-	2040-
			in	Materials	2030	2040	2050
	Spin Curre Generation	ent n	40	2D transition metal dichalcogenides (MoS ₂ , MX ₂)			
		-	42	Optically generated spin current (Bi2Te3 on GaAs)			
	Magnetic manipulat	ion	40	Multiferroics (BiFeO ₃ , LaBiFeO ₃ , TbMnO ₃ , LuFeO ₃ /LuFe ₂ O ₄)			
	using		40	Magnetostrictive (Fe3Ga, Tb _x Dy _{1-x} Fe ₂ , FeRh)			
	magnetoe	lectric	41	Exchange Bias (Cr ₂ O ₃ , Fe ₂ TeO ₆)			
5 L	ס		41	Co, Fe, Ni, CoFe, NiFe, CoFeB (In production in connection with STT RAM and magnetic information storage, permanent magnets, etc)			
ntin			41	Heusler alloys (X ₂ YZ, XYZ: Co ₂ FeAl, Mn ₃ Ga)			
d moo		-	43	Antiferromagnetic materials (CuMnAs, Mn ₂ Au, MnN, NiO, Mn(II)Au, CoO, RuO ₂)			
eter (ete Magnetic	-	45	Nanocarbon and molecular thin films on ultra- thin metal thin films or 2D materials			
Materials	-	45	Molecular thin film magnets (Phthalocyanines α-CoPc, carbon based molecules)				
Č,	с С		44	2D van der Waals materials			
Orde ack	ack Jic	41	Synthetic antiferromagnetically coupled materials (TaN/Pt/Co/Ni/Co/Ru/Co/Ni/Co/TaN)				
	Icetra	acetra Id log	41	Ferrimagnetic materials (AIO/TaN/Pt/Co/Gd/TaN)			
		ar	41	Magnetic logic (Pt/Co/AIO)			
			42	Metals (Cu)			
			42	Metals (Ag, Co, Al)			
	Interconnect and interlayer materials	ect ayer	42	Metal semiconductor (Ru poly-Si, NiSi, CoSi, NiGe, TiSi)			
			42	Interlayer dielectrics (SiO ₂ , SiN, SiCOH, polymers)			
			42	Superconducting materials			
Kev	Research a	ctivity		Industrial prototype	at industria	l scale	

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- 153 **The main 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, High-frequency Devices*, and *High-throughput Testing*, each underpinned by world-class scientists and engineers, with dedicated specialist technical staffing
- Development of techniques to effectively and efficiently embed new materials into
 high performance, energy efficient devices, including interfacing with the external
 environment.
- 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 accessible materials databases, and simulation and modelling development across the length scales from atoms to devices.

- 169 Investment to support the development of new computing architectures, and next
 170 generation wide-bandgap semiconductors for power electronics.
- Funding approaches to support UK-wide collaborations between academia and
 Industry.
- 173 Investments and incentives for industry to undertake research, and lead and develop
 174 exploitation strategies.
- 175 Influencing policy, including setting power consumption targets, supporting the
 176 circular economy through end of life considerations, and removing reliance on scarce
 177 materials
- 178 It was recognised that any material and technology development in this area needs a
 179 sustainable and stable resource supply as well as end of life recycling options to enable
 180 the sustainable, long-term use of these technologies.
- 181

182 For **research and technology enablers**, the 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.
- 194 > Recyclability and recovery of materials, including identifying incentives, targets and
 195 life-cycle analysis when selecting materials and processing routes, and considering
 196 availability of scarce materials and the whole-life energy cost of manufacture and
 197 use.
- Partnerships to stimulate the exchange of ideas between academia, industry and research institutions (both within the UK and outside). This should include provision of incentives for industry to co-develop fundamental research programmes from the outset, and embedding of Universities into a lab-to-product research and development culture
- 203
- 204 For **development and scale-up**, the 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, large-scale integration of III-V semiconductors with silicon, and scale-up of wide bandgap semiconductors and silicon photonics to wafer fab.

- Development of the 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 scaleup, 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 4th 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.

226 MATERIALS FOR POWER ELECTRONICS

227

228 BACKGROUND

229 Power electronics is the key technology to control and convert the flow of electrical energy 230 from the source to load-side consumption. Applications include consumer products, 231 electricity generation from wind and solar energy and electrical vehicles. Currently, the 232 energy losses from power electronics are high and savings of more than 50% could be achieved Error! Bookmark not defined. with the development and use of low-loss power s 233 234 emiconductor devices⁷. For example, advanced power electronics could reduce the electrical energy consumed by motor drives by 20-30% in the developed world Error! Bookmark n 235 ot defined. Advanced materials for power electronics can contribute towards these targets. 236

- The current, most widely used material in power electronics is silicon. Advanced fabrication processes and sophisticated electronic device designs have optimized the silicon electronic device performance almost to their theoretical limit ⁸. To further improve the performance of power electronic devices new materials need to be developed that can operate at higher voltages, faster switching speed, and at higher temperature. Not only will this lead to more efficient power conversion solutions, but these will also be lighter and smaller, with less
- 243 cooling requirements.
- 244

245 THE STATE-OF-THE-ART AND CURRENT CHALLENGES⁷

The current, most widely-used material in power electronics is silicon (Si). Si-based power electronic devices have some critical limitations, such as:

- High losses due to the low critical electric field (25 V/µm) of Si that leads to unipolar devices (MOSFETs, Schottky diodes) with high resistance and therefore high conduction losses.
- Low Switching Frequency due to the need for bipolar devices (IGBTs, thyristors) in order to keep conduction losses low.

253 Material research activities⁹ have been focusing on improved switches, for example having 254 higher blocking voltage, on-state current density, and switching frequency. Many 255 developments are also taken place on the device level with integration of logic and power 256 circuits in a single chip, reliability improvements, thermal management and packaging.

257

258 MATERIAL DEVELOPMENTS

The crucial materials' property for high performing power electronics devices is a high critical electric field. Materials with a critical electric field higher than Si enable power electronic devices to withstand higher voltages for a given drift region width. Alternatively, they can be exploited to produce much more efficient devices at a given voltage, with reduced losses and faster switching, the result of the drift region having been scaled down. Other important

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⁷ ARPA-E_Power_Electronics_Paper-April2018.pdf

⁸ DOI: 10.1002/zaac.201700270

⁹ 'Power semiconductors – state of the art and future trends', Vitezslav Benda, Czech Technical University in Prague, Transaction on Machine, Power electronics and Drives ISSN: 2229-8711 Online Publication, June 2011

factors include a wide bandgap which enables high temperature operation, and a high thermal conductivity which improves the dissipation of heat, reducing operational temperatures. This improvement in the thermal management reduces external heat sink requirements and lowers cost. A high charge carrier saturation velocity also helps increase switching frequencies.

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New material developments in this domain have been focussed on developing and testing wide band gap (WBG) semiconductors, SiC and GaN, and ultra-wide band gap (UWGB) semiconductors, diamond, Gallium Oxide and Aluminium Nitride (as well as more novel materials such as Boron Nitride (BN). Developments on silicon¹⁰ are taking place at the device level, in the form of integration of logic and power circuits on a single chip and in form of improvements on the reliability and thermal management and packaging.

276

277 Wide band gap materials

SiC and GaN address the performance shortcomings of Si, however, their non-negligible
 defect densities and high synthesis costs are limiting factors for large scale applications¹¹.

281 SiC is, of all "beyond Si" contenders, the most technologically mature materials system. 4H-282 SiC unipolar devices (MOSFETs, Schottky diodes) of high quality and increasing maturity 283 and reliability, are available from a number of international suppliers in the voltage range of 284 600 to 3300 V. Drivers of device development are the electric vehicle and solar inverter 285 markets. However, a number of materials issues are preventing the production of devices 286 at other voltages. Bipolar devices, potentially rated up to 30 kV per device, are not currently 287 possible due to the number of defects in the substrate, and in the epitaxy, which reduces 288 the carrier lifetime. Furthermore, all substrates are highly n-type doped, the absence of p-289 type substrates, making it a significant processing challenge to make n-channel IGBTs. 290 Finally, high voltage devices require thick epitaxially grown drift regions, which is currently 291 prohibitively expensive due to slow growth rates and hence throughput. The UK is taking the lead in resolving many of these issues¹², addressing improvements in epitaxial growth 292 293 processes and device design and development.

294

295 A large number of different stacking sequences of the Si-C double layer exist resulting in 296 various stable crystal polytypes which exhibit differences in their electronic properties. 297 including their band gap and charge carrier mobility. 4H-SiC is the polytype that is in 298 production, as detailed above. 3C-SiC, which must be grown upon another substrate such 299 as silicon, is attractive due to its potential compatibility with existing silicon lines. However, 300 its material quality is currently poor, the number of defects very high due to its growth on a 301 different substrate. With capability in the UK to grow both polytypes, and to fabricate high 302 voltage devices, a significant opportunity exists to strengthen its position in this growing 303 market.

304

¹¹ Energy Environ Sci (2019), 12, 3338

¹⁰ https://www.sciencedirect.com/topics/materials-science/high-power-electronics

305 **GaN devices** are being manufactured internationally however, the technology maturity is 306 slightly behind SiC¹⁵. GaN possesses excellent characteristics when compared with silicon 307 with a high breakdown capability, high blocking voltage using thinner devices, higher 308 electron mobility than silicon and silicon carbide, and higher critical field resulting in a thinner 309 more highly doped drift layer and thus lower on-resistances. In combination this results in 310 reduced system size and weight and an increased efficiency. It has a higher bandgap than 311 silicon (3x) and SiC (1.1x) and a critical electric field strength 11 times larger than Si. 312 Ongoing materials development towards achieving the theoretical limit of the materials is 313 ongoing as well as improving doping capabilities. In particular, dopant control (principally p-314 type) for GaN requires more development. This is an important area of research to enable 315 the development of high performance vertical devices with effective termination structures¹³, a type of device structure which is important for reducing switching losses and therefore 316 317 essential for more energy efficient performance as they can support higher current densities 318 within a smaller footprint. The current focus of materials development is on controlling the 319 number of defects in GaN which is limiting the size of size at which wafers can be grown. 320 Issues with bowing and thermal effects on large GaN on Si wafers limits the effective wafer 321 size, an aspect needing further development. Furthermore, development is directed towards 322 optimising the UK capability in regrowth of GaN on GaN substrates to enable very thick 323 (~100 µm) active layers in devices. Overall, the GaN material now needs to bridge the gap 324 from a laboratory-based material and device development towards volume production within 325 the UK. 326

Implementation **Required Activities** Scale-up of GaN materials for device applications ST Scale-up of 4H-SiC materials for high voltage device applications ST Development of efficient thermal management, including heterogeneous ST integration Dopant control (principally p-type) for 3C-SiC, and GaN ST - MT Solve issues with Issues with bowing and thermal effects on large GaN on Si ST - MT wafers Materials for device application beyond Si (2-300V), 300-900V GaN, >SiC for MT Automotive applications * ST = short term (now-2030), MT = medium-term (2030-2040), LT = long-term (2040-2050)

327

328 Ultra-wide band gap materials

Ga₂O₃ offers the potential for high voltage operation and low cost wafer production^{14,1516}. Gate-to-drain electric field strength of >3.8 MV/cm have been shown in beta-Ga₂O₃ metal oxide semiconductor field effect transistors, a value which exceeds theoretical limits for GaN and SiC, while still affording scope for improvements¹⁷. Currently, Ga₂O₃ devices have an issue with heat dissipation that can be addressed by using diamond as a heat sink. Development of efficient thermal management methods which can be integrated into the growth process are critical for device development. Further research into p- and n-type

¹³ https://www.nature.com/articles/s41598-019-45177-0

¹⁴ http://ww2.che.ufl.edu/ren/paper/2017%20p23.pdf

¹⁵ Z. Hu IEEE Electron Device Letters 39, 6 (2018) ¹⁶ S. P. Bassa, January 2 2022 (2012)

¹⁶ S. B. Reese, Joule 3 899 (2019)

¹⁷ A.J. Green, IEEE Electron Device Letters 37, 7 (2016)

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Roadmapping workshop for Henry Royce Institute for materials for Low Loss electronics

doping capabilities is needed. Currently p-type doping in Ga₂O₃ is quite problematic as
doped materials tend to display low mobility. Furthermore, limits exist in the capability of
high background n-type doping as Ga₂O₃ needs a high concentration of acceptor dopants.
Modelling and simulation is an important aspect of research for both improving the Ga₂O₃
material performance as well as enabling device design development. Solutions that link in
with device processing and packaging methods are needed also.

342

For **diamond**, doping remains a key research area. A breakthrough in doping is fundamental for diamond to fulfil its ultrahigh bandgap potential. Future research activities need to demonstrate relevant diamond transistor architectures. However, developing the materials growth capabilities of diamond is also of interest for other power electronics devices due to its thermal properties and thus its potential to act as a heat sink.

348

354

The development **AIN** and **AIGaN** materials for power electronic devices is still in the early stages. Applications are envisaged in the medium-term (2025-2035) potentially for 12kV and high frequency operation. The research challenges are focused on high quality growth of these materials and specialist facilities are needed for growing these high mole fraction materials. Issues with regards to how to achieve the required doping need to be addressed.

355 Other materials

Further research is required for **BN** and **B(AI)N**, and the applications could be realised in the long-term (2035+). It is not clear presently if the performance of these materials would superior to the other UWBG ones discussed in this and previous sections. However, large scale computational screening has identified nine oxides, four nitrides and three carbides as possible not yet developed materials to outperform Ga₂O₃. A screening of 863 materials, taking into account heat dissipation as a performance factor¹⁸. has shown that there is scope for fundamental research for power electronics research of the future.

363

Required Activities	Implementation timescale *
Development of BN and other promising candidates for future device applications	LT
* ST = short term (now-2030), MT = medium-term (2030-2040), LT = long-term (2040-2050)	

364

365 Device developments

For all power electronic devices research is required on the materials used for device processing, e.g. dielectrics, contacts, ultra-conformal high-K dielectrics, soft magnetic materials for power inductors and transformers, die-attach, interconnect, encapsulation materials for power packaging, thermal interface materials for cooling, and feedstock materials for additive manufacturing for heterogeneous integration¹⁹. This is essential in order to develop reliable devices. There is a high innovation potential in research on novel insulators.

373

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¹⁸ P. Gorai Energy and Environmental Science 12, 3338 (2019)

¹⁹ https://www.mdpi.com/journal/materials/special_issues/materials_power_electronics

Required Activities	Implementation timescale *
Ability to control rapidly changing magnetic fields	ST - MT
Passive components development like high-frequency inductors	МТ
Smart power IC, where the logic device sits alongside the power substrate).	MT
Systems to deliver integrated working devices	MT
* ST = short term (now-2030), MT = medium-term (2030-2040), LT = long-term (2040-2050)	

374

UK CAPABILITY 375

The EPSRC Centre for Power Electronics²⁰ has strongly supported the development of SiC 376 377 material, devices and applications in the UK, unifying research efforts from across academia 378 and industry. Work within this Centre has helped to pioneer a range of high voltage SiC power devices, including the epitaxy and the device development. Within the UK, epitaxial 379 growth of SiC is available from the University of Warwick²¹ and Clas-SiC²² in Scotland, with 380 volume production taking place at the IQE plant in Newport²³. SiC device development 381 382 capability exists at the Universities of Warwick and Newcastle, and in Clas-SiC, while device 383 design expertise exists in the Universities of Cambridge and Nottingham. Ion implantation 384 capabilities are available at the University of Surrey²⁴. There are no suppliers of SiC 385 substrates in the UK.

