



# Innovations to decarbonize materials industries

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**Abstract** | Materials science has had a key role in lowering CO<sub>2</sub> emissions from the electricity sector through the development of technologies for renewable energy generation and high-performance energy storage. However, outside of the energy sector, there remain considerable greenhouse gas emissions linked to materials production, particularly due to growth in the built environment infrastructure, transportation and chemicals manufacture. This Review focuses on the challenge of reducing the emissions impact of materials production. We assess the potential for decarbonization in the cement, metals (including steel and aluminium) and chemicals manufacturing industries, including the potential to reduce emissions from the inputs to the production and the transformation processes, as well as through the design of desired outputs. We also address underexplored research areas and outline opportunities for the materials community to reduce emissions by leveraging innovations along length scales from atoms to materials markets.

We are at a tipping point in the anthropogenic influence on Earth's climate. Abrupt and irreversible climate changes now seem more likely at lower global average temperatures than previously thought. The 2018 Intergovernmental Panel on Climate Change (IPCC) Special Report suggests that these tipping points could be exceeded between 1 and 2 °C of warming; however, current voluntary pledges maintain a range closer to 3 °C (REF<sup>1</sup>). Even this limit requires urgent action across our society. There must be regulatory activity by governments to support technology development and set a price for carbon emissions, individual actions by citizens to demand policy change, technologists anticipating and innovating around the needs of this new era, and scientists advancing knowledge frontiers.

Materials have long had a role in transitioning between industrial eras. Now, the materials community's most pressing role is to decarbonize society. Advances in materials science will continue to enable carbon-reduced electricity grids, usher in efficient separation technologies and facilitate low-emissions transportation. However, growth in materials consumption also increases greenhouse gas (GHG) emissions — an issue that must be confronted. In this Review, we focus on the role that the materials community has had — and must continue to have — to address the adverse effects of materials production. We identify priority research areas for reducing GHG emissions and outline their limitations. We explore the resulting decarbonization strategies across different length scales. The recognition

that materials properties are governed over a range of length scales is central to materials science and engineering, with the performance at larger scales (such as complex industrial structures) governed by the behaviour at smaller scales (such as atoms). By reviewing approaches to materials innovation towards decarbonization along different length scales, we describe the various materials challenges and highlight areas of cross-disciplinary collaboration needed to address these challenges.

Growing global demand for materials puts ambitious climate targets at risk unless industrial emissions fall. Production facilities are designed to operate for 20 years or more, meaning that, to meet, for example, targets set for 2050, all processes must be low or zero emissions by 2030, or earlier, and be compensated by negative emissions<sup>2</sup>. The materials that generate the most GHGs in their supply chains are cement and concrete, iron and steel, and petrochemicals, which are our focus herein. This prioritization is determined by GHG intensity of production per unit mass and total production volume, which are individual considerations (for example, per unit mass, cement and concrete have lower GHG emissions than other commodity materials, but have vast production volumes) (FIG. 1). We also discuss aluminium, the second most produced metal after iron, because of its growing role in lightweighting.

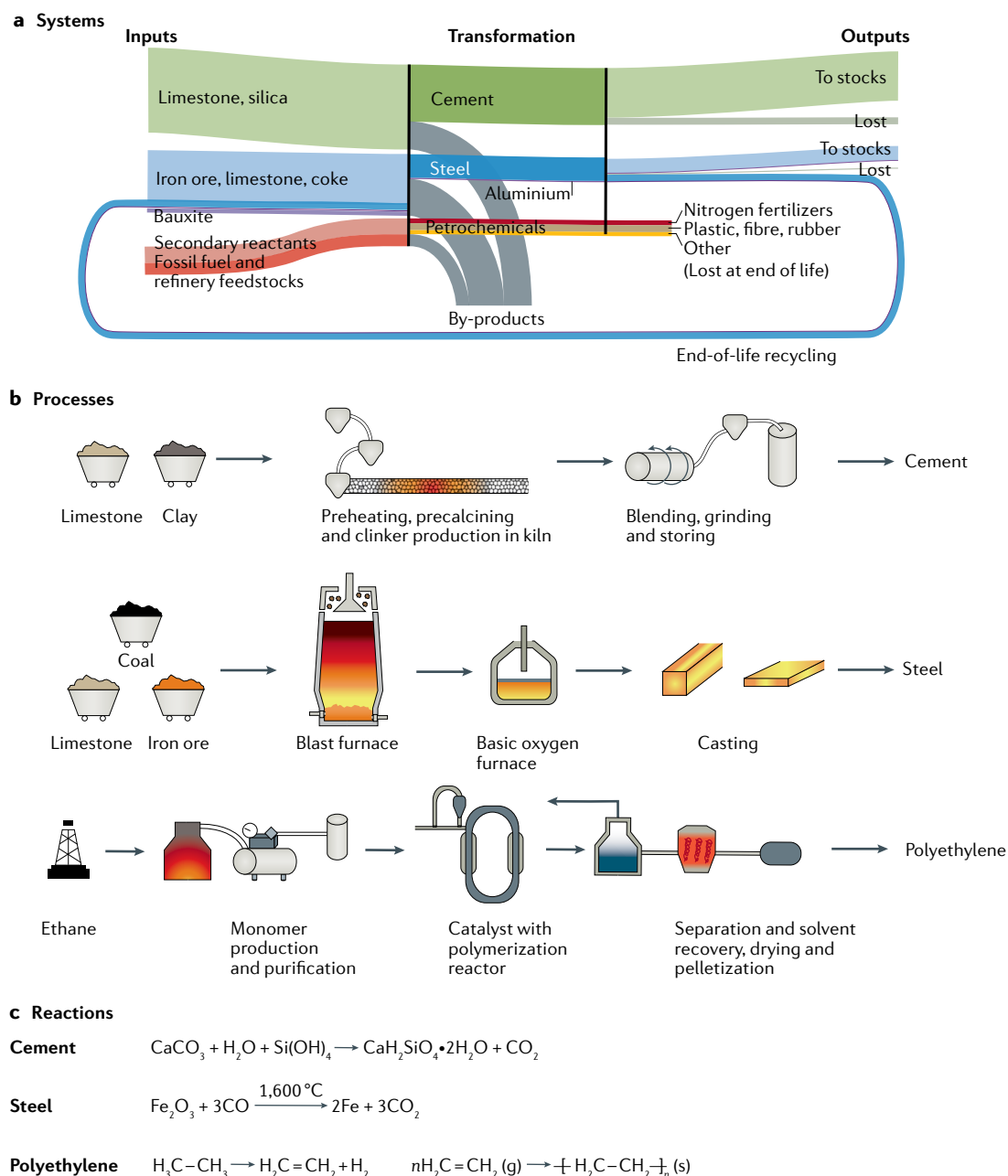
Over the past decade, attention has been paid to the potential for low-CO<sub>2</sub> production technologies across the minerals, metals and petrochemicals industries, with more recent efforts focusing on deep decarbonization

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**Fig. 1 | Length-scale considerations in the decarbonization of cement, steel and petrochemicals.** The decarbonization of cement, steel and petrochemicals requires processes to be linked across different length scales, including system-level mass flows (panel **a**), industrial processes (panel **b**) and key chemical reactions (panel **c**). At the system level (panel **a**), massive quantities of raw materials are extracted and transformed to supply the global demand for cement, metals and petrochemicals (the thickness of the lines is based on production volume in 2017). For petrochemicals, the flows are separated by the largest product categories: fertilizer > plastic, fibre, rubber > and other). The end-of-life recycling loop is relevant only for steel and aluminium; the recycling loop for plastics is too small to be visible. Example industrial production pathways are shown for cement, steel and polyethylene (panel **b**). For cement, the majority of emissions occur during calcination of limestone to clinker (the precursor to cement), which involves decomposition of  $\text{CaCO}_3$  to  $\text{CaO}$  (releasing  $\text{CO}_2$ ) and subsequent reaction with a silicon species in aqueous environments to produce calcium silicate hydrate (panel **c**). For steel, chemical reduction of iron ore in a blast furnace at  $1,600^\circ\text{C}$  releases  $\text{CO}_2$ . Most emissions during petrochemical production are energy related; the reaction shown (panel **c**) is for polyethylene polymerization, which is the dominant plastics flow by mass. Data available in the Supplementary information.