386

387 The UK has a strong footing in GaN growth capacity within academia (for example at the Universities of Sheffield²⁵, Cambridge²⁵ and Nottingham²⁶). Foundry capability exists at IQE 388 389 and with some III-V on Si capability at Newport Wafer Fab for up to 200 mm wafers. 390 Swansea hosts Ga₂O₃ MOCVD growth facilities which is an excellent first step in developing 391 a UK capability. No dedicated reactors are available, however, within the UK for novel 392 materials beyond Ga₂O₃ and hence materials produced tend to suffer from inferior quality. 393 This has resulted in outsourcing of AIN and AIGaN wafer growth. In general, a review of 394 epitaxy facilities within the UK is needed. Capabilities need to be updated to keep up with 395 international competition if the UK wants to stay relevant in the power electronics sector. 396

397 Whilst the UK is very strong in compound semiconductor technologies and bringing these 398 through TRLs 1-3, the transition into the higher value TRLs for the applications markets is 399 behind this. It is vital that the infrastructure is put in place to avoid a cyclic opportunity cost 400 on UK technologies being developed and then exploited overseas. Indeed, substantial 401 investments are being made in Europe, America and Asia in order to attain dominance in 402 the development of next generation low loss electronics markets, and it is imperative that 403 the UK is in a position to compete internationally.

- 404
- 405

- 22 https://www.clas-sic.com
- 23 https://www.iqep.com/about-iqe/

- ²⁶ Molecular Beam Epitaxy (MBE)

²⁰http://www.powerelectronics.ac.uk/

²¹ https://warwick.ac.uk/fac/sci/eng/research/grouplist/electricalpower/peater/sicepitaxy

²⁴https://www.ion-beam-services.com/ ²⁵ Metalorganic Chemical Vapour Deposition (MOCVD)

406 UK COMMUNITY RECOMMENDATIONS

407 There is an enormous market opportunity for SiC devices, especially for automotive 408 applications, but in order for the UK to compete internationally, investments are needed. 409 The community recommends investments into new and existing SiC facilities in industry and 410 academia. A further two epitaxial growth facilities (up to 6" wafer size) in academic 411 institutions would help tackle the fundamental issues that remain in the growth of the 412 material. Further investments into existing and new SiC fabrication facilities, with >6" 413 wafer size capability would enable translation of research into the commercial space. This 414 will allow the UK research and industrial communities to continue to compete internationally 415 and take a lead in this rapidly expanding field. In particular, SiC fabrication capabilities need 416 specialist equipment, such as high-temperature furnaces for annealing and oxidation, 417 and PECVD systems, along with the capability any Si fabrication facility will require. More 418 **GaN** regrowth capability is needed within the UK, including 'fast' epitaxy to enable the 419 formation of ultrawide (~100 µm) layers. There is also a need for an expansion and 420 enhancement of fabrication capabilities expansions, such as access to state-of-the-art gate recess capability (digital etch). In addition to growth and fabrication facilities this needs 421 422 to be accompanied by state of the art standards and reliability testing facilities.

423

424 For developing both **SiC** and **GaN** devices not only significant capital investments required, 425 but also continuous and consistent funding for fabrication-related projects, and to develop 426 the UK's skills and to establish a highly trained workforce. It is important that the UK can 427 demonstrate a sovereign capability in this strategically-important area, as well as continuing 428 to undertake international co-development, especially with European partners post-Brexit. 429 Enhanced doping capabilities are needed, especially p-type doping, on the national level 430 such as pulsed epitaxy for dopant control. Co-location of epitaxial growth and fabrication 431 centres is essential for ensuring that material and device developments progress to higher 432 TRL levels (e.g. prototyping and manufacture). For early TRL developments, a virtual centre 433 would enhance the UK effort. A dedicated facility supported by characterisation experts for 434 a wide range of characterisation methods such as DLTS, Hall, CV, fast-transient analysis is 435 needed to enable material parameter (mobilities, phonon modes, lifetime etc.) extraction 436 and thus support new device design. There are significant limitations in translation of 437 academic knowhow into an industrial setting with limited access to testing facilities. A UK 438 pilot line facility is needed to enable new materials developments to be tested in an industrial 439 manufacturing setting without contaminating existing fabrication lines. These investments 440 are essential to provide rapid, efficient access of the whole UK community to state of the art 441 tools and to allow the UK to compete internationally.

442

Future development is needed of **Ga₂O₃**, together with expanding capabilities for halide vapor phase epitaxy (HVPE), and low-cost polycrystalline materials growth. Demonstration of working Ga₂O₃ devices is needed by 2025 in order to remain competitive with the international developments in this rapidly-growing field. There is also a need for fundamental discovery-led research into future wide band gap materials for power electronics and high temperature operation, taking into consideration the abundance of source materials, the need for recycling, and the importance of sustainability over the full materials life cycle.

451 MATERIALS FOR CMOS

452

453 BACKGROUND

454 Complementary metal–oxide–semiconductor (CMOS), is a well-established semiconductor 455 fabrication process that is used for constructing both digital integrated circuits e.g. 456 microprocessors, memory chips and analogue ones such as RF circuits and sensors. CMOS 457 and related technologies are vital for designing high performance, low power devices^{27,28}. 458

459 The semiconductor manufacturing industry particularly those related to small scale 460 electronics are scaling down devices continuously. Due to the dramatic reduction in device 461 size, numerous challenges are surfacing related to energy consumption, heating, connectivity and integration of new materials. To overcome these challenges disruptive 462 463 innovation in materials and devices is required, in two broad areas (a) increasing the device 464 functionality or productivity without increasing the power consumption and (b) reducing the 465 energy consumption in the next three decades. Substrate development is also essential for 466 heat dissipation.

467

However, there are many issues into integrating novel materials with CMOS processing,
such as differing processing temperatures, achieving stable interconnections between the
different materials or avoiding contamination.

471

472 THE STATE-OF-THE-ART AND CURRENT CHALLENGES

473 CMOS for high-performance electronics is right at the theoretical limit. Most industrial drive 474 is focused in reducing transistor size to improve performance per square inch. Challenges 475 need to be addressed in order to reduce the power consumption by 90%, by 2050, and 476 minimise the cooling requirements while retaining comparable length scales without 477 compromise to performance i.e. speed.

478

Enhancing the current device functionality: Due to the high barrier to enter the market, new low power technology ideally possess the following features: (i) they are "drop-in" replacement for CMOS FETs; (ii) they are compatible with CMOS processes; and (iii) they significantly improve performance, reduce cost, or add novel functionality beyond the current capability of CMOS. In order for an 'enhanced CMOS technology' to be adopted, there is an absolute requirement that the replacement significantly outperforms its existing CMOS alternative.

486

487 Despite the scaling and energy challenges of CMOS and the quest for "beyond CMOS" 488 technologies, the industry continues to innovate and invest in CMOS based devices. This is 489 highlighted by planned multi-billion dollar investment in silicon fabrication facilities in 2020 490 and beyond. Thus, there is significant barrier for adoption of any new technology. Ideally,

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 ²⁷ Omura, Y., Martino, J.A., Raskin, J.P., Selberherr, S., Ishii, H., Gamiz, F. and Nguyen, B.Y., 2015. Advanced CMOS-compatible Semiconductor Devices 17. The Electrochemical Society.
 ²⁸ https://ieeexplore.ieee.org/stamp/stamp.jsp?tp=&arnumber=4098005

- 491 any new technology must be CMOS compatible and offer new functionalities that enhance 492 the current CMOS capabilities.
- 493

495

494 Materials challenges for CMOS integration include the following:

- 496 1. Interface engineering to optimise metal/semiconductor junctions and reduce contact 497 resistances.
- 498 2. Interconnects need to be optimised There is an urgent need to develop low dielectric 499 constant (k < 2) materials. High k dielectrics are not available for most new 500 semiconductors which is an issue not only at the device level but also at the system 501 level. The absence of low k materials leads to large resistance-capacitance power 502 dissipation. This is where a lot of thermal impedances and thermal mismatch occurs due 503 the difference in the thermal coefficient of expansion of materials. This is a problem 504 which spans from the micro-level through to the system level.
- 505 3. Ability to downscale to the nano-scale.
- 506 4. Ability to move from 2D to 3D.
- 507 5. Etching and processability of different materials and their compatibility with CMOS 508 processing.
- 509 6. Operating temperature range between different materials.
- 510

511 With regards to the reduction in energy consumption per switching for low-voltage 512 devices, the signal-to-noise ratio is a key limitation. Reduction of the device operating 513 voltage requires improvements in signal-to-noise ratio to allow efficient power utilisation and 514 optimisation. A reduction of parasitic losses such as heat generation via Joule heating, 515 through negative capacitance for example, is necessary.

516

MATERIALS FOR ENHANCING CURRENT FUNCTIONALITY 517

The limitation of traditional CMOS technology is the struggle to improve performance, 518 519 reduce power consumption and increase bit density while maintaining or reducing wafer 520 cost. To go beyond traditional CMOS we need to add functionality to CMOS while in parallel 521 reduce the energy consumption. For the future, the focus is on high mobility, low leakage 522 materials to improve performance without increasing power consumption. A summary of the 523 performance of different materials beyond Si in terms of carrier mobility and energy bandgaps can be found in reference ²⁹. Furthermore, key advances can be made by adding 524 525 materials which can be actively tuned to enhance functionality for example by adding 526 ferroelectrics, plasmonic or magnetic materials. Growth of heterogeneous materials on 527 large-area silicon platforms (8"-12") to enable large scale manufacturing is a challenge.

- 528 529
- 530

²⁹ High mobility materials for CMOS applications, Chapter 2: Opportunities and challenges of multiscale heterogenous material integration on Si platforms for enhanced functionality and performance, Aaron V.-Y Tean, NUS, Singapore. ISBN 978-0-08-102062-3 IfM Education and Consultancy Services

531 Heterogeneous Material integration with CMOS

532 Heterogenous material integration with CMOS has taken place for over a decade for 533 example by using silicon-germanium (SiGe).

534 535

Silicon Carbide (SiC) integrated with CMOS has been demonstrated already in both digital and analogue circuits extending the operating temperature up to 500 °C³⁰ which is not possible with Si alone. SiC is also of interest for CMOS integrated RF applications. The SiC growth capabilities are discussed in the power electronics section of this report.

540 541

550

542 Piezoelectric materials can be integrated into transistor gate stacks to improve MOSFET 543 behaviour as well as add sensing capabilities. Using nitrogen-polar AIN as part of the gate 544 stack allows for example the detection of different magnitudes of force applied to the device. 545 This opens the doors to applications ranging from varying sensor systems, niche RF 546 applications, actuation and to energy harvesting³¹. Dielectric materials which enable this 547 technology are Si₃N₄, AIN, ZrO₂, HfO₂ or HfSiO₄. While large area and large volume growth 548 and fabrication capability is available these are not suitable to trial and develop niche 549 applications, where intermediate-scale facilities are needed.

551 The development of **2D** and **thin film** materials compatibility with Si is an active research 552 activity. Graphene has promise in terms of performance however interfacing graphene with other materials such as electrodes is a challenge. High quality CVD grown graphene can be 553 554 used as a plasmonic material adding further functionality. Proof of concept for its use for 555 optical switching/signal processing has been demonstrated and could be manufactured within the next 5 years. The main challenges lie in dry transfer or low temperature deposition 556 557 methods on top of CMOS without contamination. Graphene can be grown in-situ on Si and 558 alternative substrates (SiC, BN saphire and GaN) without the need of dry transfer has been 559 demonstrated by the companies such as EMBERION and PARAGRAF. Early proof-of-560 principle on a single device scale are in the public domain for graphene and ferroelectrics 561 however, a proof of scalability is still outstanding.

GaN is an important material for future RF microwave devices for high frequency communication. Of particular interest here is the integration of efficient RF communication with CMOS on the same chip. In particular, in the area of **5G operation and beyond**. The 5G materials demands are substantial and the UK research in materials for 3G and 4G has been central to defining new modalities – this must continue with 5G. The challenge is achieving sub-100 mV switching at 50 GHz operation enabling agile antennas (beyond 5G). In the longer term 6G (>50 GHz) development will push all technologies and materials.

570 571

562

572

³¹ H. Winterfeld et al. Journal of Material Science: Materials in Electronics 30 11493 (2019)

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³⁰ https://iopscience.iop.org/article/10.1088/1361-6641/aa59a7/pdf

- 573 Integration with microelectromechanical systems
- 574 [No Information from the workshop further information is needed, please.]

575 Monolithic integration of different device functionalities

576 Silicon waveguides on thick layers of silica, integrated onto silicon are important for a range

577 of applications. This includes silicon photonics, inertial sensing and quantum technologies.

578 Research activity focused on interfaces is required. Interfaces need to demonstrate low loss

579 dielectric properties. Multiple research and development capabilities are required spanning

580 physics, modelling, structure-functionality relationships and final device performance

581 prediction.

582

Required Activities	Implementation timescale *
Fast materials evaluation and testing capability including in operando testing and device testing on the die. Testing needs to fit with existing processes, and needs to be coupled with site-specific off-line quality assurance, as well as on-line monitoring.	ST
Model performance of RF switch.	ST
Big data intelligence, 4 th Industrial Revolution strategy for manufacturing to accelerate product development.	ST
Scoping of scenarios for developing power consumptions for policy. RE, PR, scalability is known, DE loss, RF switch.	ST
Modelling (including ab Initio modelling) of the system is needed that includes structure-functionality relationships and final device performance prediction capacity by intelligent behavioural design.	ST-MT
Understand the device scaling behaviour more generally	ST - MT
Fundamental physics research on fermi levels, bandgaps, etc. is needed	ST - LT
Understand the effect of defects on material and device performance	ST - LT
Research on interfaces that need to show low loss dielectric properties. Multiple research and development capabilities required (physics, modelling, structure-functionality relationships and final device performance prediction.)	ST - LT
Research and development of new 2D materials to perform different functions beyond plasmonics	MT - LT
Development of high quality, new piezoresistive composites materials. Using the state-of-the-art, they are only just good enough versus other systems.	MT - LT
Optimisation of metallic conductors and development of new oxide conductors	MT - LT
Pilot capability for niche applications and demonstration of scale-up, e.g. piezoelectrics on silicon and silicon waveguides. This needs to be accompanied with suitable certification to match industry requirements (which is normally available in Universities)	ST - LT
Improvement of 12" high quality Piezoceramic materials growth for RF switch applications and development of UK manufacturing capability	ST-MT
Improvement to yield and performance of piezoelectric devices	ST-MT
"Tools" (MBE, PLD, CVD) development for new materials systems for quality, uniformity, functionality. Tool manufacturers are keen to do this but are not UK based. This will also have to address the adaptation of the in Laboratory-to- Fab toolsets	MT - LT
Make up-to-date equipment for monolithic integration to be available to academic researchers, such as pick-and-place, wafer-, and on-chip bonding (to demonstrate integration capabilities).	MT - LT
End-users need to be brought in	MT - LT
* ST = short term (now-2030), MT = medium-term (2030-2040), LT = long-term (2040-2050)	

583 INTEGRATION OF NEW MATERIALS INTO CMOS TO REDUCE584 ENERGY CONSUMPTION

585 Power consumption in CMOS is typically due to charging and discharging of capacitors 586 (dynamic power consumption), short circuit paths and leakages from diodes and transistors. 587 As devices scale down, static power dissipation when devices are on stand-by mode also 588 become significant. The challenge is developing and implementing technologies which 589 reduces the power consumption of current technology by at least a factor of 100 while 590 retaining comparable length scales and performance.

591

592 To reduce power consumption of CMOS devices per switching requires optimisation at all 593 levels i.e. the technology used to implement the digital circuits, as well as the circuit design 594 and architecture³². The primary strategy for reducing power consumption is reducing and 595 controlling the threshold voltage. For this the signal-to-noise ratio is a key limitation.

596

597 There are four possible ways: (i) energy filtering in tunnel FETs, (ii) inter voltage amplification 598 using negative capacitance gates, (iii) metal insulator transitions using phase change 599 materials (i.e. colocation of memory and computing which is covered in more detail in the 600 beyond CMOS materials section of this document), and (iv) internal transduction such as 601 spin FETs.

602

603 Tunnel field-effect transistor development and integration with CMOS

604 Tunnel field-effect transistors (TFETs) enable the device to be switched off more effectively 605 that a more conventional transistor. For example, TFET logic consumes only 54% of total CMOS power³³. A number of TFET designs depend on heterojunctions of different materials 606 such as GaSb/InAs^{34,35}. Interfaces play a critical role in device optimisation for power 607 efficiency as a poorly controlled interface tends to induce leakage currents through high 608 level of traps and defects³⁶. Development of homo-junctions where only one junction 609 material is used and optimisation of the doping levels could help solve this issue. TFETs 610 611 also face scale-down challenges. The need to fabricate very thin body dimensions to 612 achieve good electrostatics and the requirement for high guality III-V materials and their oxides to remove the effects of trap-assisted tunnelling are challenges. The former could be 613 614 addressed by using atomically thin 2D semiconductors. 2D semiconductors are ideally 615 suited for TFETs and provide unique CMOS compatible process advantages. 8" 616 compatibility is important for any technology development. Here the focus needs to be on 617 medium scale innovation.

618 **Negative capacitance materials**

Negative capacitance is an important strategy for reducing energy consumption which could be integratable into a CMOS stack. Negative capacitance circuits are analogue building blocks that can be used to compensate for undesired parasitic capacitance, bandwidth enhancement of amplifiers, equalization filters design without passive inductors,

³² https://ieeexplore.ieee.org/document/371964

³³ https://ieeexplore.ieee.org/stamp/stamp.jsp?arnumber=7006647

³⁴ https://ieeexplore.ieee.org/document/6724559

 ³⁵ https://ieeexplore.ieee.org/stamp/stamp.jsp?arnumber=7006647
 ³⁶ https://semiengineering.com/tfets-andor-mosfets-for-low-power-design/

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etc^{37,38}. Negative capacitance materials are simple ferroelectric materials and their feasibility has been demonstrated. However, it is challenging to achieve non-hysteretic negative capacitance FET using ferroelectric materials. Further research needs to be focused on compatibility and integration with CMOS using low-temperature deposition methods for as well as on improving the yield and performance of those materials.

628

629 There is no manufacturing of negative capacitance materials in the UK currently. Manufacturing facilities exist in Finland (DCA³⁹) and the Netherlands (Solmates⁴⁰). It is 630 631 important to create an ecosystem and establish an upstream industry e.g. chemical 632 manufacturing. To address this knowledge gap, it is important to develop a clear 633 understanding of which applications could benefit the most from these materials. Deposition 634 capabilities of high-quality films on 12" wafers need to be developed. Negative capacitance 635 ferroelectric layers should be CMOS compatible and need to be trialled initially to develop 636 capability in the UK to stimulate industrial uptake.

637

Research is required in both fundamental material understanding and development as well
as manufacturing process capability and equipment. A list of the different research activities
proposed is shown in the table below.

641

Required Activities	Implementation timescale *
Develop controlled etching capability	ST
Develop and improve testing equipment for Traps	ST
Validate testing method and develop new testing standards for various material systems	ST
Eliminate hysteresis for negative capacitance materials	ST - MT
Matching of negative to positive capacitor to achieve steep switching and improve understanding for device design	ST - MT
Non-native dielectric knowledge could be leveraged to understand trap distribution time-constant and space-location. Progression of native to non- native dielectrics. Getting control of dielectrics, profound understanding of various dielectrics rather than silicon e.g. Gallium Nitride. Maintain activity on all Nitride based structures e.g. Gallium Nitride.	ST - MT
Develop understanding what is going on in process chamber relating to deposition, particularly understanding dimensions like flow rate, pressure, energy control, charge, chemical composition, material properties and using big data simulations to get meaningful results to control process.	ST - MT
Understanding and controlling material properties for device performance and in particular research in doping and contacts especially to wide-bandgap materials	ST-MT
Understanding process variables and linking to product performance especially in CMOS.	ST - LT
Understand process dimensions and process control using Big- Data Analytics for control strategy in manufacturing processes.	ST - LT
Improve ability to generate 2D Hole gasses	ST - LT
Use Density function theory for modelling and simulation and T-CAD models for a range of materials	MT - LT

³⁷ https://ieeexplore.ieee.org/document/6240619

40 https://www.solmates.nl

³⁸ https://doi.org/10.1038/s41598-019-45628-8

³⁹ https://www.dca.fi

Develop a common platform - Gap in ALD and ALE, Select Area Deposition infrastructure	MT - LT
Develop equipment and technologies to understand process chambers relating to deposition. Furthermore, equipment and processes to capture flow rates, pressure, energy control, charge, chemical composition and material properties and then applying appropriate big data analytics to get meaningful results for robust process control to get appropriate product performance	MT - LT
* ST = short term (now-2030), MT = medium-term (2030-2040), LT = long-term (2040-2050)	

642

643 INTERCONNECTS

644 Interconnects are a critical research area that needs to be developed in parallel with other 645 material developments for integration with CMOS. Currently Cu is used as interconnect 646 material, but it exhibits issues such as increased scattering at the surface and grain-647 boundary interfaces when it is scaled down⁴¹.

648

Development of new, low k dielectrics and highly conducting materials is necessary to
overcome the limitations of Cu. New conductors have been investigated such as silicides
and materials that have different conductance mechanism e.g., carbon.

652

Silicides have low resistance, good process compatibility with Si, make good contact with other materials and show little electromigration ⁴². **Carbon-based materials** such as multiwalled Carbon Nano-Tubes (CNT), mixed CNT bundles and multilayer graphene nanoribbons (GNR) are emerging as promising materials for interconnects⁴³.

657 Additional materials' development to use for Cu barriers is also required to prevent Cu 658 diffusion e.g. Ta(N), Mn(N) etc. or materials to improve the adhesion properties of low-k 659 materials⁴¹.

660

661 SUBSTRATE DEVELOPMENT FOR HEAT DISSIPATION

662 The development of future low loss electronic devices, including (a) the integration of new 663 device functionalities with CMOS, (b) the enhancement of power electronic performance, 664 and (c) the development of new computing architectures, are all underpinned by the 665 development of suitable substrates. High thermal conductivity materials are needed in which 666 the thermal expansion of the substrate is matched to that of the active layers, and with high 667 interfacial adhesion to integrated metal surfaces or other films. The substrates need to be 668 large area, and have low defects, low bow, and be robust to thermal cycling. They also need 669 to have low electrical loss.

670 Low-loss dielectric substrates

High resistivity Si is well established and commonly used, especially in optoelectronic
 integrated circuits. Additional research is needed for large wafer diameters and for RF
 applications. p-type Si is currently used for GaN growth for power electronics.

674

⁴¹ 'The International Roadmap for devices and systems: 2017' - Copyright © 2018 IEEE

⁴² Prof. Krishna Saraswat Lecture notes, Stanford University

⁴³ https://www.tandfonline.com/doi/abs/10.1080/00207217.2017.1285436?scroll=top&needAccess=true&journalCode=tetn20

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675 Silicon Carbide (SiC) substrates are becoming widely used in power electronic devices, as 676 well in other applications such as the development of photovoltaic cells. They are also being 677 used as the host substrates in low-loss applications of GaN-based materials. However, due to 678 the strong Si–C covalent bands, it is hard to fabricate high density SiC substrates at low 679 processing temperatures without the use of additives or external pressure⁴⁴.

680

681 **GaN** has several advantages for use in optoelectronic and high power and high frequency 682 electronic devices. The issues are the lattice mismatch between GaN and conventional 683 substrates such as sapphire, silicon or silicon carbide resulting in poor crystal quality and hence high dislocation density, pits and cracks that affect carrier transport. Therefore, there 684 is a strong need to develop bulk free-standing GaN substrates^{45,46}. There have been 685 686 successful methods to grow bulk GaN. However, there are still issues with large scale thick GaN growth due to wafer bow. Additional issues exist around the scalability of the 687 688 fabrication methods and cost. Polycrystalline AIN needs developing for growth of GaN (CTE 689 matched substrate) for power electronics.

690

694

702

705 706

691 Development of Ga_2O_3 , and substrate technologies is required to overcome the limitations 692 in existing materials. Development activities need to include growth, contacting, processing 693 and testing.

Diamond has excellent thermal properties and therefore the potential to act as a heat sink. This particularly important for power electronic devices and diamond is considered as a substrate for RF electronics applications. Diamond is also used for optical sensing/single photon applications. There are several material issues to overcome for the fabrication and use of diamond substrates such as ability to fabricate large size substrates that are dislocation free, and of low resistivity⁴⁷. Diamond is required to be doped to make it useful for the design of devices, which has been difficult to achieve.

Sapphire (Al₂O₃) and MgO single crystals can both be made in large areas and both have
 good thermal conductivities and low microwave dielectric loss.

Required Activities	Implementation timescale *
Addressing limitations of the Laboratory-to-Fab toolsets, which need to be adapted	ST
Analysis and testing that fit with processes, and with the need for site- specific off-line quality assurance, as well as on-line monitoring.	ST
Pilot capability to take SiC and GaN from University facilities to wafer fabrication. Deposition is needed, but also suitable processing, patterning, and annealing.	ST - MT
Modernising testing and analysis equipment for high power applications. There are opportunities for manufacturers to develop new test equipment for RF and power applications.	ST - MT
* ST = short term (now-2030), MT = medium-term (2030-2040), LT = long-term (2040-2050)	

707

⁴⁴ doi: 10.1016/j.jeurceramsoc.2014.06.006.

⁴⁵ https://aip.scitation.org/doi/full/10.1063/1.4959073

⁴⁶ https://iopscience.iop.org/article/10.1088/1361-6463/aaaf9d

⁴⁷ https://doi.org/10.1016/j.diamond.2016.03.013

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708 UK COMMUNITY RECOMMENDATIONS

The materials challenges identified are mainly around the translation pathway from 709 710 academia to manufacturing. Having 8" compatibility is important, but the focus should not 711 be on foundries but on providing innovation on the medium scale. III-V on silicon for lasers 712 needs to be scaled from academia to industry, with buffers needed for scale up to 12" wafers. 713 The UK has an 8" CMOS line, and 4" and 6" experimental lines. It is of importance 714 to establish equivalent modelling and simulation methods to obtain good yields as well as 715 detailed simulations of all aspects of the fabrication process. As more, and different, 716 materials are envisaged for incorporation with CMOS, it will be critical to consider cross-717 contamination issues. As materials are scaled up from research, interface and defect control 718 will become critical. Materials will need development and optimisation, and growth 719 methods/toolsets will need to be adapted accordingly. This requires dedicated materials 720 research scientists.

721

In order to advance niche applications, a short term focus on developing patterning and structuring with the aid of a foundry service is needed for small scale production (1000 die per annum). Integration of new materials such as piezoelectrics on silicon for sensing, niche RF applications and actuation (MEMs, and IoT) to demonstrate feasibility are important. Large area and large volume capability is available, however this is not suitable for niche applications, where cost effective intermediate-scale facilities are needed. Such a foundry would need to support a disparate materials set while avoiding potential contamination.

730 There is a recognition that excellent research is being undertaken by UK scientists and 731 engineers in academia, but the UK lack the Institutes and Centres seen in Europe, the US 732 and far-East (e.g. IMEC, the Fraunhofers, Chalmers, TNO and the National Labs in the US) 733 to take new materials and devices from TRL3 to TRL7. Such Centres embed a culture of 734 translation of ideas to commercialisation, and have industry embedded within them. The 735 advantages of such a National Institute are retaining expertise in materials and devices 736 through core groups of long-term scientists, engineers and technicians. The UK provides 737 outstanding training for people in materials science and engineering however, retention of 738 these talents within the UK is currently challenging. Institutes, separated from 739 individual University, help retain talent and serve as links to other international Institutes and 740 Centres. DARPA for example has funded a \$1.5B Electronics Resurgence Initiative, 741 illustrating the importance of electronic materials and their commercialisation.

742

There is a need to support start-ups in accessing equipment and specialist staff especiallyas devices become more complex and involve many materials and interfaces.

745

746 UK expertise is focused on the know-how of complex materials and technologies for the 747 future. These need to be tested and proved, ready for scale-up from research. Simulation 748 and modelling feedback is needed for studying interfaces, defects, and reliability analysis is 749 becoming more and more crucial.

- 750
- 751 752

753 MATERIALS FOR MORE THAN MOORE

754

755 The long-term goal is to realistically power computationally intensive, by current standards, 756 tasks through green energy such as solar and wind. For a step change in the energy efficiency of computing we need to move away from ferrying electrical signals around 757 758 electronic chips in series, develop more advanced signal multiplexing and continue to 759 increasingly co-locate memory and processing. New hardware solutions need to be found 760 to support the fast evolving software developments. New building blocks need to be found 761 and improved not restricted to CMOS technology, with appropriate properties and energy 762 efficiencies from the outset.

763

Required activities	Implementation timescale
Electrical applications powered autonomously	МТ
Boosting silicon capabilities	МТ
Fully autonomous remote applications which are self-powered and utilise local energy harvesting	LT
Achieve conventional computing at a fraction of the current energy consumption.	LT
Unsupervised learning integrated into a dynamic environment such as controlling interfaces for autonomous vehicles.	LT
* ST = short term (now-2030), MT = medium-term (2030-2040), LT = long-term (2040-2050)	

764

765 NEUROMORPHIC COMPUTING

766 Neuromorphic computing refers to computing which emulates the neural structure of the 767 human brain. This is especially suitable for develop computing hardware and software which tackle data intensive problems however which do not require high accuracy, i.e. task which 768 769 the human brain excels at such as image recognition. Existing computing and logic 770 architectures are extremely good at deterministic problems but are very inefficient and power 771 intensive at solving indeterminate problems e.g. image recognition. One way of realising 772 neuromorphic computing is via artificial spiking neural networks. In a spiking neural network 773 neurons fire independently but are linked and thus a fired neuron changes the electrical 774 state of connecting neurons. This leads to information being encoded in the signal itself but 775 also in their timing and thus learning occurs by a dynamical remapping of the synapses in 776 response to stimuli.