(>50% reduction in emissions)<sup>3</sup>. Industrial emissions reductions became part of mainstream global discourse in the early 2000s<sup>3</sup>. Earlier European efforts, such as those related to the Kyoto Protocol, did not focus on shifts in

industrial technologies to achieve stated 2020 targets<sup>4,5</sup>. Even in the materials community, the focus has been on decarbonization through the energy sector (for example, through energy generation and storage technologies,

such as wind turbines, solar cells, fuel cells and batteries)<sup>6</sup>. More recent studies have documented the decarbonization potential along different pathways, namely, energy efficiency, materials efficiency and recycling, as well as carbon capture and storage<sup>7,8</sup>. Many of these strategies are dependent on the availability of emissions-free electricity<sup>8–11</sup> and rely on industry to use commercially available technologies to reduce industrial emissions in the short term and develop low-carbon technologies in the long term<sup>8,11</sup>. Given the long time frames for adopting

and scaling new technologies, materials efficiency — that is, delivering the same service with less virgin material — provides the principal lever for GHG reduction in the near term. For example, it is estimated that 35–40% of residential life cycle emissions within G7 countries and 50–70% of emissions within China and India could be eliminated in 2050 by leveraging materials efficiency strategies<sup>12</sup>. The most influential measure in these reductions was to increase the intensity of use, pointing to the important role of legislation to drive necessary change. There are barriers to realizing all of these strategies associated with lack of policy incentives, profit-making inertia and carbon-emitting technology lock-in<sup>13</sup>. Technical progress might reduce the barriers to overcome these obstacles by lowering the cost of promising innovations.

This Review overlays the central disciplinary commitment of the materials community to link atomistic and molecular structure to macroscopic properties onto the crucial innovations needed to substantially reduce global emissions. We assert that achieving the necessary advances to accelerate emissions reduction requires materials discoveries to be linked across length scales (FIG. 1): from consideration of the interaction of atoms and molecules through reactions, to the resulting microstructure governed by processing parameters, to the influence of reactor design on chemical transport phenomena and, finally, the systems-level implications of new technology. Advancing this capability will require knowledge about the behaviour of materials at each length scale, coupled with advances in predictive tools to inform that behaviour across the characteristic dimensions. The heterogeneous, large-scale and complex nature of industrial processes is a challenge to realizing the benefits borne by materials production innovations. Through this lens, we highlight areas requiring further investigation and emphasize where priorities should be placed, given temporal constraints and the need for unprecedented scaling.

First, we provide an overview of the sources of emissions in the cement, metals and petrochemical industries, outline broad strategies for mitigating GHG emissions and estimate the mitigation potential of proposed technologies. We then consider the role of the materials community in reducing emissions at the key stages of the production processes.

### Emissions from materials production

GHG emissions from materials production arise (BOX 1) from the burning of fossil fuels to generate the energy required to reach high temperatures<sup>14</sup>, apply pressures or separate constituents<sup>15</sup>. There are also direct GHG emissions from chemical reactions within the production processes (FIG. 1c). Reducing emissions requires changing the fuel mix for energy generation, altering the chemical processes to eliminate direct CO<sub>2</sub> emissions, as well as capturing and sequestering GHG gases that cannot be eliminated. Strategies to decarbonize must also involve measures to reduce materials demand through manufacturing efficiency, using the right amount of material for a given application, extending the lifetime of products and improving materials recovery. The current demand, projected future demand and associated GHG emissions for cement, metals and petrochemicals are given in TABLE 1.

#### Box 1 | Emissions from materials production

Concrete is the most used material in the world after water, far outpacing other building materials<sup>219</sup>. Concrete's functionality, low cost and widespread availability will continue to make it a key building material for the foreseeable future. Although concrete has a low greenhouse gas (GHG) footprint per unit weight relative to other materials considered here, because of the scale of its use, there are opportunities to lower global GHG emissions. Concrete is a mixture of fine and coarse aggregates, water and a hydraulically activated binder, most commonly, ordinary Portland cement (OPC). Extraction of aggregates has a low GHG impact; thus, the OPC in concrete largely determines the GHG footprint<sup>220</sup>.

The energy emissions from OPC are primarily due to the burning of fossil fuels to generate the heat necessary for calcination at 900 °C and sintering at 1,450 °C. The chemical process emissions are due to fugitive releases during the calcination of limestone to clinker (calcined, quenched material that is the reactive constituent in cement), which involves decomposition of CaCO<sub>3</sub> to CaO, thereby, releasing CO<sub>2</sub>. The production of 1 kg of OPC releases ~0.86 kg of CO<sub>2</sub>, equivalent on average, although this can vary by ~30% based on local parameters, such as fuel mix and kiln efficiency<sup>89</sup>. Approximately 45–60% of total emissions from cement production are process emissions, with the remainder largely due to energy generation<sup>220</sup>. Global process emissions of cement production are ~1.5 Gt of CO<sub>2</sub>, representing ~4% of the total global GHG emissions<sup>221,222</sup>. As energy emissions are slightly less than process emissions in cement production, it is estimated that global cement production constitutes ~7–8% of total global GHG emissions.

The most energy-intensive step in primary metal production is the reduction of metal oxides into metal and oxygen, which typically requires a reductant<sup>164</sup>. GHG emissions from steel is dominated by the blast furnace–basic oxygen furnace route, which uses coking coal (used for 70% of steel production) and can accommodate up to 30% scrap<sup>155</sup>. Carbon is typically used to reduce iron ore in a blast furnace at 1,600 °C, yielding liquid iron saturated with carbon and a mixture of CO<sub>2</sub> and CO. Most of the carbon must then be removed to produce useful steel products, generating more CO<sub>2</sub> (REF. 223). For aluminium, nearly 20% of its total production emissions are associated with the production and oxidation of the carbon anodes used during electrolytic extraction (most of the remaining emissions are due to the carbon intensity of the grid that provides the electricity for electrolysis)<sup>224,225</sup>.

The petrochemical industry faces unique challenges along the road to decarbonization, as it uses fossil fuels as both energy and feedstock. This industry emits 1.5 Gt of CO<sub>2</sub> per year globally<sup>24</sup>, amounting to 5% of total global GHG emissions (or 18% of industrial CO<sub>2</sub> emissions). Of this, 0.5 Gt of CO<sub>2</sub> is attributed to the annual extraction of ~500 million tonnes of fossil feedstocks, such as coal, natural gas and crude oil, for chemical production. The rest is from process emissions due to the manufacture of chemical products. Seven large-volume commodity chemicals — ammonia, ethylene, propylene, methanol and BTX aromatics (benzene, toluene, xylene) — underpin the industry and account for 60% of the total process-related emissions<sup>24</sup>. The remaining emissions are due to the tens of thousands of commodity, specialty and consumer chemicals derived from these chemical building blocks.

More than 85% of the emissions from chemicals production are energy related and are emitted when fuels are combusted to provide energy directly or indirectly in the form of steam. Many processes, such as steam methane reforming to produce syngas and H<sub>2</sub>; steam cracking of light alkanes, naphtha and gas oil to produce major olefins<sup>226</sup>; and the processing of aromatics in oil refineries<sup>227</sup>, require high temperatures above 700 °C. Other processes involving gaseous reactants, such as the reaction of CO and H<sub>2</sub> to produce methanol or the reaction of H<sub>2</sub> with air-separated N<sub>2</sub> to form ammonia in the Haber–Bosch process<sup>174</sup>, require high pressures in excess of 200 bar. Several separation and purification processes used in the chemical sector are also energy intensive.

### Future demand for materials

Since 1990, global demand for steel, aluminium, plastics and cement has grown by 2–3.5 times. Demand for these materials will increase further by 2050 (TABLE 1). Demand for infrastructure increases with economic growth in developing nations. Although per capita cement and steel demand have historically levelled off with economic growth, aluminium and petrochemical demand may not because of dominant uses in shorter-lifetime products, such as packaging<sup>16</sup>. However, globally, demand for materials is also changing in response to decarbonization efforts in the building, power and transportation sectors. The material intensity of new energy technologies may be higher than for existing technologies<sup>17</sup>, although estimates indicate that material demand will still be driven by economic growth, rather than an energy transition<sup>18</sup>. Demand for copper, crucial for electrification, may be 30% higher with the necessary energy transition compared with similar estimates using current energy carriers<sup>19</sup>. These increases are not believed to be limiting and correspond to an additional amount equivalent to only 2 years of current production for copper<sup>20</sup>. However, today's supply of minor metals, such as lithium, cobalt and rare earth elements, which are vital to clean energy technologies, is vulnerable to disruption, and these resources must be secured responsibly<sup>21</sup>.

Steel and cement are also key materials for renewable energy infrastructure and carbon capture technology. Wind turbines, for example, rely on steel for most components and cement for the foundation<sup>22</sup>. Peak steel demand for renewable energy infrastructure is likely to coincide with the peak in wind energy capacity, as the steel in turbines is highly recyclable and can be used for next-generation turbines after the 20–30-year lifetime<sup>22</sup>. There are also opportunities for materials substitution: high-strength steel can reduce cement demand and decrease emissions<sup>23</sup>, and, thus, could shift steel production in decarbonization scenarios. Furthermore, a shift from steel to aluminium (and polymer-based composites) in the transportation sector could be driven by the desire to increase fuel economy through lightweighting.

Although global petrochemical consumption is difficult to track, it is increasing in developing countries and has levelled off in wealthy developed nations<sup>24</sup>.

### Strategies for mitigating GHG emissions

Roadmaps for these industries describe how new technologies can be implemented to meet future emissions targets. The goals vary by industry but aim to be consistent with a 50% chance of limiting the average global temperature increase to 2°C (2DS; within the framework of the modelling and analysis in the International Energy Agency's (IEA's) Energy Technology Perspectives project)<sup>21</sup>, which are then mapped to target total emissions reductions from current or past levels by 2050.

The roadmap for the cement industry evaluated four main strategies towards limiting the rise in global temperatures to <2°C above pre-industrial levels<sup>25</sup>. Meeting the GHG reduction targets in this scenario would require the industry to decrease its global direct CO<sub>2</sub> emissions by 24% from current levels, which is equivalent to cumulative reductions of 7.7 Gt, by 2050 (including expected increases in demand). Technological and economic feasibility assessments determined that 15% of these reductions would come from improvements in thermal energy efficiency and the use of alternative fuels in cement plants and kilns, and 37% from a decrease in the clinker proportion in cements. The remaining 48% of reductions would need to come from carbon capture in cement plants.

The steel industry can exploit various strategies to decrease emissions in line with 2DS<sup>10</sup>. There are opportunities to increase the energy efficiency of steelmaking through approaches such as coke dry quenching, recovery of waste heat and gases, and continuous casting<sup>26</sup>. Although the steel industry has greatly reduced its energy use since the 1960s, and existing efficiency and waste-heat-recovery technologies can be leveraged to further decrease the energy intensity of steel production by an estimated 15–20%, these reductions are insufficient to achieve 2DS<sup>11</sup>. Implementation of material efficiency strategies would reduce demand by

Table 1 | Global CO<sub>2</sub> emissions associated with the production of different materials

Material	Global CO <sub>2</sub> emissions associated with production in 2000 (Mt CO <sub>2</sub> per year) <sup>210</sup>	Global CO <sub>2</sub> emissions associated with production in 2017 (Mt CO <sub>2</sub> per year)	Current global average specific CO <sub>2</sub> intensity (kg CO <sub>2</sub> t <sup>-1</sup> material)	Global production in 2017 (Mt per year)	Business-as-usual demand in 2050 (Mt per year)
Cement	1,588	2,200 (direct) <sup>25</sup>	860 (OPC with additional processing) <sup>89</sup> ; 540 (direct) <sup>25</sup>	4,050 (REF. <sup>211</sup> )	4,682 (REF. <sup>25</sup> )
Steel and iron	1,319	3,700 (2,600 direct) <sup>27</sup>	2,000 (1,400 direct) <sup>27</sup>	1,736 (total crude steel) <sup>212</sup>	2,100 (final end-use); 2,535 (crude steel) <sup>27</sup>
Aluminium	324	1,000 (REF. <sup>213</sup> )	14,400 (primary) <sup>213</sup>	64.3 (primary) <sup>a</sup> ; 92 (plus secondary) <sup>213</sup>	110 (primary) <sup>214</sup> ; 175 (plus secondary) <sup>32</sup>
Copper	47 (REF. <sup>215</sup> )	70 (average CO <sub>2</sub> intensity multiplied by production in 2017)	3,500 (REF. <sup>216</sup> )	20 (REF. <sup>217</sup> )	50 (REF. <sup>218</sup> )
Petrochemicals	2,013	1,500 (REF. <sup>24</sup> )	1,700 (REF. <sup>24</sup> )	960 (REF. <sup>24</sup> )	1,500 (REF. <sup>24</sup> )

Emissions from production include indirect emissions, unless otherwise noted. The specific CO<sub>2</sub> intensity for the production of each material is the current global average, although a range exists, depending on the scope of indirect emissions accounting. OPC, ordinary Portland cement. <sup>a</sup>Data from the International Aluminium Institute.

20% and contribute 40% of the total required emissions reductions. To achieve 2DS, the IEA estimates<sup>27</sup> that emissions from the steel industry must fall by  $\geq 50\%$  by 2050, requiring CO<sub>2</sub> emissions intensity to decrease to 600 kg of CO<sub>2</sub> per tonne of steel. To meet this target, blast furnace production would need to decline from 70% to 30% and scrap-based electric furnace production double, while innovative technologies that incorporate carbon capture and use hydrogen would need to grow to account for nearly 40% of steelmaking. Promising mitigation measures include production using an electric arc furnace with decarbonized electricity and hydrogen direct reduced iron, using bioenergy and electrolysis<sup>11</sup>.

In the petrochemical industry, meeting targets for 2DS requires a 30–45% decrease in global GHG emissions from current levels<sup>24</sup>. Several strategies could effect this transition; assessments suggest that process intensification and energy efficiency improvements can make up to 25% of this target. These improvements include better heat integration<sup>28</sup> to meet the endothermic demand of some processes with the exothermicity inherent in others, membrane separation<sup>29</sup> to replace inefficient cryogenic separation, innovative chemical looping<sup>30</sup> systems that use redox catalysis to potentially increase selectivity, eliminating exergy loss by coupling process heat needs and enabling in situ product separation. Another 25% reduction depends on coal being replaced with natural gas. Plastics recycling and alternative feedstocks can contribute an additional 15% reduction, but a substantial 35% share needs carbon capture and utilization within the chemical industry.

In considering the role of materials science in decarbonizing materials production, we compare and prioritize the array of reported potential technologies (FIG. 2). The technologies are compared by specific decarbonization potential (that is, reduction in CO<sub>2</sub> emitted per tonne of material produced, relative to current specific CO<sub>2</sub> intensity), implementation potential (that is, maximum market share in 2050) and technical readiness (left parts of FIG. 2). An overall mitigation target in 2050 (the blue line in the left parts of FIG. 2) is calculated for each industry as the difference between CO<sub>2</sub> emissions in the business-as-usual case (in which current average CO<sub>2</sub> intensity stays constant alongside projected 2050 demand in TABLE 1) and target emissions in 2050. Here, the target by 2050 is to reach half of the level of emissions in 2000 (TABLE 1), as originally stated by the IPCC<sup>31</sup> (note that this target may vary from the 2DS emissions targets in the roadmaps described above). Individual technologies group by high mitigation potential but limited potential market share or by high potential market share but low mitigation potential. However, all fall below the total industry mitigation target; therefore, to meet the target, a range of technologies must be implemented in concert. The individual technologies can be assembled considering the specific CO<sub>2</sub> mitigation potential and the relevant material volume to explore how the total 2050 mitigation target could be met (right parts of FIG. 2).

Rapid decarbonization is constrained by factors that include the availability of alternative input materials,

market penetration of decarbonized electricity, the presence of incumbent manufacturing infrastructure, and the rate of scale-up and deployment of new technologies. For example,  $>70\%$  of electricity must come from renewable energy sources in 2050 to hold global temperature rise within 2 °C up to 2100 (REF.<sup>32</sup>). Renewable sources currently provide  $\sim 15\%$  of total demand; the significance of the required change cannot be underestimated. The most promising materials innovations must be identified and pursued considering these constraints. The portfolios of technologies presented in the right parts of FIG. 2 are not a singular answer but a starting point to illustrate potential impact and barriers to implementation. Specific constraints are discussed in subsequent sections, but a few concepts apply generally. It is well documented that new technologies require decades to reach widespread implementation and tend to scale at a rate of no more than 1% per year<sup>33</sup>; 2050 was chosen as a snapshot in time, but emissions must continue to decrease beyond 2050. The IEA projects limited potential for carbon capture and storage by 2050: for cement, 550 Mt of CO<sub>2</sub> per year at 25% of ordinary Portland cement (OPC) plants; for petrochemicals, 160 Mt of CO<sub>2</sub> per year alongside the steam reforming of natural gas; and, for metals, 200 Mt of CO<sub>2</sub> per year from blast furnace–basic oxygen furnace plants. Technologies at early stages of development should not be expected to contribute substantially to near-term goals but will have an important role in the latter half of the century.

Even with an ambitious scenario envisioning vast changes in industrial practice, mitigation targets are at great risk. Closing this gap requires further scrutiny, technical insight and creativity. We urge the materials community to take a leading role engaging in these realities and we review the opportunities for materials scientists guided by this context.