777

Intel's most recent Loihi chip includes 8,000,000 neurons optimised for spiking neural networks performing tasks with 10,000 times energy efficiency at 1000x faster performance when used for applications like sparse coding, graph search and constraint-satisfaction problems (Intel's neuromorphic loihi processor scales to 8M neurons, 64 cores⁴⁸). Beyond von Neumann computing solutions developed by IBM and brought to market contains 256 million 'neurons' per system, *True North* architecture e-brain chips project. Both platforms are still largely based on CMOS transistors the former on 14nm CMOS technology and the
 latter on 40 nm CMOS technology⁴⁹.

786

787 Neuromorphic computing and artificial intelligence go hand in hand. The first generation of 788 Al developed by Intel was rule based and emulated classical logic in order to draw reasoned 789 conclusions in a very specific and well-defined problem domain, thus performing tasks more 790 energy efficiently. Efforts of the second generation of neuromorphic computing are focused 791 on sensing and perception. Thus, target areas are deep-learning networks and the analysis of a video frame. The next generation, as Intel sees it, will extend artificial intelligence 792 793 towards mimicking human cognition. The focus will be on interpretation and autonomous 794 adaptation, addressing the lack of context and common-sense understanding present in the 795 second-generation artificial intelligence chips. In order to achieve this, a key factor is the 796 development of neuromorphic computing and probabilistic computing tool boxes. The latter 797 creates algorithmic approaches to dealing with uncertainty, ambiguity and contradiction in 798 the natural world. In summary, neuromorphic computing enables unsupervised learning and 799 probabilistic computing will enable a computer to cope with the chaos of the natural world. 800 Combined artificial chips will move towards matching a human's flexibility, and ability to learn 801 from unstructured stimuli with the energy efficiency of the human brain, estimated at 20 W 802 [Intel's neuromorphic Loihi processor scales to 8M neurons, 64 cores⁵⁰.

803

Required activities	Implementation timescale*
Research into new material platforms with designed properties for non von- Neumann computing.	ST
Improvements on CMOS based artificial intelligence based technology	ST
Improvements on supervised learning	ST
Demonstration of supervised hardware learning.	MT
Development of non-CMOS based technology including non CMOS neurons	MT
Development of Bio-inspired 3D architectures	MT
Achieve unsupervised learning and artificial intelligence which mimics human cognition with a focus on interpretation and autonomous adaptation which demonstrates common sense and understanding of context	LT
Implementation of non-CMOS based neural networks	LT
* ST = short term (now-2030), MT = medium-term (2030-2040), LT = long-term (2040-2050)	

804

805 Nano Oscillator networks

Taking inspiration form the brain's neurons which behave like non-linear oscillators which develop rhythmic activities and interact to process information, artificial networks of coupled oscillators have great potential for high density, low power neuromorphic computing⁵⁰. The key challenge to high-density, low-power neuromorphic computing is the realisation of large networks (initially 2D to be expanded into 3D long term) of oscillators in the order of 10⁸ devices which fit on a reasonable sized chip. In other words, each oscillator needs to

⁵⁰ J. Torrejon Nature 547 428 (2017)

⁴⁹ B. Linares-Barranco Nature electronics 1 100 (2018), Memristors fire away

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812 possess a lateral dimension which is less than 1µm and does not suffer from noise and 813 stability issues⁵². CMOS oscillatory networks are under investigation, such as ring oscillators 814 and Schmitt trigger-based oscillators however challenges with frequency tunability, complex circuit design involving 10-20 transistors and high-power densities persist^{51,52}. Laboratory 815 816 based prototypes of non-CMOS alternatives are emerging. Under consideration are Joule 817 heating, PrMnO₃⁵³, volatile filamentation, TaO_x (not area scalable) ^{5354,}, metal to insulator 818 transition VO₂ and NbO₂ ^{55,56,57} and magnetic switching-based oscillators ^{52,58}. Classification 819 of 512 visual patterns into a set classes using a network of 3x3 thermally coupled vanadium dioxide oscillators and one output neuron⁵⁹ (Joule Heating oscillators basic operation 820 821 criteria's have been demonstrated using coupling elements which include a capacitor and a resistor ⁵³). 822

823

824 Spintronic oscillators are nanoscale pillars composed of a single magnetic layer or of two ferromagnetic layers separated by a non-magnetic spacer. An applied input charge current 825 826 is converted into a spin current exerts a torque on the magnetisation of the ferromagnetic 827 layers and generates sustained precession of the pillar's magnetisation. The frequency of the precession has an intrinsic memory with regards to past inputs (of the order of a few 828 829 hundred nanoseconds) and is sensitive to, i.e. is influenced by the oscillation of neighbouring 830 oscillators ⁵². The latter aspect of magnetic oscillators is a key advantage as the nanooscillator precession is modulated by radio waves however, importantly active oscillators 831 832 also emit radio waves and thus oscillators in the network interact with each other without the 833 need to implement physical interconnects. This enables wireless communication between 834 oscillators i.e. between neuron layers on the chip⁶⁰. Vowel recognition using coupled nano 835 - oscillators was demonstrated by using 4 coupled nano-oscillators achieving a recognition rate of 85 % using an automatic real time learning rule. This was achieved by tuning their 836 837 frequency via two strip lines situated above the network ⁶⁰.

838

Required activities	Implementation timescale*
Exploration of new materials which consider the whole ecosystem of neurons and synapses	ST
Development of improved oscillator coupling and synchronisation	ST
Solve challenges associated with size, agility and reproducibility	ST
Achievement of increased efficiency in generating oscillation	ST
Identification of materials which are cost-effective	ST
Improvement of grown materials quality i.e. reduction of defects	ST
Improvement in interface control	ST
In case of magnetic oscillators the following materials properties need optimisation: efficient generation of spin currents, voltage control of	ST

⁵¹ F.C. Hoppensteadt IEEE Trans Neural Netw 11 3 734 (2000)

⁵⁷ Y. Zhou IEEE Electron Device Lett. 34, 2, 220 (2013)

⁵² S. Lashkare IEEE 39, 9 (2018)

⁵³ A.A. Sharma IEEE J. Explor. Solid-State Comput. Devices Circuits, 1, 58, (2015)

⁵⁴ T.C. Jackson IEEE J. Emerg. Se. Topics Circuits Syst, 5, 2, 230 (2015)

⁵⁵ N. Shukla Sci. Rep. 4, 4964, (2014)

⁵⁶ L. Gao Appl Phys Lett, 11, 10, 2, (2017)

⁵⁸ Romera Nature 563, 230 (2018)

⁵⁹ A. Velichko Electronics, 8, 1, 75 (2019)

⁶⁰ A. Slavin IEEE TM 45, 1875 (2009)

anisotropies, more efficient spin torques and efficient manipulation of spin current polarisation	
Engagement between academia and industry to establish the future potential of oscillator networks	ST
Development of modelling tools which span length scales from the atomic scale, device scale through to the integrated scale to improve hardware design	MT
Development of proof of principle chip for industry	MT
Identifying and solving manufacturing and scale up issues	MT
Continue the exploration of new materials, considering the whole ecosystem of neurons and synapses	MT
Integration of prototype with computational hardware	LT
Development of hardware connects and software to utilise oscillator chip	LT
Demonstration of large-scale manufacturability and scale up	LT
* ST = short term (now-2030), MT = medium-term (2030-2040), LT = long-term (2040-2050)	

839

- 840 The main **bottle neck** is that there are no pilot plant for translation of proof of principle to 841 prototype.
- 842

PROBABILISTIC COMPUTING 843

844 Probabilistic computing hardware and software addresses the challenge of handling the 845 uncertainty and noise which is inherent in data generated from real world events. Modern 846 computing needs to be able to handle and understand uncertainties in order to respond to 847 dynamic environments. This is of importance in autonomous systems where the system 848 needs to be able to understand uncertainties in sensory input in order to make appropriate 849 decisions. High level brain function emulating neural network models which are capable of reasoning and memory recall, often require the presence of noise⁶¹. However, probabilistic 850 851 computing is not only a building block for artificial intelligence but can also aid in handling 852 errors in current semiconductor chips.

853 Software developments are steadily moving forward. Intel accelerated its investment into modelling the potential impact of probabilistic computing on artificial intelligence in 2018⁶². 854 855 Materials for probabilistic computing are predominantly in the proof of principle and thus 856 academic domain. Hardware implementations of probabilistic computing use a robust classical entity which fluctuates in time between well-defined 0 and 1 states⁶³. A proof of 857 858 principle device consisting of an asynchronous probabilistic computer based on engineered 859 unstable magnetoresistive random-access memory units (CoFeB/MgO/CoFeB based structure) was achieved⁶⁵. An alternative approach is demonstrated through thermal 860 861 diffusion of topological magnetic quasi particle entities referred to as skyrmions⁶⁴.

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⁶¹ Jordan Scientific reports 9 18303 (2019)

⁶² Probabilistic computing takes artificial intelligence to the next step" <u>https://newsroom.intel.com/editorials/probabilistic-computing-takes-</u> artificial-intelligence-next-step/#gs.8iwgq6 ⁶³ W.A. Borders Nature 573, 390 (2019)

⁶⁴ Zazvorka Nature Nanotechnology 14 658 (2019)

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Required activities	Implementation timescale*
Exploration of proof of concept materials and devices.	ST
Design of new hardware aligned to software developments.	ST
Design and materials optimisation	MT
System integration	MT
* ST = short term (now-2030), MT = medium-term (2030-2040), LT = long-term (2040-2050)	

- 863 The main **bottle neck** is the development of hardware and fusion with software
- 864

865 EDGE COMPUTING AND AUTONOMOUS SMART SENSORS

866 Edge computing refers to performing data analysis closer to the point of its creation, i.e. 867 close to the sensor Conventional vision, audio and electromagnetic sensors generate large volumes of redundant data⁶⁵. Transmitting raw data from thousands of sensors to a central 868 processing unit is bandwidth limited and can be costly. An alternative is to bring the 869 870 computation closer to is generation i.e. performing computation locally and transmit relevant data reducing cost and improving latency issues⁶⁶. Efficiency is at the heart of edge 871 872 computing and it is a necessity for the internet of things. Furthermore, utilising neuromorphic 873 sensors which produce spiked outcomes in an asynchronous and event-based manner will 874 further reduce data volume. Ultimately edge computing provides faster more relevant and 875 more reliable experiences and helps uncovers business opportunities by tapping into a fast amount of unanalysed and underused data ⁶⁸. 876

"By year-end 2023, more than 50% of large enterprises will deploy at least six edge
computing use cases deployed for IoT or immersive experiences, versus less than 1% in
2019" ⁶⁷. In particular, applications which rely on fast responses and which require ultralow
latencies (below 1 ms) will rely more and more on edge computing such as autonomous
vehicles, augmented and virtual reality and, industrial robots⁶⁸.

882

883 Types of edge computing include the combination of light sensing electronics with a neural 884 network on the same chip. This approach allows the photosensitivity of the light-sensing 885 diodes to be adjusted externally which enables the filtering of useful information at the point 886 of creation and reduces the demand on the computational image recognition algorithm. This is particular useful for driverless cars and industrial robots ⁶⁹. Commercial products are 887 888 being launched. Sony announced the release of the world's first image sensor with 889 integrated AI earlier this year, its IMX500 sensor which integrates processing power and 890 memory enabling machine learning-powered computer vision tasks⁷⁰.

⁶⁵ P. Kirkland, "Neuromprphic engineering taking AI to the edge" Leonardo

⁶⁶ "What is edge computing" IBM <u>https://www.ibm.com/uk-en/cloud/what-is-edge-computing</u>, M. Satyanarayanan, Nature Electronics 2, 42 (2019)

⁶⁷ Exploring the Edge: 12 Frontiers of Edge Computing, Gartner T. Bittman, Distinguished VP Analyst - Exploring the Edge: 12 Frontiers of Edge Computing, Gartner Research

⁶⁸ K. Kitayama APL Photonics 4 9 090901 (2019)

⁶⁹ MIT technology review https://www.technologyreview.com/2020/03/04/916701/ai-chip-low-power-image-recognition-nanoseconds/ 2020

⁷⁰ "Sony's first AI image sensor will make cameras everywhere smarter", https://www.theverge.com/2020/5/14/21258403/sony-imagesensor-integrated-ai-chip-imx500-specs-price, 2020

Required activities	Implementation timescale*
Addressing niche connectivity, information and security challenges	ST
Development of self-powered units (link to PV and thermoelectric strand)	ST
Matching hardware to the software algorithm	MT
Application specific neuromorphic sensor development	MT
* ST = short term (now-2030), MT = medium-term (2030-2040), LT = long-term (2040-2050)	

891

892 ALL OPTICAL AND OPTOELECTRICAL COMPUTING

893 Using light as medium for data transport through intensity modulation for example has the 894 advantage of operating at the speed of light. Translating the advances made in the 895 communications field, where encoding information as optical signals is the norm, onto on-896 chip optical computing requires devices which work seamlessly in the electrical and optical 897 domain without the need for repeated electrical-to optical conversion. Nanophotonics is an energy efficient and fast way of processing data on a chip overcoming the shortcomings of 898 899 electric circuits in terms of signal transportation and resistance-capacitance delays which 900 are increasingly problematic as bit rates increase⁷¹. However, integration of optical and 901 electronic architectures is challenging due to the fundamentally different interaction volumes of electrons and photons⁷². Crucial developments needed are integrated light sources, 902 903 photodetectors and modulators. Combining elements concepts from the fields of photonics, 904 electronics and plasmonics limitations can be overcome.

905 While integrated hybrid chips using light and electronics components in combination utilising 906 their respective advantages for improved performance are not realised yet advances in new 907 materials, our understanding of light at the nanoscale and increasing integration density of 908 devices are indicators towards achieving all optical or hybrid computing. Laboratory proof of principle devices towards optical and optical and electrical hybrid functionalities 909 exist^{73,74,75,76,77,78}. One such example uses a combination of waveguide-integrated 910 911 plasmonic nanogaps with phase change memristive cells (Ge₂Sb₂Te₅) to create an electro-912 optical memory cell with a switching energy of 16 pJ and an active area of 0.05x0.05 µm² 913 ⁷³. Similar outcomes can also be achieved by replacing the phase change material by 914 magneto-optical materials. Another example uses InGAs, and a InP photonic-crystal 915 platform with an imbedded InGaAsP nanocavity to demonstrate the first experimental proof 916 of optoelectronic integration at only 2 fF with data rates of 40Gbit/s and an energy consumption of 42 42 aJ bit^{-1 73}(Advances in silicon photonics is another avenue to achieve 917 918 optic based computing in the long run as it builds upon fabrication capabilities developed for 919 CMOS 79).