### Role of materials science and engineering

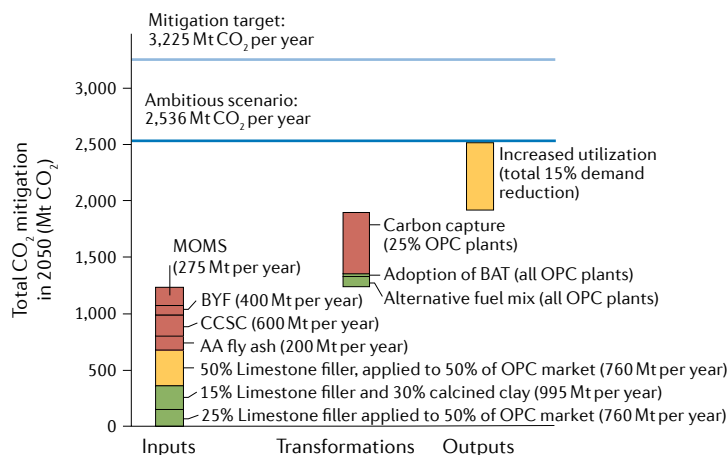
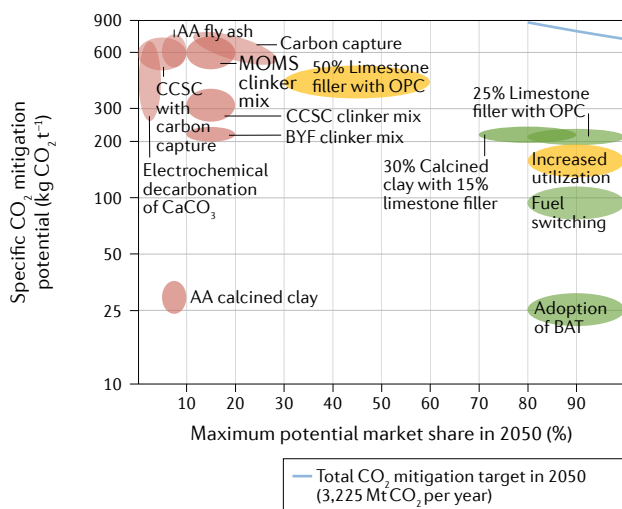
Materials production involves the transformation of raw feedstock and energy (inputs) into outputs that provide services desired from the material. Reducing emissions within the inputs, transformations and outputs requires technical challenges to be solved across length scales from the atomic level up to the industrial-scale deployment of low-carbon technologies. These solutions must comprehend both the continuous chemical processing of materials and the discrete physicochemical link between structure and properties.

### Inputs to the production process

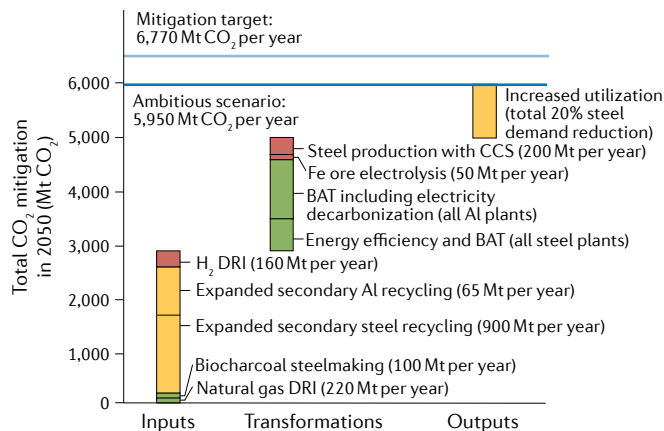
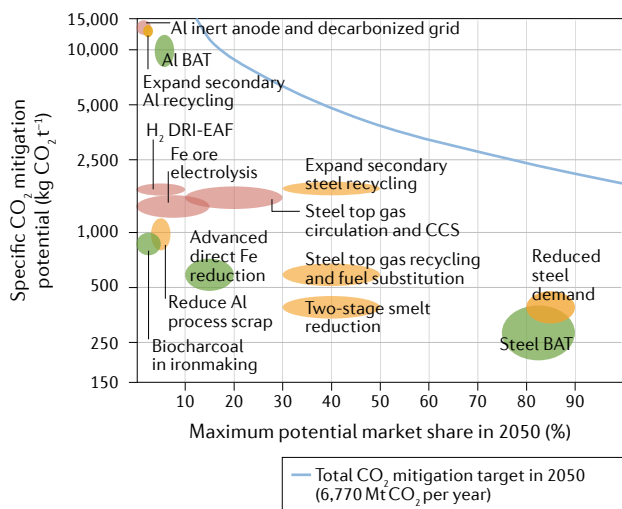
Key materials opportunities to reduce emissions for the inputs to a production process involve the use of alternative feedstocks (including increased use of secondary material) or use of CO<sub>2</sub> as a feedstock. This section covers opportunities that use raw materials with lower embodied CO<sub>2</sub> or that yield lower emissions during processing. We begin by describing the use of secondary raw material, because increased secondary production of steel, aluminium and plastics offers considerable near-term opportunities, whereas broader alternative feedstocks might have a notable role in the petrochemical and cement industries in the medium to long term.



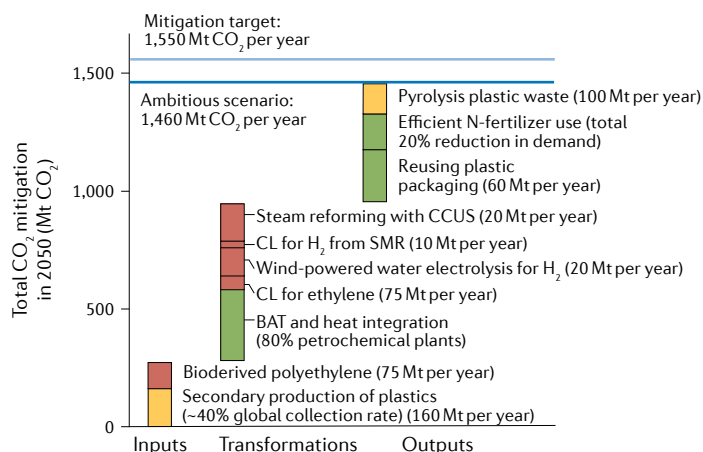
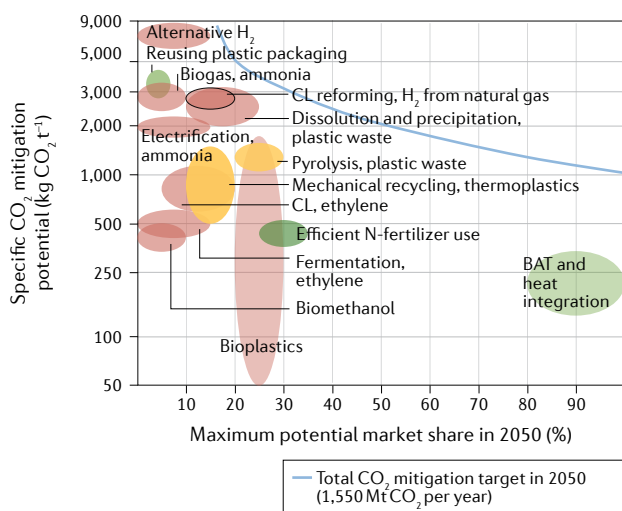
## a Cement



## b Metals



## c Petrochemicals



**Use of secondary material.** Recycling is the process of separating sufficiently pure feedstocks from waste streams for use as an input material with a potentially reduced GHG emissions impact (if the impact to reprocess does not exceed that of virgin material). The degree

of separation required varies based on the recycling process and the degree of mixing of the macroscopic components, as well as the composition of the materials themselves (such as cement from aggregate, alloying elements within a metal or polymer blends).

◀ **Fig. 2 | Estimating the decarbonization potential of materials production technologies.** The left part of each panel shows the potential for CO<sub>2</sub> mitigation by strategy and their potential market share in 2050 for cement (panel **a**), steel and aluminium (metals, panel **b**), and petrochemicals (panel **c**). Estimates for specific CO<sub>2</sub> mitigation (details in the Supplementary information) are plotted on a logarithmic scale. The potential market shares in 2050 are plotted as the maximum portion of the industry that the strategy could be applied to. The main considerations determining potential market share are raw material availability, the portion of industry the strategy applies to and technology readiness. The colour of the bubbles is a qualitative categorization of the technical readiness. Green indicates that the strategy is well understood and has been demonstrated in practice, but non-technical barriers (cost and consumer participation) may hinder further implementation. Orange indicates that the concept is well proven and likely scalable, but further technical study is required to support widespread implementation. Red indicates that the strategy is relatively new and further investigation is required to determine industrial feasibility or that the technology requires extensive changes to current practice (such as new equipment and infrastructure) that require a timeline beyond 2050. The blue line denotes a total industry mitigation target in 2050, calculated as the difference between CO<sub>2</sub> emissions in the business-as-usual case (current average CO<sub>2</sub> intensity stays constant alongside projected 2050 demand in TABLE 1) and target emissions in 2050 (half of 2000-level emissions). The right part of each panel shows example scenarios that aim to meet the 2050 climate targets for the different industries, constructed by assembling the individual technologies shown in the left parts of each panel. The values in the parentheses are the quantities of material in 2050 that a technology might be applied to. The scenarios are ambitious but realistic, accounting for time to develop early-stage demonstrations and the infrastructure likely available for renewable energy, carbon capture and hydrogen production in 2050 as determined by the International Energy Agency and other literature (details in the Supplementary information). AA, alkali activated; BAT, best available technology; BYF, belite-ye'elinite-ferrite; CCS, carbon capture and storage; CCSC, carbonatable calcium silicate clinkers; CCUS, carbon capture, utilization and storage; CL, chemical looping; DRI, direct reduced iron; EAF, electric arc furnace; MOMS, magnesium oxides derived from magnesium silicates; OPC, ordinary Portland cement; SMR, steam methane reforming.

For cement (and concrete in its end-product form), the crystalline network of covalent bonds that forms during the hardening reaction cannot be broken down chemically (except by slow weathering and carbonation); therefore, cement cannot be traditionally 'recycled' but concrete can be ground for use as an aggregate in road bases, construction fill, soil stabilization, asphalt concrete and Portland cement concrete. The performance of recycled aggregate may be inferior to that of natural aggregate because of residual adhered mortar, potentially requiring additional processing or cement to maintain performance (thereby, limiting the benefit)<sup>34,35</sup>. A portion of cement may also remain unhydrated, and this material could be recovered for use as clinker (this is not current practice).

If combusted, the mass of plastic discarded annually (260 Mt) would correspond to 2% of global CO<sub>2</sub> emissions. Alternative end-of-life treatments to incineration typically result in emissions savings, but the magnitude depends on the intensity of processing and the suitability of the recyclate to displace primary production<sup>36</sup>. Polymers (particularly thermoplastics) can be recycled mechanically by breaking the secondary bonds between the covalent chains during melting, allowing new shapes to be cast without changing the chemistry of the polymer chains. Only a few plastic types, most notably polyethylene terephthalate (PET)<sup>37</sup>, have mature mechanical recycling technology in place, yet, the recycling rates are low (<20%). Chemical recycling<sup>38</sup> of polymers breaks the covalent bonds in thermoplastics and thermosets to recover the constituent monomers; examples include

chemolysis<sup>39–41</sup> of PET to produce ethylene glycol and a terephthalate; pyrolysis<sup>42</sup> of polyolefins to produce naphtha<sup>43</sup>, diesel<sup>44</sup> and gasoline-range<sup>45</sup> hydrocarbons; thermal depolymerization of polystyrene<sup>46</sup> to yield light aromatics; and alkaline hydrolysis of common polycarbonates to give bisphenol A<sup>47</sup>. Approaches have been developed to increase the degradability of thermosets through the insertion of cleavable backbone bonds that remain amenable to traditional curing methods<sup>48</sup>. However, the energy required to break bonds and separate oligomer mixtures may cancel any environmental benefits of chemical recycling<sup>49</sup>. Dissolution and precipitation processes, which do not break or reform bonds, can be used to separate polymer mixtures, as well as remove colourants and additives through filtration to produce higher-purity resins, and may offer a less energy-intensive approach if solvents with high dissolution capacity and simple recovery routes can be developed<sup>50</sup>.

Biological recycling uses biodegradable enzymes to catalyse polymeric breakdown. The type of backbone bond is a major determinant of biodegradability: non-hydrolysable C–C bonds lead to recalcitrant polymers such as polyethylene and polypropylene, whereas PET features hydrolysable ester linkages that permit enzymatic degradation. Certain enzymes such as cutinases<sup>52,53</sup> hydrolyse PET to produce ethylene glycol and terephthalic acid, which can be repolymerized to bottle-grade PET<sup>53</sup>. PET hydrolase from the bacterium *Ideonella sakaiensis* completely degrades and assimilates PET<sup>54</sup> to form CO<sub>2</sub> and H<sub>2</sub>O. Being biochemically inert, polyethylene requires abiotic stimuli<sup>55,56</sup>, such as mechanical forces, ultraviolet irradiation or oxidizing agents, to break down the long polymer chains into short-chain hydrocarbons suitable for enzymatic biodegradation. Although some microbial agents can depolymerize polystyrene<sup>57</sup>, the enzymes are not well understood. Biodegradability studies on polypropylene and polyvinyl chloride, two of the major large-volume polymers, are also lacking. Additionally, thermally stable enzymes that can act on crystalline portions of polymer matrices are needed<sup>51,54,56</sup>. Not much is known about the GHG impact of industrial biorecycling, but as the temperature of enzymatic activity (50–70 °C)<sup>54</sup> is much lower than that in chemical recycling, GHG emissions could be lowered if enzyme production is not energy intensive. Advances in predicting the 3D structures of proteins may accelerate the development of effective enzymes<sup>58</sup>.

Metals can be melted, refined and recast with no degradation in bond strength, but losses inevitably occur through contamination with elements that are difficult to refine<sup>59</sup> (FIG. 3). Increasing use of end-of-life scrap is a dominant, accessible strategy to decarbonize metal production (FIG. 2b, left). Owing to the expanding scrap supply, secondary production may account for ≥50%<sup>60</sup> of the steel and 35%<sup>61</sup> of the aluminium global markets by 2050 (FIG. 3b). New technologies and practices are needed to support this transition<sup>62</sup>. However, technologies to decarbonize primary production will have the most impact before secondary production dominates; thus, the timing of these investments must be executed carefully. Here, we discuss current practice in steel and

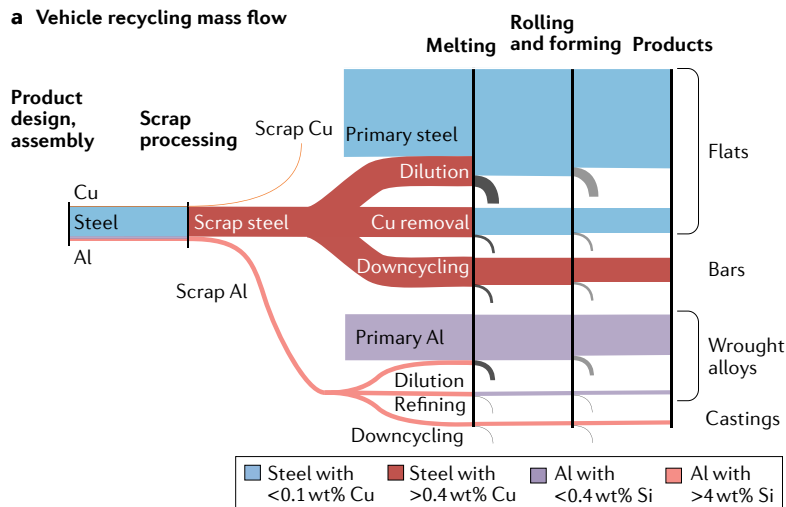
aluminium recycling, and technical interventions that could reduce GHG emissions.

Final products are inevitably a mix of materials. For example, in a vehicle, electrical copper wiring and motors are affixed within a steel frame, and multiple aluminium alloys are used for the engine block (cast alloys, which can be high in silicon, iron and copper) and the body (wrought alloys, with a lower concentration of alloying elements) (FIG. 3a). Vehicles, a main input into the steel and aluminium recycling streams, are shredded upon disposal to physically liberate the different materials. The widely used ‘hammer shredding’ technique entwines ductile copper wiring onto steel pieces, such that subsequent magnetic separation is only partially effective<sup>63</sup>. Aluminium can be separated from steel by density or eddy current separation, but advanced sensing is required to then sort this stream into distinct alloys<sup>64</sup>. Processes to refine key contaminants, including copper from a steel melt<sup>65</sup>, or silicon and iron from an aluminium melt<sup>66</sup>, are not available commercially. The main refining technique in steel recycling is oxidation by slagging, but copper is not preferentially oxidized over iron, and, thus, remains in the melt. Aluminium is

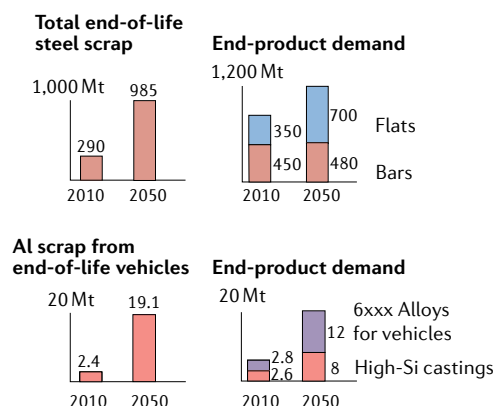
simply remelted, acting as a sink for other elements present<sup>67</sup>. Contaminants within the melt can be detrimental to the final product properties. Liquid copper embrittles steel grain boundaries during subsequent hot rolling (known as surface hot shortness) and deteriorates surface properties<sup>68</sup>. There are complex physical metallurgy challenges encountered during aluminium recycling<sup>69</sup>. Iron and silicon are particularly pervasive and decrease the formability and mechanical properties of aluminium, including ductility and fatigue resistance. Thus, strict tolerances for contaminants are set. Only long steel products (bars and sections typically used in construction and infrastructure) can tolerate the concentration of copper typical in end-of-life scrap. Thus, steel from a shredded vehicle cannot be recycled into a high-quality sheet for a new vehicle, while unsegregated aluminium can typically be cast but not recycled to wrought alloys (FIG. 3a).