⁷¹ K.Nozaki, Nature Photonics 13, 454 (2019)

⁷² Within sight of computing at the speed of light (2019) <u>https://www.technologynetworks.com/informatics/news/within-sight-of-computing-at-the-speed-of-light-327869</u>, Farmakidis, Science Advances 5, 11 (2019)

⁷³ Farmakidis, Science Advances 5, 11 (2019)

⁷⁴ P. Markov ACS Photonics 2, 1175 (2015),

⁷⁵ A. Joushaghani Opt. Express 23 3657 (2015)

⁷⁶ Y. Lu, Nano Letters 17 150 (2017)

⁷⁷ M. Rude ACS Photonics 2, 669 (2015)

⁷⁸ C. Rios Nat Photonics 9 725 (2015)

⁷⁹ A comprehensive outlook is given on power efficient optical communication technology is given in the "Roadmap on silicon photonics" D. Thomson et al Journal of Optics, 18, 7 (2016) and the health of the UK photonics community is attested by "The health of photonics" an Institute of Physics report (2018). All optical logic includes concepts of cavity-based all optical flip-flops and logic gates, all optical gates

Required activities	Implementation timescale*
Improvement of electron to photon and photon to electron conversion	ST
Communication between industry and academia outlining integration challenges	ST
Improving fatigue issues of hybrid systems	ST
In case of all photonic systems address limits in the power efficiency of silicon based light sources	ST
Reduction of Si waveguide losses to below 2dB/cm	ST
Power efficient on chip integration of lasers through low loss interfaces between III-V and silicon on insulator waveguides within laser cavities	ST
Heat flow management for III-V materials	ST
Small size, large bandwidth, power efficient optical electrical optical converters	ST
Utilisation of AI to accelerate materials discover	ST
Initiate dialogue with photonics community to accelerate hybrid schemes	ST
Investigation of new multifunctional materials ongoing to the long term e.g. 2D materials (large scale manufacturing needs to be addressed in parallel) and heterostructures	ST
Development of reconfigurable system in form of active reconfiguration through 'Etch-o-sketch' type systems, plasmonic particles.	MT
Overcoming miniaturisation challenges concerning operation.	MT
Addressing of integration challenges	MT
Development of advanced hybrid systems converting information from spin to photon. Addressing of issues of gain and amplification (into long term)	MT
Development and implementation of proof of concepts of 3D optical integration	MT
Overcome technological problems with multiplexing. Optimisation of jitter noise instead of amplitude noise levels	MT
Demonstration of chip integration of long distance optical connects	MT
Solve electronic transduction challenge by improving interfaces between electronics and photonics/optoelectronics	LT
* ST = short term (now-2030), MT = medium-term (2030-2040), LT = long-term (2040-2050)	

920

921 MATERIALS ORDER PARAMETER COMPUTING

922 The goal here is to move away from charge current driven devices and move towards for 923 example spin currents. This has the potential to lead to dissipation less information transport, eliminating Joule heating losses. These thermal effects limit current CMOS technology and 924 925 preventing devices to operate below around 0.5 V⁸⁰. For this computing, interconnects and 926 memory needs to be redesigned to rely on order parameters such as polarisation, 927 magnetisation, antiferromagnetic order, strain and exhibit collective switching where the 928 target volume switches its order parameter collectively when the input driving signal exceeds 929 a threshold. Furthermore, the output is required to be interconnectable to further logic 930 devices. The transferred output signal then is needs to be able to act as an input signal i.e.

based on semiconductor optical amplifiers and nanoscale all-optical logics which are summarised in the following road map (Minzioni et al Roadmap on all-optical processing J. Opt. 21 063001 (2019)

⁸⁰ S. Manipatruni et al Nature 565, 35 (2019)

Roadmapping workshop for Henry Royce Institute for materials for Low Loss electronics

achieve a switching event. The last piece of the puzzle is reversibility i.e. once the state is
toggled further input from the circuit can reverse the order parameter back to its initial state.
Of interest here are ferromagnetic, ferroelectric or ferroelastic materials.

934

935 The building blocks for achieving new logic devices beyond CMOS are devices which 936 outperform CMOS and offer further multi-generational scalability. Key considerations are 937 operation voltage, interconnects and energy consumption⁸⁰. Fundamentally, the challenges 938 in order parameter devices for computing are efficient order parameter switching and 939 effective order parameter detection additionally to the challenge of the interconnects. A 940 comprehensive review of desired parameters operation at 420 K is given in reference ⁸⁷ and 941 summarises to the following: an element size of 10 x10 nm² operating at switching energies 942 of 1-10 aJ, switching voltages of 100-300 mV, switching speeds of 10-1000 ps, write errors of 10⁻¹ for stochastic computing and 10⁻¹² for von Neuman computing applications. Coupled 943 with electrical and spin current interconnects of 30 nm width and 100nm to 0.1 mm length 944 945 and switching voltages and currents of 100 mV and 1-10 µA, in case of optical connects 200 nm width and >100 μ m range with a spin to optical conversion at < 10 aJ (10⁻¹⁸J) per bit, 1 946 947 Gbit s⁻¹.

948

949 In memory Computing

950 Resistive memory devices, referred to as memristors, are a relative mature concept, with 951 much research having been done in the last >10 years. Resistive switching materials enable 952 the merging of information processing with memory, and thus reducing the level of electrical 953 signal retrieval and sending from the central processing unit to the external memory across 954 the computing chip. This greatly increases energy efficiency. This class of materials includes 955 transition metal oxides (resistive materials), phase change materials, magnetic multilayer 956 systems and other systems (e.g. ferroelectrics). Potential applications include non von 957 Neumann computer architectures with reduced energy consumption and increases 958 processing speeds. These systems are central to low power AI computing. AI computing is 959 currently using massive amounts of power with an upwards trend. While the state of the art 960 material, Ge₂Sb₂Te₅ (a phase change chalcogenides), is still the favoured alloy, it is 961 approaching its performance limits. For higher endurance and lower switching energy the 962 development of current materials by sophisticated materials engineering in addition to research on new material compositions is urgently needed. Resistive switching materials 963 964 are already commercialised for high performance SSD applications.

A memristor is a two-terminal variable resistor. Its resistance changes depending on the signals applied. Furthermore, resistance state is memorised in the OFF state i.e. when no signal is applied, i.e. non-volatile. Ideal materials candidates for memristors are a long retention characteristic, fast switching and an ultra-low power consumption. Some laboratory demonstrator memrisitive systems have the ability to support a multitude of resistive states.

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- 974

975 Oxides

976 In the case of transition metal oxides the main bottle neck are limitations in the long-term 977 stability of independent states. Resistive material random access memory is based on 978 thermal, electrically or ionic stimulated changes of the resistance state of a metal-insulator-979 metal structure⁸¹. Material systems include (Ta₂O₅, HfO₂ and TiO₂⁸²). Self-learning spiking 980 8 x 8 crossbar array on a single chip with 64 synapses and 8 leaky integrate-and-fire 981 neurons have been demonstrated. The synapses were built with non-volatile HfO-based synaptic drift memristors, and the 8 neurons with volatile silver-based diffusive memristors⁸³. 982 Resistive material technology is scalable beyond current CMOS technology⁸⁴. HP envisions 983 984 technology capabilities of 10 times the performance of NAND flash at 10 times less power 985 consumption coupled with a longer life-time. Other companies which have invested in resistive random access memory are Panasonic, Toshiba and Micro⁸⁴. A two neuron 986 network consisting of Pt (10 nm)/TiO₂ (25nm)/Pt(10nm) demonstrating reversible 987 unsupervised learning was demonstrated⁸⁵. The key challenges are engineering materials 988 989 to be highly uniform, with ability to scale. There are strong UK efforts in promoting this area including e.g. two Royal Academy Chairs in Emerging Technologies. Connection of efforts 990 991 across the U.K. will strongly enhance the UK capability is this field.

992

993 Phase change materials

994 Phase change materials are more reliable than resistive materials but are also more affected by power and scalability issues ⁸⁴. Phase change materials have great potential for 995 996 applications due to performance and cost benefits and could promise a universal storage 997 class memory replacing SRAM, DRAM, NOR flash and NAND flash. Suppliers including 998 Micron, IBM, Intel, Samsung and SK Hynix are pursuing development of the technology ⁸⁶. 999 However, an impact on the market is only envisioned when current 3D NAND flash has 1000 reached its 10 nm limit at the end of the decade. Phase change memory is based on a 1001 controlled temperature induced transition from a crystalline state to an amorphous state⁸³. A successful demonstrator using one million phase change memory devices to perform high 1002 1003 level computing was made doped Ge₂Sb₂Te₂ (d-GST) integrated into 90 nm CMOS 1004 technology. Energy efficiency of correlation computations of two order of magnitudes with the material used being doped Ge₂Sb₂Te₅ (d-GST) integrated into 90 nm CMOS technology 1005 87 1006

1007

1008 Ferroelectric materials

Non-volatile memory in which bits are stored in form of stable polarisation states can be
achieve using ferroelectric materials. This is at an earlier stage of development than the
aforementioned systems, with critical materials challenges being uniformity of operation and
toxicity. Ferroelectric based memory enables low power performance and fast write speeds.
Commercialised narrowly in 1990 using perovskite materials. However historically the
severe challenge of integrating perovskite or layered perovskite ferroelectric materials into

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⁸¹ R. Waser Nature materials 6, 833 (2007)

⁸² S. Stathopoulos Scientific reports 7 17532 (2017)

⁸³ Wang et al, 1, 137 (2018)

 ⁸⁴ Would the real flash storage successor please stand up? (2014) <u>https://www.computerweekly.com/feature/Would-the-real-flash-storage-successor-please-stand-up? ga=2.176675939.735273345.1592576100-881259463.1592576100</u>
 ⁸⁵ A. Sebastian, Nature communications 7 12611 (2016)

1015 CMOS processes and realising three dimensional structures has hindered scaling below

1016 100 nm and thus limited device density and market uptake. The discovery of hafnium oxide

- 1017 has changed this⁸⁶.
- 1018

1019 The most commonly studied material for memory applications is PbZr_xTi_{1-x}O₃ (PZT). PZT 1020 materials have a permanent polarization value of ~ 10-40 µC/cm², a permittivity of ~ 300-400, and a coercive field of ~ 50-70 kV/cm. However, fatigue problems set in if the active 1021 1022 part of the device is coupled with a metallic contact such as Pt. A problem which can be 1023 avoid by using an oxide electrode. A leadfree alternative material system, SrBi₂TaO₉ reaches polarisation values of 5-10 µC/cm² with a coercive electric field of 30-50 kV/cm and 1024 does not suffer fatigue issues when paired with metal electrodes. On the other hand, BiFeO₃ 1025 1026 has excellent ferroelectric properties, however it is almost a wide band gap semiconductor, 1027 rather than an insulator which is a disadvantage for applications. Furthermore, it is a 1028 complex material with non-uniformity issues. Its magnetic properties and potential for 1029 optoelectronics applications makes it attractive for other applications. As switching of a 1030 ferroelectric material requires a limited number of electrons to form a sizable energy barrier of 1 eV (1-10), ferroelectric materials which exhibit magnetic properties are key for very 1031 1032 energy efficient hybrid applications where the polarisation induces a magnetisation reversal in a neighbouring ferromagnetic laver⁸⁷. 1033

Due to the ability to grow ferroelectric thin films fluorite based ferroelectric materials such as Si doped HfO₂, undoped HfO₂ and solid solutions of HfO₂-ZrO₂ are of interest. They have already been used as dielectrics in CMOS technology and thus provide an excellent solution for next generation ferroelectric computing applications. However, reproducibility, wake-up effects, and cycling fatigue are problems as well as the large coercive field. Again, advanced materials control and engineering are challenges to addressed⁸⁶.

1040

1041 Piezoresistive Materials

1042 Combining piezoeletric materials, materials in which a large volume change occurs under 1043 the application of an electric field, with a material which undergoes a hysteretic metal to 1044 insulator transition under pressure is a way to achieve a memristive transistor which is not subject to the voltage limits of a field effect transistor⁸⁸. Gigahertz switching speeds can be 1045 1046 achieved⁸⁹. PZT is currently the dominant material with regards to achieving high strains 1047 and forces at a given voltage, however the relaxor material (1-x)[Pb(Mg1/3Nb2/3)O3] x[PbTiO₃] (PMN-PT) is gaining traction⁹⁰ due to its high piezoelectric coefficient. Thin film 1048 1049 growth development is focused on pulsed laser deposition growth due to its compatibility 1050 with CMOS technology. However, growth of single phase formation of perovskite PMN-PT 1051 systems is still a challenge. Advances towards growth on Si involve adding lattice matched 1052 substrates or template layers such as Si/STO/SRO or Si/TSZ/CeO/LNO. On the memristive 1053 side, a material with a large and hysteretic change in resistance is needed which is driven 1054 by a change in pressure. Proof of principle efforts are focused on rare earth

⁹⁰ Baek et al. Science 334 6058 (2011)

⁸⁶ C S Hwang Advances in non-volatile memory storage technology 2nd edition 393 (2019) and references within

⁸⁷ S. Manipatruni et al Nature Physics 4, 338 (2018)

⁸⁸ J. B. Chang et al. Nanotechnology 26, 37 (2015)

⁸⁹ D. Newns et al. J Appl. Ohys 111 084509 (2012)

1055 monochalcogenides such as SmSe which are deposited using highly controlled state 1056 techniques P.M. Solomon Nano Letters 15, 2391 (2015)⁹¹. An effect first observed in 1970. 1057 Switchable films can be achieved using sputtering methods. Piezoelectric memristors are at 1058 TRL 3-4 currently. Improvements need to be made on with regards to the materials interfaces and the guality of the piezoresistive material which will require modelling and a 1059 1060 fast tracking of materials evaluation. A concern is also the incorporation of lead which may be problematic in the future due to its toxicity and life cycle concerns. However, innovation 1061 1062 in other materials families such as Heusler compounds, other chalcogenides and oxides are 1063 promising and will be needed to be moved towards an industry prototype.