Managing contamination early in the supply chain is the simplest and lowest-energy solution<sup>70</sup>. Ideally, products would be designed for easy disassembly, such as detachable copper wiring harnesses from vehicles, to prevent issues downstream<sup>71</sup>. When recycling a mixture

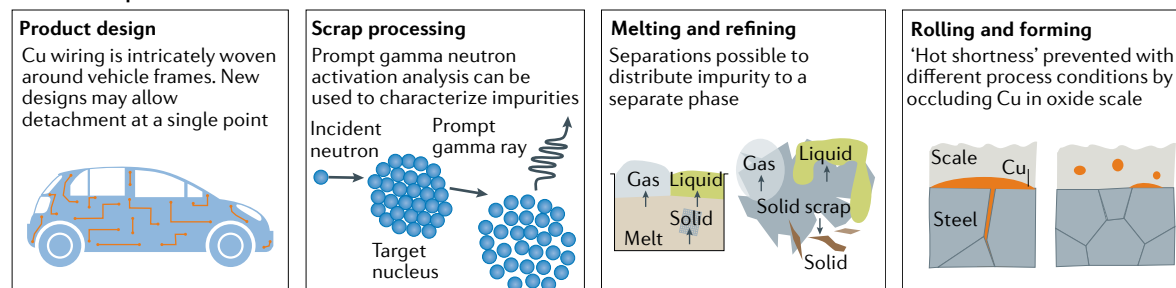
#### a Vehicle recycling mass flow



#### b Supply and demand dynamics



#### c Technical practice



**Fig. 3 | Mass flow dynamics and technical practice behind metal recycling from end-of-life vehicles.** The simplified Sankey diagram (panel a) shows the mass flow of metal from a discarded vehicle. Three distinct recycling scenarios are shown for scrap steel and aluminium, as illustrated by the flow splitting into three possible pathways: dilution, high-value recycling as enabled by copper removal (for steel) or refining (for aluminium) and downcycling. These pathways are dictated by compositional requirements. Typical scrap steel contains 0.4 wt% copper<sup>75</sup>, while mixed wrought and cast aluminium alloys contain 4 wt% silicon<sup>189</sup>. Tolerances for high-quality products

(flat sheets and coils for steel, or wrought alloys for aluminium) are 0.1 wt% copper and 0.4 wt% silicon, respectively. Scrap can be directly downcycled to tolerant applications (bars and castings). Demand for bars and castings has historically been greater than the scrap supply (panel b; data from REFS<sup>81,83</sup>). However, the scrap supply will expand, while demand for impurity-tolerant products will plateau. Managing impurities by dilution requires excessive primary material (3:1 primary to scrap ratio for steel and 10:1 for aluminium). To enable closed-loop recycling, technical practice can be improved, from product design through to thermomechanical processing (panel c).



of metals, inefficiencies arise from the inability to quantitatively characterize solid scrap. Sensing and sorting aluminium by alloy (primarily cast and wrought classes) would enable source separation. Current sensing methods may use X-ray detection or spectroscopy<sup>64</sup>. Laser-induced breakdown spectroscopy is promising, owing to its multi-elemental high throughput with high accuracy<sup>72</sup> and ability to distinguish between wrought and cast aluminium. For external impurities, such as copper wiring dispersed in steel scrap, liberation can be improved by shredding the material to a higher density or using a trommel screen<sup>73</sup>. Such techniques can greatly decrease copper content to facilitate the production of some high-value flat steel products. However, in the current market, steel scrap is typically graded by eye; therefore, incremental changes in concentration may not be detected and financially compensated. To measure the bulk composition of a scrap stream, an excitation source with a high penetration depth is needed. Prompt gamma neutron activation analysis is well established in the mining industry and its application is expanding to scrap metal<sup>64</sup>. A potentially lower-cost alternative is to use cameras and artificial intelligence to monitor and estimate the impurity content of an incoming scrap stream<sup>74</sup>. Further collaboration between materials physicists, computer scientists and scrap processors will enable practical, fast and low-cost characterization to incentivize rigorous impurity handling.

There is scope to develop new separation processes. Over decades, refining processes have been developed to manage impurities in ore. Recycling employs a subset of these processes and, thus, has not been fully adapted to treat the variable mix of elements in today's alloys and products. In principle, separation routes can be devised by exploiting a difference in physical or chemical properties, although industrial viability is critical. A framework to systematically evaluate the range of separation routes and estimate specific energy and material consumption from governing thermodynamic and kinetic relationships can reveal promising opportunities<sup>75</sup>. For example, melting copper away from steel scrap during preheating may obviate this contaminant (with the technical challenge of controlling process conditions to promote non-wetting behaviour)<sup>76</sup>.

There is also an opportunity to accommodate impurities with enhanced understanding of composition–processing–property relationships. Surface hot shortness caused by copper and tin in steel can be minimized by adjusting conditions during hot rolling (temperature, gas composition and oxidation time), to control the diffusion of copper and oxidation of iron<sup>77,78</sup> (FIG. 3c). Furthermore, the addition of other elements can change the behaviour of copper. For example, nickel increases the solubility of copper in austenite<sup>79</sup>, whereas silicon can cause copper to occlude in the oxide scale<sup>80</sup> (FIG. 3c). Overall, the tolerance limits set today are empirical and cautious, but further investigation will support decisions to adjust composition and process variables in real time to accommodate a wider range of scrap inputs.

The development of practical, targeted technical solutions must also be guided by an understanding of the larger recycling system. The current practice of 'downcycling' can be economically and environmentally

viable, providing there is demand that would have otherwise been met by primary production. The point at which new technologies must be introduced to avoid the accumulation of unrecyclable scrap can be difficult to identify but can be estimated by analysing the mass flow of metals and contaminants at a regional or global level. Such analyses (for example, FIG. 3b) show that, owing to the growing scrap supply, alongside plateauing demand for impurity-tolerant 'sinks', the presence of contaminating elements will likely limit the amount of steel scrap that can be recycled globally by 2050 (REF.<sup>81</sup>) (and already constrains domestic recycling within the United States)<sup>82</sup> and already limits aluminium recycling regionally<sup>83,84</sup>. Process fundamentals, technical practice and the use of scrap at a systems level are linked, and these dynamics must be investigated<sup>85,86</sup>. To fully utilize scrap, research to characterize thermodynamic and kinetic phenomena to facilitate separation or establish key composition–processing–property relationships should be guided by needs and opportunities identified at the million-tonne scale.

**Alternative raw materials.** Use of alternative raw materials in cement and petrochemicals has a high impact potential (FIG. 2a, left). Alternative feedstock use in steel smelting includes biomass carbon (charcoal) as the fuel and reducing agent, but projected use is limited to 5% of global production, owing to concerns about land use<sup>27</sup>, and, therefore, we do not explore this alternative further.

OPC is the most common cementitious binder because the raw materials are widely available, it can be reliably manufactured to exact specifications and there is extensive empirical data on the performance of concrete made with OPC. However, there is renewed interest in alternatives to OPC that have lower production emissions<sup>87</sup>. Alternative clinkers and cements contain various active mineral phases and, thus, have different GHG emission profiles<sup>88</sup>. The chemistries of most cements derive from the oxides lime (CaO), silica (SiO<sub>2</sub>) and alumina (Al<sub>2</sub>O<sub>3</sub>)<sup>89</sup>. The potential implementation of these alternative clinkers to displace OPC in 2050 is investigated in FIG. 2a. We distinguish alternative feedstocks based on four criteria. First, whether the feedstock would provide a complete substitute for precursors to OPC; examples include magnesium oxides (MOMS) or belite-ye'elimite-ferrite (BYF). Second, whether the feedstock would partially replace or supplement OPC within a blended system; this strategy is more viable in the near term because of its similarity to current practice, such as the use of calcined clay<sup>90,91</sup>. Third, the role of the alternative material in the binding reaction, namely, whether it is pozzolanic (broadly, an aluminosilicate that reacts with calcium hydroxide to form calcium aluminosilicate hydrate products, abbreviated as C-(A)-S-H, with variable aluminium content)<sup>92</sup>, involved in alkali activation (such as alkali-activated fly ash or calcined clay, yielding sodium aluminosilicate gel)<sup>93</sup> or added as a filler (such as limestone). Fourth, whether the curing reaction is through carbonation (that is, reacts with CO<sub>2</sub>, such as carbonatable calcium silicate clinker (CCSC))<sup>94</sup> or hydration<sup>95</sup>. The alternative binders may be from natural (that is, calcined clays) or waste sources<sup>96</sup>.