1064

1065 Magnetic materials

1066 Magnetic materials, while more reliable than resistive materials are more affected by power and scalability issues⁸⁴. The devices based on the former is commercially available however 1067 cost is an issue ⁸⁴. A commercially niche products based on spintronics is Magnetic RAM 1068 1069 which utilises magnetic fields to switch a soft non-volatile magnetic layer in a magnetic 1070 tunnel junction configuration. The first generation RAM works on a two-state system where 1071 the effective resistance of the MTJ changes as the soft layer is switch between parallel and 1072 anti-parallel alignment with a fixed hard magnetic layer where the switching is driven by a 1073 small magnetic field. The second generation of MRAMs utilises spin polarised currents to 1074 switch the soft layer via spin torques. Inefficient conversion between charge currents to spin 1075 currents is currently limiting the writing endurance and the energy efficiency⁹². Magnetic 1076 random access memory struggles with the write error rate which is linked to the write 1077 voltage. Fast switching times in the order of 2-3 ns are needed for commercial products. 1078 The next generation, utilising out of plane spin torques acting on out of plane magnetised layers is promising an optimised performance⁹³. State of the art research demonstrated 1079 1080 electrical switching of Magnetic tunnel junction in 0.2 ns in a 23 mT static in plane field using 1081 a combination of spin transfer torque and spin orbit torque at a critical switching energy of 0.5 pJ using a 1082

- 1083 W (3.7 nm)/Co₂₀Fe₆₀B₂₀ (0.9 nm)/MgO (~1 nm)/Co_{17.5}Fe_{52.5}B₃₀ (1.1 nm)/W (0.3 nm)/Co
- 1084 (1.2 nm)/Ru (0.85 nm)/Co (0.6 nm)/Pt (0.8 nm)/[Co (0.3 nm)/Pt (0.8 nm)]₆ junction⁹⁴.
- 1085

Required activities	Implementation timescale*
Close collaboration between hardware development and software development	ST-LT
Achieve better understanding of fundamental physic and chemistry involved in the motion of ions, electrons and magnetic domains	ST-MT
Improvement of device performance through optimisation of materials properties.	ST
Improvement of interface control and design to enhance electrochemical processes, device and bit stability, improve switching characteristics and to	ST

mram ⁹⁴ E. Grimaldi Nature Nanotechnology 14, 111 (2020)

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⁹¹ D. Newns et al. J Appl. Ohys 111 084509 (2012)

⁹² IEEE International Roadmap for Devices and systems (2017 Edition)

⁹³ 11 Myths about MRAM B. Hoberman (2017) <u>https://www.electronicdesign.com/technologies/memory/article/21802179/11-myths-about-</u>

reduce the overall power consumption, improve write-ability, yield and minimise writing energies	
Improve latency time and current densities	ST
Reduce memristor size while maintain performance	ST
Development of MTJ memory cells which are of comparative size to transistors while retaining stability against thermal fluctuations and which are addressable with very small current densities.	ST
Survey properties of less explored memristive materials such as antiferromagnetic phase memory.	ST
Translation of proof of principle multistate memristors to prototype	ST
Modelling across all length scales from atomistic, to device through to the architecture scale	ST
Development of benchmarking framework enabling a direct comparison between the different materials and technologies	ST
Development of selection criteria for materials discovery.	ST
Scale up of commercial production capabilities of materials as they become technologically ready	ST
Development of techniques for non-destructive probing of ferroelectric with high special and resolution	ST
Address scalability challenge of PbZr _x Ti _{1-x} O ₃ ferroelectric materials	MT
Development into lead free alternatives with improved performance	ST-MT
Address fatigue and coercive field challenge of fluorite based ferroelectric materials	MT
Catalogue matching materials properties to neuromorphic computing hardware and software	MT
Development of interface outputs and interconnects able to address large arrays of elements	MT
Optimisation of materials and device architecture to achieve noise suppression and optimise error correction	MT
Development of practicable co-processor or special purpose processor such as a neuromorphic processor	MT
Development of high quality, new piezoresistive composites materials. Using materials modelling.	MT-LT
Investigation into structure-functionality relationship of piezoelectric memristors	ST-MT
Scale down of piezoelectric memristor device size	ST-MT
Volume scale up and commercialisation.	LT
Achievement of cost reduction.	LT
Improvement of bit switching speeds through improved knowledge of dynamic effects	LT
* ST = short term (now-2030), MT = medium-term (2030-2040), LT = long-term (2040-2050)	

1086

The main **bottle necks** are lack of volume characterisation equipment, lack of large-scale
(8" inch wafer growth) compatible prototyping line and limited access to high end (single nm
write-line, large wafer compatible) lithography tools.

1090

1091 CHARGE TO SPIN CURRENT CONVERSION

1092 In order to convert charge currents to spin currents, in order to manipulate a magnetic 1093 material, or to convert a spin current to a charge current, to sense a change in a magnetic 1094 material, requires materials with large spin orbit coupling. Conversion occurs either via the 1095 spin Hall effect or the inverse Spin Galvanic effect (or Rashba Edelstein effect).

Heavy metals: Pt 95, Ta, Ir, W 1096

1097 Topological oxides: Bi₂O₃ ⁹⁶, SrIrO₃ ⁹⁷, SrTiO₃/LaAlO₃ ⁹⁸

Topological materials and superlattices: Bi_{1.5}Sb_{0.5}Te_{1.7}Se_{1.3}⁹⁹, Bi₂Se₃¹⁰⁰, α-Sn¹⁰¹, 1098 1099 BiSb¹⁰²

- Two-dimensional transition metal dichalcogenides: MoS₂, MX₂.¹⁰³ 1100
- 1101

1102 Topological materials have great potential in spin based technologies, however, they are at 1103 the fundamental research level. Understanding their physics and materials processing 1104 needs fundamental development. Their potential lies in their linear dispersion which results 1105 in high mobility and low electrical losses. Furthermore, they can be used to carry 1106 dissipationless currents. Their potential in active parameter tunability and reconfigurability 1107 might open many new avenues for innovation.

1108

1109 **MAGNETOELECTRIC MATERIALS**

1110 An exceptionally energy efficient charge driven switching phenomena is based on charge 1111 switching a ferroelectric material which in turn switches a ferromagnet via magnetoelectric 1112 switching. This efficiency is due to the limited number of electrons which are required to form an energy barrier of 1 eV (1-10 electrons) in ferroelectric materials. Magnetoelectric 1113 1114 materials can then induce a magnetisation reversal in a magnetic material ⁹³. The switch in the ferromagnet is then read back via spin to charge conversion through strong spin-charge 1115 coupling such as topological materials via the Rashba-Edelstein or topological two 1116 dimensional electron gases ^{93, 82}. 1117

1118 Fundamentally, the challenges in spintronic devices for computing are efficient spin 1119 switching and effective spin detection additionally to the challenge of the interconnects. In 1120 order to tackle these challenges, the following materials are of interest.

- Multiferroics: BiFeO3 ¹⁰⁴, LaBiFeO3 ¹⁰⁵, TbMnO3 ¹⁰⁶, LuFeO3/LuFe2O4 ¹⁰⁷ 1121
- Magnetostrictive: Fe₃Ga¹⁰⁸, Tb_xDy_{1-x}Fe₂¹⁰⁹, FeRh¹¹⁰ 1122

¹⁰⁶ Kimura, T., et al., Nature 426, 55 (2003)

- ¹⁰⁹ Ryu, J., et al. Jpn J. Appl. Phys. 40, 4948 (2001)
- ¹¹⁰ Cherifi, R. O. et al. Nat. Mater. 13, 34 (2014)

⁹⁵ Zhang Nature Physics 11, 496 (2015)

⁹⁶ Karube, S., et al., Applied Physics Express, 9, 3 (2016)

⁹⁷ Pesin, D. et al. Nat. Phys. 6, 376 (2010)

⁹⁸ Varignon, J., et al., Nat. Phys. 14, 322 (2018) ⁹⁹ Shiomi, Y. et al. Phys. Rev. Lett. 113, 196601 (2014)

¹⁰⁰ Fan, Y. et al. Nat. Mater. 13, 699b(2014)

¹⁰¹ Rojas-Sánchez, J.-C. et al. Phys. Rev. Lett. 116, 096602 (2016) ¹⁰² Khang, N. H. D., Nat. Mater. 17, 808 (2018)

¹⁰³ Wang, G. et al. Nat. Commun. 6, 10110 (2015)

¹⁰⁴ Heron, J. T. et al., Nature 516, 370–373 (2014)

¹⁰⁵ Chu, Y. H. et al., Appl. Phys. Lett. 92, 102909 (2008)

¹⁰⁷ Mundy, J. A. et al. Nature 537, 523 (2016)

¹⁰⁸ Srisukhumbowornchai, N. et al., J. Appl. Phys. 90, 5680 (2001)

- 1123 Exchange bias: Cr₂O₃ ¹¹¹, Fe₂TeO₆ ¹¹²
- 1124
- 1125 Magnet Materials
- 1126 Nominal Ferromagnet: Co, Fe, Ni, CoFe, NiFe
- 1127 **Heusler alloys:** X₂YZ and XYZ alloys (for example, Co₂FeAl, Mn₃Ga)
- 1128

1129 Materials within all four classes need extensive materials engineering to improve interfaces 1130 for integrated devices, operation temperature range, processing temperature compatibility 1131 and performance metrics to achieve the desired 1-10aJ performance and a device size of 1132 <10 nm. For example, spin to charge conversion efficiency (Inverse Edelstein length (IEL)) 1133 of 2.1 nm was demonstrated in (001) α -Sn (30 monolayers)/Ag (2 nm)/Fe (3 nm)/Au (2 nm) 1134 at room temperature¹¹³.

1135

1136 SPIN CURRENT DRIVEN DEVICES

Spintronic materials are a versatile group of materials suitable for hybrid non-volatile charge
- spin architecture such as integrated MTJs for in memory computing or domain wall logic
architectures or volatile nano-oscillator based (See previous sections).

1140 Magnetic Racetrack Memory and Logic

1141 Magnetic logic and racetrack memory embody fully solid state devices without any moving parts. Magnetic domains are moved by fields and or currents from stationary read and write 1142 1143 elements. Both magnetic domain logic and racetrack memory are based on moving and 1144 manipulation of information, in form of magnetic domain walls, via spin polarised currents. 1145 Current state of the art racetrack memories combine out of plane easy axis materials, 1146 interfacial driven effects such as Dzyaloshinsky-Moriya interactions and proximity effects created by interfacing ultrathin ferromagnetic thin films with heavy metals in addition to a 1147 1148 non-magnetic spacer layers to control the long range dipolar interactions. These 1149 heterostructures are commonly referred to as synthetic antiferromagnetic material systems. 1150 In systems consisting of TaN/Pt/Co/Ni/Co/Ru/Co/Ni/Co/TaN domain wall velocities can reach 750 m/s with driving currents of the order of 10⁸ A/cm² ¹¹⁴. Alternative, using stacks 1151 based on ferrimagnetic materials such as AIO/TaN/Pt/Co/Gd/TaN enable additional 1152 1153 tunability of parameters. Domain wall velocities reach 400 m/s at a current density of 10⁸ 1154 A/cm²¹¹⁵. State of the art logic elements are demonstrated in Pt/Co/AIO with single NOT gate operation in an area of 0.8x1 µm² at 20 pJ with a predicted down scaling of 20 aJ if a 1155 footprint of 10 x 10 nm² was achieved ¹¹⁶. 1156

1157 Key materials parameters for success are perpendicular magnetic anisotropy, stable 1158 homochiral Néel domain walls, and large spin currents with controlled polarisation. The latter 1159 is created from a charge current through the spin Hall effects or interface effects such as 1160 the Rashba Edelstein effect and materials with large conversion efficiencies are of interest. 1161 Heavy metals such as Pt possess an efficiency in the order of 10-30%. Interfaces between

- ¹¹³ J.C. Rojas-Sanchez, PRL 116 096602 (2016)
- ¹¹⁴ S. Yang Nature Nanotechnology 10, 221 (2015)
 ¹¹⁵ Blaesing et al Nature Communications 9 4984 (2018)
- ¹¹⁶ Z. Luo Nature 579 (2020)

¹¹¹ Street, M. et al. Appl. Phys. Lett. 104, 222402 (2014)

¹¹² Wang, J. et al., J. Phys. Condens. Matter 26, 055012 (2014)

- 1162 heavy metals and Co induces the required perpendicular magnetic anisotropy and the
- 1163 Dzyaloshinsky-Moriya interaction which stabilises homochiral Néel domain walls. However,
- 1164 materials with larger charge to spin current conversion have been demonstrated such as 1165 Bi₂Se and $Cr_xBi_2Se_3$ ^{117,118,119,120}. Material scarcity is a potential concern for spintronics
- 1166 applications as they currently rely on Co, Pt, boron and rare earth metals and thus a large
- 1167 proportion of the product price will be set by the materials price.
- 1168

1169 INTERCONNECT MATERIALS

1170 Interconnect Materials

- 1171 Noble metals: Cu, Ag, Co, Al, SiO₂
- 1172 Metal-semiconductor: Ru poly-Si, NiSi, CoSi, NiGe, TiSi
- 1173 Interlayer dielectric: SiN, SiCOH, polymers

1174 Spin Based Interconnects

1175 Spin current interconnects are a potential candidate for low loss transmission of signals. 1176 While in theory spin currents propagate dissipationless and thus could lead to energy 1177 efficient interconnects. A key materials problem to address is spin scattering. The direction 1178 of the spins is not conserved i.e. the spins can flip their direction when undergoing a 1179 scattering event. This means frequent spin signal repeaters or regenerators would need to

1180 be added in order to transmit signal over the distances required on current chips ⁹³.

1181 Superconductor Based Interconnects

- 1182 These material groups are very early in their development but promise zero resistance conduction of electrical signals. However, there are issues relating to operation temperature 1183 1184 and functionality. Operation temperature lies 40 K below 300K and is an issue for domestic applications. Superconducting SQUID loops and superconducting interconnect have the 1185 1186 potential to enable quantum computing and high power computing where low temperature 1187 operation is less of an issue and speed and low loss operation are of importance. Progress is being made in developing interfacing memory. The UK is behind the research and 1188 1189 development curve.
- 1190

1191 MAGNETO-OPTIC DEVICES

1192 Linked to the optical computing themes are materials which change their order parameter 1193 through light bridging non-volatile computing, efficient switching and fast operation. Optical switching of magnetic materials is a process mediated by magnetic dichroism and/or thermal 1194 1195 effects. Magnetisation reversal using light has unprecedentedly low heat load (<6 J cm⁻³)¹²¹. 1196 Interference enhanced absorption of light through microstructuring of the magnetic film was shown in GdFeCo¹²². Proof of concept, single-pulse switching of Co/Pt multilayers within a 1197 1198 magnetic spin-valve structure ([Co/Pt]/Cu/GdFeCo) has been demonstrated¹²³. Optically 1199 driven MTJs exhibit very fast switching speeds however they need high optical pulse

¹¹⁷ Zhang Nature Phys (2015)

¹¹⁸ Demasius Nat Com (2016)

¹¹⁹ Nayaj Si Adv (2016) ¹²⁰ Zhang Sci Adv (2016)

¹²¹ Alexey V. Kimel and Mo Li, Nature Reviews Materials 4, 189 (2019)).

¹²² M. Savoini, et al. Phys. Rev. B 86, 140404(R) (2012)

¹²³ A. lihama Advanced Materials, 30, 51 (2018)

energies to switch and due to growth incompatibilities the resulting poor MgO tunnel barrier
leads to very low read out signals. GdFeCo is a good proof of principle material with
switching times of 30 ps, however performance below 200 nm is impossible due to thermal
stability issues¹²³. Therefore, new materials for optical switching need to be developed.
Other avenues combine optical switching with domain wall race track elements using
Pt/Co/Gd heterostructures¹²⁴. Ultrafast nonthermal photo-magnetic switching has been
demonstrated in less than 20 ps at 20 aJ in a transparent YIG:Co film¹²⁵.

1207 It is also possible to optically generate a spin current, in contrast to switching a magnetic 1208 volume through light. For example in GaAs through illumination of circular light an current of 1209 200 pA/W was then generated at the surface of the topological insulator Bi₂Te₃ at 20K¹²⁶.