The substitution of any of these binders for OPC in concrete is not straightforward. Final concrete properties are governed by the microstructure and morphology of the binder reaction products, as well as the integration with fine and coarse aggregates, water and other additives<sup>97</sup>. Concrete mixtures are designed to meet myriad performance targets, including early (on the order of days) and late (on the order of months) compressive strength, durability, stiffness, constructability and finish targets. Use of alternative cementitious binders will modify performance in many of these categories. The challenge for the materials community is to better understand the role of alternative feedstocks in a binder and to then expand the database of performance information for these materials to accelerate their adoption, given local availability for these materials<sup>98</sup>.

The most fundamental considerations for determining the final properties are the available chemical species, the ratio between water and solids, and the pH of the solution. The available chemical species determine the resulting inorganic polymer binder network. C-(A)-S-H, for example, exhibits a layered structure, with alternating layers of Ca–O and silicate chains, and with water and Ca<sup>2+</sup> ions (as well as other ions) in the interlayer space<sup>99</sup>. Aluminium ions are also commonly incorporated and can occupy bridging sites that link dimers of silicate tetrahedra to increase the average chain length of C-(A)-S-H (REFS<sup>100–102</sup>). Predictive tools that leverage solution thermodynamics can be used to predict phase formation based on Gibbs energy minimization by accounting for the dissolution of solid reactants and precipitation of products<sup>103</sup>. Elucidating the specific chemical arrangement of that product phase is also important to determine the role and ratio of each of the available species in the final network. As an example, first-principles calculations predicted the incorporation of aluminium in C-(A)-S-H, with bridging Al(IV) species behaving as network formers<sup>104–106</sup>. Kinetic considerations are similarly important, as they influence the achievement of many of the performance targets. Incorporation of alternative feedstocks typically slows reaction kinetics<sup>97</sup>. At a macroscale, alternative feedstocks also influence the rheological properties of the cement, affecting the viscosity of the paste and surface finish, the required pumping pressure and the setting times<sup>107</sup>.

Increasing the proportion of filler can result in massive emissions savings. The proportion of limestone filler is typically 10%, but increasing the proportion up to 50% is a promising strategy to halve the CO<sub>2</sub> intensity<sup>89</sup>. The finely ground filler also has physical effects, such as providing additional surface area and increasing the number of heterogeneous nucleation sites for hydrate precipitation<sup>108</sup>. The evolution of the microstructure affects the resulting porosity, including the shape and connectivity of the pores<sup>109</sup>. This connectivity dictates the mechanical behaviour of the hardened paste and system durability, which is related to its resistance to acids, sulfates and carbonation (depending on the system). Computational simulations of the pore structure and chemistry have helped elucidate the concentration dependence of diffusion coefficients and chloride

binding<sup>110</sup>. Comprehensive simulation strategies that can capture the breadth of possible microstructural and chemical possibilities hold promise towards the design of improved concretes from both technical and sustainability perspectives<sup>111</sup>.

Finally, system-level implications are informed by whether a feedstock can be used in existing cement kilns, and the supply chains for these systems will vary depending on which materials are being used<sup>88</sup>. Given the large volumes required and the local nature of cement production, reserves of potential feedstocks must be localized and plentiful. The degree of market penetration of the alternative clinkers in the left part of FIG. 2a has been projected while accounting for the reported availability of these materials<sup>89</sup>. For example, calcined clays are of particular interest because of the sheer size of the reserves<sup>90</sup>, and, in many regions, supplies of commonly used blast furnace slag and fly ash are decreasing<sup>112,113</sup>.

The petrochemical industry can be decoupled from its dependence on fossil fuel feedstock if alternative and industrially viable renewable sources of carbon, hydrogen, nitrogen and oxygen atoms can be found; these can be bio-based or obtained from water, air and captured CO<sub>2</sub>. There are two parallel research directions relating to bioderived feedstocks: using bioderived renewable feedstocks to make conventional chemicals and monomers, and designing chemistries for new bio-based polymers with improved properties. Thermoset and thermoplastic polymers account for ~40 wt% of the production volume of petrochemicals, with fertilizers accounting for another ~30 wt%. Owing to the large volume and the materials focus herein, we concentrate on alternative feedstocks towards polymer end products.

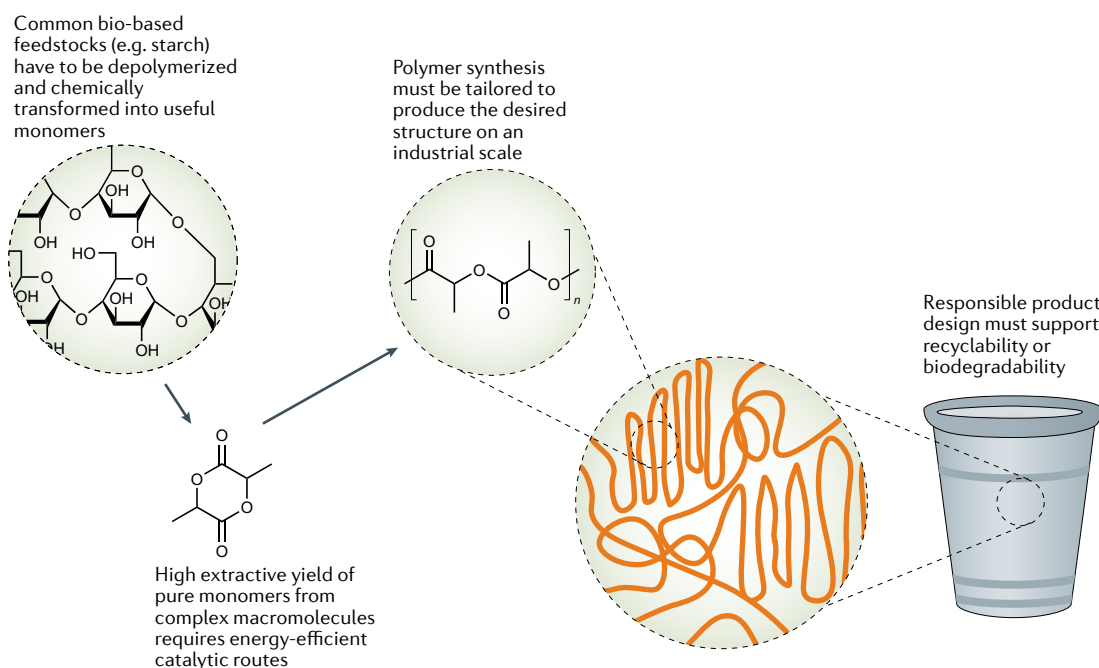
At the laboratory scale, monomers for conventional polymers can be synthesized from renewable bioderived<sup>114</sup> and biosynthesized C<sub>2</sub>–C<sub>6</sub> platform chemicals<sup>115,116</sup>. These monomers include ethylene from the catalytic dehydration of bioethanol sourced from algae and biomass<sup>117</sup>, terephthalic acid from furfural derived from inedible cellulosic biomass<sup>118</sup>, and styrene and acrylates from phenylalanine potentially sourced from biofuel wastes<sup>119</sup>. Beyond monomer production, the polymerization processes and polymer properties are identical to those of their petrochemical-derived counterparts, allowing easy integration within the current infrastructure. Bioplastics have a wide range of CO<sub>2</sub>-mitigation potential (FIG. 2c, left). Life cycle assessments indicate GHG emissions savings for bio-based PET<sup>120,121</sup>, and high-density and low-density polyethylene<sup>122,123</sup>, albeit with results strongly depending on the scope and boundaries of the life cycle assessment, as well as the biomass source<sup>124,125</sup>. Polylactic acid (PLA) is an industrially produced biopolymer with mainstream packaging applications<sup>126</sup>. However, its potential use as a substitute for other polymers is limited<sup>127</sup> by its inferior barrier properties compared with polyethylene, lower impact resistance than PET and lower fatigue modulus than polypropylene. However, copolymers, blends, stereocomplexes and composites of PLA<sup>128</sup> and other biopolymers are being explored to tune the physical and chemical properties for large-volume uses,

while still being biodegradable. Studies have indicated possible GHG savings of up to 40%<sup>53</sup> and 55%<sup>54</sup> when PET is replaced with PLA or polyethylene furanoate, respectively.