1210

1211 ANTIFERROMAGNETIC DEVICES

Antiferromagnets materials which possess magnetic order but do not have a net 1212 1213 magnetisation, exhibit very fast dynamics and thus are of interest for fast computational 1214 approaches. Furthermore, they are sources and detectors of THz radiation. Antiferromagnetic materials open the door for faster operation for the same energy. Another 1215 1216 advantage is their resilience to radiation and magnetic fields¹²⁷. Electrical control of the 1217 orientation of the spins in CuMnAs on GaAs at THz frequency has been demonstrated¹²⁸. 1218 CuMnAs can be growth with molecular beam epitaxy on GaP at temperatures between 220 and 230 °C which is well below the CMOS circuit tolerance of 400 °C¹²³. As GaP is lattice 1219 1220 matched to Si integration with CMOS is possible. Memory cell fabricated from Mn₂Au have 1221 been demonstrated¹²⁹. Furthermore, optical writing is possible in CuMnAs nanostructures 1222 grown on GaP substrates with a single 100 fs laser pulse¹³⁰. By realizing detection of the 1223 antiferromagnetic state via optical reflectivity the tool-box of electrical and optical writing and 1224 readout is achieved. Additionally to CuMnAs and Mn₂Au electrical control has also been 1225 shown in metallic MnN¹³¹ and in insulating NiO¹³² interfaced with a large spin–orbit coupling 1226 material such as Pt¹³³. Other potential materials with room temperature antiferromagnetic 1227 order include Mn(II)Au, NiO, CoO, RuO₂ and several perovskites.

1228

1229 TWO DIMENSIONAL MATERIALS

1230 The electronic properties of 2D materials encompass a wide range and includes 1231 semiconducting, insulating and metallic behaviour (including superconducting). They can 1232 have magnetic and ferroelectric phases. They are easily doped and hence can be designed 1233 to cover a broad range of parameters. Furthermore, two-dimensional transition metal 1234 dichalcogenides for examples are interesting candidates for spin to charge conversion.

1235

¹²⁵ A. Stupakiewicz, et al. Nature 542, 71 (2017)

¹³² T. Moriyama, Tet al. Sci. Rep. 8, 14167 (2018)
 ¹³³ J. Shi et al Nature electronics 3, 92 (2020)

¹²⁴ M. L. M. Lalieu, et al Nature Communications 10, 110 (2019)

¹²⁶ Y.Q. Hiang, Nature Communications 8 15401 (2017)

¹²⁷ K. Olejník, <u>Nature Communications</u> 8, 15434 (2017)

¹²⁸ K. Olejník, et al. Science Advances, 4, 3 (2018)

¹²⁹ S. Y. Bodnar, et al Nat. Commun. 9, 348 (2018)

¹³⁰ https://arxiv.org/abs/1909.09071

¹³¹ M. Dunz, preprint arxiv.org/pdf/1907.02386.pdf (2019)

1236 Key limitations for widespread industrial uptake are that their scalability is highly material 1237 dependent and that some of the characteristics are so far only accessible at low 1238 temperatures. Insulating 2D materials so far can only be grown in atomic-sized flakes. 1239 However, for viable industry uptake large scale, good quality growth is necessary, and 1240 technologies will have to be developed towards this goal. The creation of heterostructures 1241 of 2D materials allows a flexible tuning of properties. Dry transfer techniques are crucial tool 1242 kits for laboratory based proof of principle device engineering. Reliable heterostructure 1243 development requires O₂ free atmosphere or immediate passivation of the top layer to prevent device breakdown. Some heterostructures can be drawn by chemical bath 1244 1245 deposition. Industry manufacturing requires integration of different materials, including 1246 integration with Si. Industrial uptake of 2D materials so far is limited to passive thermal 1247 management.

1248

1249 Magnetic two-dimensional systems are interesting candidates for the study of low-1250 dimensional magnetic behaviour. Transition metal phosphorus trisulfide (or thiophosphate). 1251 TMPS3, is an example which can host several transition metals such as Mn, Fe, Co, Ni, Zn 1252 and Cd, at the TM site and thus gives access to a fast variety of possible properties. It is a 1253 little explored field which has potential for many novel fundamental insights¹³⁴. With new physical phenomena one expects a substantial shift in our ability to control and investigate 1254 nanoscale phases¹³⁵. The current fabrication method via exfoliation is a drawback for 1255 1256 commercialisation. Other growth methods need to be developed. Other techniques can 1257 produce magnetic monolayer such as chemical vapour deposition and molecular beam 1258 epitaxy. Most of the magnetic van der Waal materials are layered, cleavable transition-metal 1259 chalcogenides and halides. As such they are usually comprised of a layer of metal ions 1260 between layers of chalcogens or halides. Diverse magnetic and electronic properties have 1261 been found in these systems which include ferromagnetic semiconductors, such as 1262 $Cr_2(Si,Ge)_2Te_6$ and MSe_2 (M = V, Mn), itinerant ferromagnets, such as Fe_3GeTe_2 , and 1263 insulating antiferromagnets (AFMs), such as MPX₃ materials where M refers to the transition metal and X to S or Se. Materials development challenges to overcome are materials 1264 1265 discover, growth, stability, exposure to Oxygen and reproducibility.

1266

1267 ORGANIC AND MOLECULAR SPINTRONIC MATERIALS

1268 The main advantage of organic materials in general is the ease by which they can be 1269 processed. They have a low thermal budget. However, the challenge with the performance 1270 of organic materials lies in their low operational frequency which is a limiting factor for some 1271 applications. The main processing issues are stability, printability and reconfigurability, i.e. 1272 the integration of organics with inorganic contacts as well as the diffusion that can occur in 1273 the organic material itself. A crucial engineering step in organics is encapsulation, ensuring 1274 oxygen does not enter the system. Furthermore, the management of lattice vibrations, 1275 phonons, is crucial which needs to be addressed for higher operation power and heat 1276 dissipation (in the spintronics space organic materials are of interest as biosensors).

1277

 ¹³⁴ Je-Geun Park J. Phys.: Condens. Matter 28 301001(2016)
 ¹³⁵ K. S. Burch Nature 563, 47(2018)

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Roadmapping workshop for Henry Royce Institute for materials for Low Loss electronics

1278 Growth of nanocarbon and molecular thin films

Over the last decade, there has been a concerted effort in the growth of high-guality organic 1279 and fullerene based, resilient thin films using techniques that are CMOS-compatible. High 1280 1281 vacuum thermal evaporation, together with spin coating and electro-spray, offer alternatives to grow hybrid devices containing molecules and carbon-based materials (e.g. 1282 1283 Phthalocyanines α -CoPc, carbon based molecules). These layers can be the active 1284 component of the device or they can be used to tune the electronic properties of adjacent layers, such as ultra-thin metals or 2D materials, via charge transfer, interface orbital 1285 1286 hybridisation and/or gate voltages.

1287

1288 Carbon based molecules

1289 Carbon-based molecules offer a sustainable alternative to heavy metals, doped 1290 semiconductors and rare earths. These abundant, light, eco-friendly materials are of interest 1291 due to the small spin orbit coupling of light elements and a lack of hyperfine interaction in 1292 12C leading to long spin coherence and diffusion times i.e. the interval before an electron spin changes its direction. However, molecular electronics and spintronics has faced 1293 1294 challenges with replicating effects seen in conventional crystalline devices due to bad 1295 reproducibility, low carrier mobility and degradation. Nevertheless, molecular spintronics has 1296 remained a fruitful field of research because of the various novel behaviours and effects 1297 which are unique to molecular systems. In particular, interfaces, that can be exploited in 1298 multifunctional devices are of interest¹³⁶. Molecular nanostructures can also be used to build spintronic devices¹³⁷ or in spin-voltage conversion structures via the inverse spin Hall 1299 1300 effect^{138,139}. There has been a concerted effort to comprehend the complex spin-dependent 1301 charge interactions between molecules and metals, in particular the formation of spin-1302 polarised interfaces and tunable surface states, where molecular materials offer unique 1303 behaviour and tunability that can be exploited to produce multifunctional devices via charge 1304 transfer and hybridisation when in contact with other materials^{140,141}. Charge transfer can 1305 take place innately due to band mismatching or be prompted by gate fields or optical irradiation. In parallel with these studies, observation and predictions have been made that 1306 1307 molecular hybridization can drastically modify the spin-texture of surface states in materials used for spin-charge conversion via spin orbit coupling or in spin capacitors^{142,143,144}. 1308

1309

Molecular layers can control and balance interactions in designer magnets. It has been observed that anti-ferromagnetic interface states form between a variety of organic molecules and Co or Fe films, resulting in changes to their magnetic anisotropy^{145,146,147}.
 High coercivity magnets are an important resource for renewable energy, electric vehicles and memory technologies. Most hard magnetic materials incorporate rare-earths such as

¹⁴⁴ Moorsom, Sci. Adv. 6, eaax 1085 (2020)

¹³⁶ M. Cinchetti et al., Nature Materials 16, 507 (2017)

¹³⁷ Wu et al., Adv. Func. Mat. 29, 1616 (2019)

¹³⁸ Ando et al., Nature Materials 12, 622 (2013)

¹³⁹ Sun et al., Nature Materials 15, 863 (2016)

¹⁴⁰ F. Al Ma'Mari et al., Nature 524, 69 (2015)

¹⁴¹ K.V. Raman et al., Nature 493, 509 (2013)

¹⁴² Stadtmueller, PRL 117, 096805

¹⁴³ Jakobs, Nano Lett. 15, 6022

 ¹⁴⁵ Gruber et al., Nature Materials 14, 981 (2015)
 ¹⁴⁶ Bairagi et al., Phys. Rev. Lett. 114, 247203 (2015)

¹⁴⁷ Moorsom et al., Phys. Rev. B . 101, 060408(R) (2020)

neodymium and samarium, but concerns about the environmental impact and supply
stability of these materials is prompting research into alternatives. A much less explored
possibility in the long-term could be the use of molecular materials to enhance the coercivity
of 3D transition metal-based ferromagnets without rare-earths.

1319

1320 Spintronics on flexible substrates and sensors

1321 Implementation of sensors on flexible substrates is of importance to enable operation on 1322 soft and elastic surfaces such as artificial electronic skin applications and for smart 1323 packaging. Furthermore, electric and magnetic field sensors are a key component of robotic 1324 systems which enable positioning and orientation in space. The challenge lies in developing a robust device while keeping costs down through simplify the processing and device 1325 1326 structures (e.g. reducing the number of layers in junctions), whilst matching the performance 1327 benchmarks necessary for the application. Recent times have seen advances such in the 1328 technology producing sensor systems consisting of 2x4 array of giant magnetoresistance 1329 magnetic sensors fabricated from permalloy (Fe₈₁Ni₁₉) Cu multilayers, an organic bootstrap shift register which controls the sensor matrix and organic signal amplifiers is 1330 1331 underway¹⁴⁸,¹⁴⁹. Fabrication of CoFeB/MgO tunnel junctions directly on flexible polyimide 1332 substrates with a 100% tunnel magneto resistance ratio has been demonstrated¹⁵⁰ as well as sensors based on heteroepitaxic Fe₃O₄/Muscovite films on flexible substrates¹⁵¹. 1333

1334

Required activities	Implementation timescale*
Development of spintronic based devices via light or currents avoiding external magnetic field routines.	ST
Integrate readout mechanisms suitable for an integrated on-chip readout.	ST
Integration of magnetic out of plane random access memory (reference to in memory computing) for non-volatile processing and logic	ST
Development of viable replacement for Pt in strong perpendicular magnetic anisotropy materials systems and SOT based devices	ST
Integration of heat assisted and microwave assisted magnetic recording for lower energy and higher density data storage	ST
Optimisation of Heat assisted recording addressing issues with optics and transducers	ST
Integration of semiconductor spintronics devices which are compatible with silicon fabrication for non-volatile logic and electromagnetic sensing.	ST
Development of spintronics devices on flexible substrates for IoT and sensing applications.	ST
Fundamental research into spin injection from and to topological Insulator and 2D interfaces for dissipationless currents especially with the long-term goal of extending the operational temperature to room temperature.	ST

- ¹⁵⁰ S. Ota Applied physics express 12 053001 (2019)
- ¹⁵¹ P-C Wu et al Asc Appl Mater Interfaces 8 33794 (2016)

¹⁴⁸ <u>https://techxplore.com/news/2020-01-fully-flexible-electronics-magnetic-sensors.html</u>

¹⁴⁹ M. Kondo Science advances 6, 4, (2020)

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Fundamental research into improving operational temperature and efficiency of spin current generation as well as into increasing the length of scatter free spin current transmission.	ST
Fundamental research into topological insulators growth to improve yield and quality	ST
Fundamental research into spin topological materials and materials properties	ST
Fundamental development of toolboxes to grow, manipulated and read out antiferromagnetic based devices	ST
Direct benchmarking of antiferromagnetic based devices against existing technology	ST
Optimisation of antiferromagnetic materials properties such as operational temperature range and bit lifetime.	ST
Fundamental antiferromagnetic materials discover.	ST
Translation of proof of principle into a prototype benchmarking device e.g. an antiferromagnets in-memory element	ST
Equipment development to improve aspects such as imaging of antiferromagnetic domains, time resolution, special resolution. Development of high frequency characterisation tools	ST
Fundamental development into modelling of antiferromagnetic modelling across all length scales and into the dynamic behaviour at high frequencies	ST
Fundamental research into antiferromagnets as THz source and detectors	ST
Linkage of spintronics and terahertz community	ST
Fundamental research and development into modelling including DFT and micromagnetic simulation, development especially in the region of antiferromagnetic behaviour and dynamics in the THz regime.	ST
Fundamental research into artificial multiferroics.	ST
Fundamental research into the development of designer materials - using known components e.g. L10 alloys	ST
Fundamental research into heterostructures of metals and oxides for memristive and racetrack applications.	ST
Fundamental research into oxide/molecular interfaces to address abundance and scarcity of materials	ST
Fundamental research into metal/molecular compounds to address abundance and scarcity of materials	ST
Close collaboration between material modelling, growth, characterisation and device fabrication for organic and molecular spintronics materials.	ST
Improvement of the reproducibility of device performance of organic and molecular spintronics materials.	ST
Understanding correlation between processing and the structure of the organic material.	ST
Improvements to wafer-scale growth and nanofabrication of organic and molecular spintronics materials.	ST
Coordination of academic research with links to industry to explore a wide variety of solutions with the goal to identify targets and materials and devices with commercialisation potential	ST
Race-track memory architecture – beating domain size limit and going into vertical integration e.g. 3D elements, controlling elements	ST-MT

Fundamental research into dynamic behaviour of magnetoelectric/ferroelectric switching. Exploration of possible materials combinations for practical magnetoelectric switching and read out	ST-MT
Unravel the fundamental interactions that control spin physics at molecular interfaces	ST-MT
Fundamental research into magnetic and multiferroic 2D van der Waals structures	ST-LT
Fundamental research into molecular based spintronics device development	ST-LT
Exploration of tunability of properties by interface hybridisation of organic and molecular spintronics materials	ST-LT
Proof of principal of Hybrid computing including optically switched magnetic materials (link to hybrid and optical computing section)	MT
Spintronic THz frequency sources and sensors for fast and efficient computing and communications	MT
Proof of principle demonstration of working magnetic and spin texture devices based on topological spin states such as skyrmions and synthetic antiferromagnetic domain wall logic.	MT
Demonstration of spintronic devices with an active magnetic/multiferroic device with a volume of less than 1,000 nm ³ and a stability of 100kBT switchable with an energy of 1 aJ ~ $6.25 \text{ eV} \sim 240 \text{kT}$	МТ
Demonstration of low stochastic errors in switching reproducibility and fatigue of ferroelectric, magnetic and multiferroic materials.	MT
Development of on chip magnet/ferroelectric state detection mechanism with high read-out voltage > 100 mV	MT
Development of material with large inverse spin–orbit effects, such as the spin galvanic effect/Edelstein effect how to achieve $\lambda_{IREE} > 10$ nm	MT
Actively tunaeble spin-orbit coupling materials	MT
Development of material architectures and device concepts for spin topological materials	MT
Solve interconnect issue of topological materials	MT
Development of actively tuneable material systems e.g. Rashba effect, permeability, permittivity, etc.	MT
Magnetic heterostructures for thermoelectric applications	MT
Demonstration of effective transduction of a spintronic/multiferroic state to a photonic state (and vice versa) enabling long distance interconnects (> 100 μ m)	MT
Demonstration of stochastic switches (spin/ferroelectric) operating near practical thermodynamic conditions in a computing architecture	MT
Optimisation of microwave assisted recording through engineering of spin- transfer oscillators	MT
Optimisation of materials properties and growth and interfaces of antiferromagnetic devices	MT
Addressing issues with interfacing organic and molecular spintronics materials with standard semiconducting devices.	MT
Agreement of standards for device performance and methodologies	MT
Connection with industry for real applications of molecular materials within current processes	MT

Material modelling and screening methods in realistic environments including defects, applied currents/voltages and magnetic fields	MT
Optimisation of organic and molecular spintronics materials and device architecture to achieve noise suppression and optimise error correction	MT
Improvement of use of recyclable and sustainable materials	MT
Equipment development to improve aspects such as imaging of antiferromagnetic domains, time resolution, special resolution. Development of high frequency characterisation tools	MT
Achieve integration into CMOS of antiferromagnetic materials based devices.	MT
Development of antiferromagnetic materials growth using CMOS compatible techniques	MT
Development of large antiferromagnet based device	MT
Industry engagement to evaluate device performance critically with attention to scale-up and integration possibilities	MT
Development of the 2D materials catalogue	MT
2D materials to be used for active thermal management	MT
Development of 2D chalcogenides and molecules and 2D materials processing techniques that are CMOS compatible.	MT
Exploitation of interface properties and control (hybrid materials)	MT
Overcome challenges in spin amplification devices, spin repeaters on a 10nm or sub-10nm length scale	MT-LT
Addressing of the interfaces challenge and spin de-coherence and scattering	MT-LT
Demonstration of optically switched materials at THz frequency, natural materials candidate are antiferromagnets	MT-LT
Continue to address challenges in growth and application of topological materials systems	LT
Charge less integrated memory and logic for ultra-low energy consumption using spin waves eliminating Joule heating losses (devices operating close to or at the fundamental thermodynamic energy limit, the landau limit). Paving the way to devices operating close to the Landau limit.	LT
Integration of magnetic, ferroelectric and multiferroic materials into the back-end of the CMOS i.e. demonstration of materials grow on an amorphous layers and at suitable temperatures at temperatures below 400 C.	LT
Demonstrate 10 billion functional spin based switches per chip utilize the extreme size, logic efficiency and three dimensional integration	LT
Development of emerging magnetic properties from non-magnetic bulk materials.	LT
Achieving permanent and tunable magnetism without using rare earth material	LT
Hybridisation of different materials systems achieving superior performance	LT
Development of single molecule properties for single molecule memory	LT
Development of permanent and tunable magnets without using rare earth materials	LT
* ST = short term (now-2030), MT = medium-term (2030-2040), LT = long-term (2040-2050)	

1335

1336 The main **bottlenecks** are poor reproducibility, degradation and lack of established 1337 standards for organic and molecular materials for spintronics which leads to problems in as well as the policy changes required to establish industrial interest in carbon-based materials to balance costs in production changes and investment in research in these materials. There are additional issues with lack of universal, established nanofabrication protocols for chemically sensitive organic materials, lack of intermediate scale test line to trial new materials and concepts, and poor of communication between industry and academia.

1345

1346 UK CAPABILITIES

1347 The UK has a large and very active spintronics, ferroelectrics, resistive memory and 1348 photonics community. With a wide set of academic laboratory-based tool kit. Furthermore, 1349 cleanroom facilities and lithography tools are available for small scale laboratory-based 1350 proof of principle devices (e.g. University of Southampton, University of Glasgow, University 1351 of Cambridge, LCN, University of Leeds, University of Manchester, etc.). The same holds 1352 for growth and deposition tools. However, commercial materials manufacturing and design 1353 knowhow for computing is less abundant. Seagate Technology holds the largest share in 1354 the UKs semiconductor and components for electronic applications in the UK, specialising 1355 in magnetic information storage and read and write heads. In general, there is a trend 1356 towards fabless production or outsourcing of production and manufacturing in countries with 1357 cheaper labour costs. However, the UK is well situated to drive the development and 1358 innovation to the industrial prototype level and needs to be ready to capitalise on the 1359 knowhow generated on the way.

1360

1361 UK COMMUNITY RECOMMENDATIONS

1362 It is widely recognised there is a strong UK academic base with great capacity for long term 1363 innovations in the development of new materials and device concepts. However, the high 1364 initial cost associated with CMOS fabrication lines, and the current trend to outsource 1365 production to other countries, has caused a void with respect to relevant industry and supply 1366 chains within the UK. As a consequence, full scale up of new concepts within the UK is 1367 extremely difficult at present, and a paradigm shift in approach is needed.

1368

1369 The UK community must focus on determining and understanding the current societal 1370 challenges. It then needs to find the necessary solutions, bringing together academic 1371 institutions, catapults and industry encompassing scientists, engineers and business 1372 economists. To enable this, the community recommends that a new Centre is established 1373 (either co-located or distributed, but with a clear central hub) to develop 'More-than-Moore' 1374 materials and device concepts focusing on low-loss electronics. This Centre would support 1375 the prioritisation of technical opportunities and identify the tangible benefits, including 1376 addressable markets and revenue streams to build a balanced UK portfolio. It would be able 1377 to appraise critically opportunities for the UK including scenario planning, from an 1378 independent perspective, and identify where targeted investment would unlock 1379 transformative opportunities for UK business.

- 1380
- 1381 It is essential that the effective teams are established to build on the UK academic strengths 1382 and take laboratory curiosities to demonstrator devices and manufacture. This requires

1383 coordination of efforts on a national level as well as collaboration internationally. It is also 1384 essential that the UK invests in equipment to improve materials growth, enabling atom to 1385 atom control, single crystal thin film growth, precise interface control, thickness control, and 1386 the growth of variety of different materials within the same system. This must be 1387 accompanied by the design of new tool sets for atomistic control. The development of 1388 internal telemetry to monitor directly gas species (e.g. ion energies, reactive and inert 1389 species) would also support the scale-up of processing tools from research to manufacture 1390 and enable co-processing of disparate materials in common pilot line tools.

1391

1392 Parallel investments will be required to deliver high spatial and/or temporal resolution 1393 techniques that enable characterisation of materials properties and mapping. This includes 1394 the development of non-destructive characterisation techniques and improvements of the 1395 lithography capabilities across the UK to <10nm. Investment is also need to maintain and 1396 enhance state-of-the facilities such as: low noise voltage and current measurements 1397 (including cryogenic capabilities), magnetometry, electron and magnetotransport apparatus, 1398 atomic scale microscopy, SEM and TEM that avoid chemical damage and degradation 1399 during the measurement, characterisation and imaging including interface sensitive 1400 techniques (SuperSTEM, TEM, SPM, XRD FMR, ARPES (especially for development of 1401 nanostructure capabilities), THz spectroscopy, nanoscale materials tomography and 1402 functional property mapping. There is also a need for vacuum suitcase technologies to 1403 enable samples to be moved between different processing and analytical tools without 1404 contamination and degradation. This needs to be supported by a central equipment and 1405 technology catalogue to capitalise on the UK capabilities that are distributed between 1406 academic and industrial institutions, with easy, transparent access to the community.

1407

1408 For development of new computing architectures, discovery, optimisation and development 1409 of materials is essential, both experimentally and theoretically, through modelling across all 1410 length scales spanning the atomistic, materials, device, architecture and the system level. 1411 An AI approach to materials discovery would identify suitable next generation materials for 1412 non von Neumann computing, especially in the area of heterostructures and 1413 antiferromagnetic materials. A key parameter that need to be considered right at the outset 1414 of the materials discovery process are the abundance, recyclability and ease of sourcing of 1415 the materials, as well as toxicity and life cycle analysis.

1416

1417 Currently, there is a bottle neck in the transition from the research environment to 1418 commercialisation. A significant limitation is the inability to test new technology for 1419 compatibility with large scale production lines. This needs to be addressed. A greater 1420 transfer of knowledge between industry and academic stakeholders is required from the 1421 outset, with more incentives for industry to participate in discovery-led and low TRL 1422 research. Innovation from the academic community must then be efficiently translated and 1423 tested on intermediate level pilot lines, prior to evaluation for manufacture.

- 1424
- 1425 1426
- 1420

1430 CONCLUSIONS, RECOMMENDATIONS AND KEY1431 MESSAGES

1432

There are significant opportunities for the UK to undertake transformative programmes of materials research and development that reduce energy consumption in electronic components and systems. By bringing together academia and industry, it will be possible to meet society's ever-increasing demands for more sophisticated electronics, whilst reducing its overall carbon footprint. This will directly support inward industrial investment, capitalise on the UK's strengths in advanced materials, and enable the UK to be an internationally leading innovator in the device supply chain, providing sovereign capability.

1440

1441 Strategic investments into UK prototyping and pilot plants, combined with high throughput 1442 device testing capabilities, will enable scale-up of devices from research to wafer-scale 1443 fabrication. Centres for growth, fabrication and characterisation are needed to develop new 1444 materials to the point of proof-of-principle and reflect optimal strategies for addressing the 1445 scale-up of the diverse range of materials needed to develop future electronic devices. 1446 Supporting and implementing new material discovery approaches was identified as a key enabler to accelerate material development, e.g. machine learning (AI) approaches, 1447 1448 together with simulation and modelling across different length scales. To achieve tangible 1449 outcomes by 2050, a clear collaborative dialogue between UK-wide academia and industry 1450 needs to be established from the outset of the materials development process, with a focus 1451 on long-term commercial exploitation.

- 1452
- 1453 Key findings include the need for:
- 1454 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.
- 1457 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.
 1459 This would be supported by UK Centres in *Materials Replacement & Recycling, High-frequency Devices*, and *High-throughput Testing*, each underpinned by world-class scientists and engineers, with dedicated specialist technical staffing
- Development of techniques to effectively and efficiently embed new materials into
 high performance, energy efficient devices, including interfacing with the external
 environment.
- 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 accessible materials databases, and simulation and modelling development across the length scales from atoms to devices.
- 1469 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.

- 1473 Investments and incentives for industry to undertake research, and lead and develop
 1474 exploitation strategies.
- 1475 Influencing policy, including setting power consumption targets, supporting the circular economy through end of life considerations, and removing reliance on scarce materials

1478 In summary a crucial pathway towards achieving commercially viable products is a close 1479 collaboration between industry and academia from initial materials discovery through to 1480 materials optimisation, prototype demonstration, scale-up and manufacture. This must be 1481 guided by clear and transparent approaches to prioritise the opportunities which will have 1482 the greatest positive impact on UK industry. Finally, establishing policies that set power 1483 consumption targets, and support the circular economy through to end of life considerations, 1484 will be a critical factor in establishing an environment where the UK takes a leading position 1485 and becomes the place for investment for the future development of low-loss electronics.

1486

Addressing the government's net zero targets necessitates the development of completely
new device concepts and architectures. This requires focused interventions now if solutions
are to be ready to meet the ambitious 2050 targets.

1490

APPENDICES

APPENDIX I: WORKSHOP DETAILS

The workshops werecommissioned by the Henry Royce Institute and delivered by IfM Education and Consultancy Services Limited.

Workshop Methodology

The roadmapping workshop methodology consisted of three parts: design, the workshops, and reporting of the workshop outcomes.

Workshop Design

During the design phase, the following activities took place:

- Discussing and designing in detail the workshop methodology and process. The workshop used the S-Plan framework developed by the IfM over several years ^{152, 153, 154}. The framework has been configured to help universities and research organisations align their research activities with industry needs, supporting decision-making and action;
- > Designing the templates necessary to support the workshop activities;
- > Agree on the detailed workshop agenda;
- > Agree to the desired workshop outputs.

Workshops Description

The roadmapping workshop process brought together around 30 participants from the research community and industry and had the following structure:

- First Session (WS1)
 - To **review** the delegate and IoP survey content submitted so far.
 - o Identify and fill in any gaps.
 - Review and feedback.
- Second Session (WS2)
 - To **discuss** topics that that would be appropriate (relevant, impactful and that experts can meaningfully contribute to)
 - To **select** the priority ideas for topic roadmapping
 - To set up the **working groups** that will be exploring each idea in Workshop 3
- Third Session (WS3)

If M Education and Consultancy Services Roadmapping workshop for Henry Royce Institute for materials for Low Loss electronics

¹⁵² http://www3.eng.cam.ac.uk/research_db/publications/rp108

 ¹⁵³ Phaal, R., Farrukh, C.J.P., Probert, D.R. (2004). "Customizing Roadmapping", *Research Technology Management,* 47 (2), pp. 26–37.
 ¹⁵⁴ Phaal, R., Farrukh, C.J.P., Probert, D.R. (2007). "Strategic Roadmapping: A workshop-based approach for identifying and exploring innovation issues and opportunities", *Engineering Management Journal,* 19 (1), pp. 16–24.

- o To explore selected key priority materials for low loss electronics
- To **scope** each priority idea
- To map the research and development path and required resources
- To describe the expected deployment and required technological and commercial enablers
- Fourth Sessions (WS4)

Additional workshops were held to encourage a wider community to be built and consulted. The format of the session was as per WS3.

- o To explore selected key priority materials for low loss electronics
- To **scope** each priority idea
- To map the research and development path and required resources
- To describe the expected deployment and required technological and commercial enablers

Session 1		
10:00 – 10:05	Welcome from HRI	
10:05 – 10:15	Introductions, objectives and workshop 1 process	
10:20 – 10:30	Discussing the content collected so far (data provenance and review process)	
10:30 – 11:30	Review pre-work and identify gaps for materials and systems (in small groups)	
11:30 – 11:55	Feedback review of group review (5 minutes presentation)	
11:55 – 12:00	Wrap-up and process feedback	
Session 2		
09:00 - 09:10	Introductions, objectives and workshop 2 process	
09:10 – 09:25	Review the short, medium and long term prioritisation results in groups	
09:25 – 09:35	Feedback of review discussion (5 minutes presentation)	
09:35 – 09:55	Set up the working groups for exploring the different topics	
09:55 – 10:00	Wrap-up and process feedback	
Sessions 3 and 4		
13:00 – 13:10	Introductions, objectives and workshop 3process	
13:10 – 14:25	Exploration of selected topics	
14:25 – 14:55	Presentation and review	
14:55 – 15:00	Wrap-up and feedback	

Indicative Workshop Agenda

Dates of Workshops

First Session:30 March 2020,Second Session:3 April 2020,Third Session:3 April 2020,Fourth Sessions:19 – 22 May 2020

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IFM EDUCATION AND CONSULTANCY SERVICES (IFM ECS)

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IfM ECS provides consultancy and executive and professional development – based on the new ideas and approaches developed at the IfM – to help policymakers and manufacturing and technology companies around the world create and capture value more effectively. Our profits are gifted to the University of Cambridge to fund future research.



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