To expand bio-based feedstock use in plastics production, materials scientists must be creative in the monomers used, polymerization methods and industrial processes (FIG. 4). To obtain useful monomers of sufficient purity, complex biomacromolecules need to be controllably depolymerized. For polysaccharides, protection–deprotection chemistry is used to navigate their multiple functionalities and prepare diverse monomers, such as alditols, lactones, aldaric acids and amino sugars<sup>129</sup>. Lignin<sup>130</sup> can be an excellent source of phenolics<sup>131</sup>; selective bond cleavage through thermochemical means such as pyrolysis and gasification have been investigated, with yields of isolated monomers of <35 wt%<sup>132</sup>. The development of monomers that are different from petrochemical-sourced small molecules invites new questions about polymerization thermodynamics<sup>133</sup>, kinetics and reaction chemistries<sup>114</sup>. The polymerization of bioderived monomers to useful polymers hundreds of nanometres long with thousands of repeating units requires understanding of the vast design space afforded by molecular weight<sup>134,135</sup>, copolymer dimensions<sup>136</sup>, end-functionalization<sup>137</sup> and various polymer architectures<sup>138</sup>. Synthesis methods such as controlled polymerization, click chemistry<sup>139</sup> and block copolymerization<sup>140</sup> are being used to explore these design parameters. Moreover, computational tools<sup>141</sup> are being used to screen the near-infinite possible polymer configurations, conformations and chemistries to understand structure–property relationships on the macro-scale and identify candidates to replace conventional polymers.

Devising synthesis routes for these new polymers and scaling them up for industrial use is a problem on a much longer time horizon. Industrial biorefinery processes such as fermentation of carbohydrates to key biofeedstocks can be energy intensive, and there are numerous opportunities<sup>142</sup> for integration with biofuels and bioenergy production to mitigate the cost and endothermicity. Also linked to scaling implications, agricultural production, separation and purification of biomass for biofeedstock generation can be economically and environmentally costly<sup>127</sup>. Commercial PLA is made from starch-rich crops such as maize that are also food sources; using lignocellulosic biomass (from forestry and agricultural wastes)<sup>143</sup> instead of virgin crops avoids competition with major food sources.

H<sub>2</sub> produced using steam methane reforming, an important feedstock to produce many petrochemicals, can be replaced by H<sub>2</sub> generated through water splitting<sup>144</sup>. Captured CO<sub>2</sub> can also be used as an alternative feedstock in the production of fundamental chemicals, greatly decreasing (even indirectly negating) the GHG emissions of a process. Both thermochemical and electrochemical processes have been proposed: catalytic hydrogenation of CO<sub>2</sub> with H<sub>2</sub> to produce methanol<sup>145</sup>, methanation of CO<sub>2</sub> through the Sabatier reaction over various catalysts<sup>146</sup>, co-electrolysis of CO<sub>2</sub> with H<sub>2</sub>O to give ethanol<sup>147</sup> and the electrocatalytic reduction of CO<sub>2</sub> into diverse chemical feedstocks, fertilizers and specialty chemicals<sup>148</sup>. Of these, ‘power-to-methane’ has been realized commercially<sup>149</sup>, while other processes rely on the development of durable catalysts with efficient hydrogenation mechanisms. Copper-based electrocatalysts designed leveraging computational approaches combined with data-driven methods exhibited increased faradaic efficiencies, owing to the ability of this approach



**Fig. 4 | Challenges in producing bio-based plastics.** Challenges in using bio-based feedstocks to produce polymers include the depolymerization of initial raw materials, subsequent polymer synthesis and product design to support recyclability or biodegradability.

to comprehensively search the materials design space for near-optimum surfaces<sup>150</sup>. Using renewable feedstocks such as water-split H<sub>2</sub> and captured CO<sub>2</sub> to thermochemically produce other chemicals such as methanol, ethylene and propylene<sup>151</sup> has also been suggested. However, the contribution of approaches that use H<sub>2</sub> and CO<sub>2</sub> as alternative feedstocks to 2050 mitigation targets must be estimated with caution. The scenario in the right part of FIG. 2c projects 20 Mt of H<sub>2</sub> produced per year for petrochemicals in 2050. Assuming an electrolyser efficiency of 45 MWh per tonne of H<sub>2</sub> (REF.<sup>27</sup>), this equates to a total power requirement of 900 TWh. Electrolysers currently have prohibitively high capital costs; thus, the feasibility of this route is still in question. Furthermore, the massive scale and installed capacity for commodity chemicals such as ethylene present barriers for new technologies, but some approaches may lend themselves to retrofitting existing plants such that feasibility can be demonstrated, thereby, potentially lowering cost for added capacity as the market continues to grow<sup>152</sup>. For example, ~20% of methanol produced in China today uses coke oven gas from the iron and steel industry as feedstock. This process uses the same technology as coal-based methanol production, but without the gasification step<sup>24</sup>. Fully utilizing gaseous by-product streams and exploring these symbiotic opportunities between industries is an important effort, because capturing CO<sub>2</sub> from the ambient atmosphere remains infeasible for the foreseeable future.

### Transformation

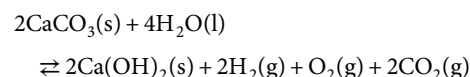
Raw material inputs enter a transformation process that can be CO<sub>2</sub> intensive because of the fossil-sourced heat required to run the process, direct evolution of CO<sub>2</sub> as a reaction by-product or both. Emissions-reduction approaches, therefore, involve shifting away from inherently carbon-dependent heating sources or drivers of a reaction. The ability to replace fuel-derived heat with electrically generated heat varies by process based on the required temperatures. We contrast lower heat requirements for steps such as heat treating, boiling, distillation and drying with processes with much higher average temperatures, such as smelting, calcining and forming. For example, reaching 1,450 °C in a cement kiln through electrically generated heat is not currently technologically or economically feasible and, thus, such an endeavour would be a solution for the distant future. Concentrated solar power shows promise for providing high-temperature process heat in some contexts, such as iron oxide smelting<sup>153</sup>. Direct electrification of high-temperature thermochemical processes such as steam methane reforming based on joule heating has been suggested<sup>154</sup>. Our focus here is on electrification for the transformation reaction, because of the notable opportunity across cement, steel and petrochemicals (FIG. 2). Use of H<sub>2</sub> as a fuel provides another strategy for metals and petrochemicals, albeit a strategy with a longer time horizon for implementation<sup>155–157</sup>.

Note that additional emissions-reduction approaches under transformation involve process intensification to increase efficiency or the capture of direct emissions. Process improvements may be weak levers on a per unit basis because industry has optimized existing

process efficiencies over many decades (and because of so-called rebound effects)<sup>158</sup>. However, these initiatives should still be pursued, as process intensification can be incorporated in the near term and the scale of the materials production industry suggests that even marginal changes can contribute to the reduction of GHG emissions (FIG. 2). Examples in the petrochemical industry, for which opportunities may be most significant, include heat integration<sup>159</sup>, membrane gas separation<sup>160</sup> and increasing selectivity through catalysis<sup>30</sup>. Effective carbon capture is a relevant strategy across all materials under consideration and the potential for impact varies based on magnitude, concentration and moisture content of the CO<sub>2</sub> stream. Materials innovations involve increasing the concentration of the captured stream through chemical looping<sup>161</sup> or membrane processes<sup>162</sup>.

**Process electrification.** There is increasing interest in electrochemical routes for industrial processes as the cost and reliability of renewable electricity continues to improve. Electrochemical routes across all the materials of interest herein offer the potential to alter direct emissions through a change in the chemical reactions and the potential to avoid separation steps (FIG. 5a). These processes are still in early phases of development and, therefore, have limited mitigation potential in 2050. The availability of decarbonized electricity may be limited in the near term<sup>33</sup>, but these approaches must still be pursued because of the potential for electrochemical production to decouple emissions from materials production. Insight across length scales has not only enabled progress but also highlights pathways for further innovation (as shown for steel electrolytic production in FIG. 5b).

For cement, a proof-of-concept, ambient-temperature, electrochemical CaCO<sub>3</sub> decarbonation process has been demonstrated<sup>163</sup>. Within the decarbonation cell, neutral-water electrolysis produces a pH gradient in which CaCO<sub>3</sub> is decarbonated at low pH and Ca(OH)<sub>2</sub> is precipitated at high pH:



Ca(OH)<sub>2</sub> requires less energy to dehydrate to CaO than is required to calcine CaCO<sub>3</sub> and reacts with SiO<sub>2</sub> to form alite (Ca<sub>3</sub>SiO<sub>5</sub>), the main mineral compound in OPC. This electrochemical calcination process produces concentrated gas streams, from which CO<sub>2</sub> can be separated and sequestered, and H<sub>2</sub> and/or O<sub>2</sub> from the process can be used to generate electric power via fuel cells or combustors. Through systems-level integration, processes could be linked within a plant to generate power or increase plant efficiency. Owing to the early stage of development, this technology will likely not appreciably contribute to 2050 mitigation.

Electrolysis of metals decouples production from CO<sub>2</sub> emissions either through high-temperature molten electrolysis or lower-temperature aqueous processes<sup>164</sup>. The main opportunity is for iron, as the electrolytic production of aluminium, manganese and magnesium is already commercially dominant. Electrochemical reduction may selectively extract elements from ore,

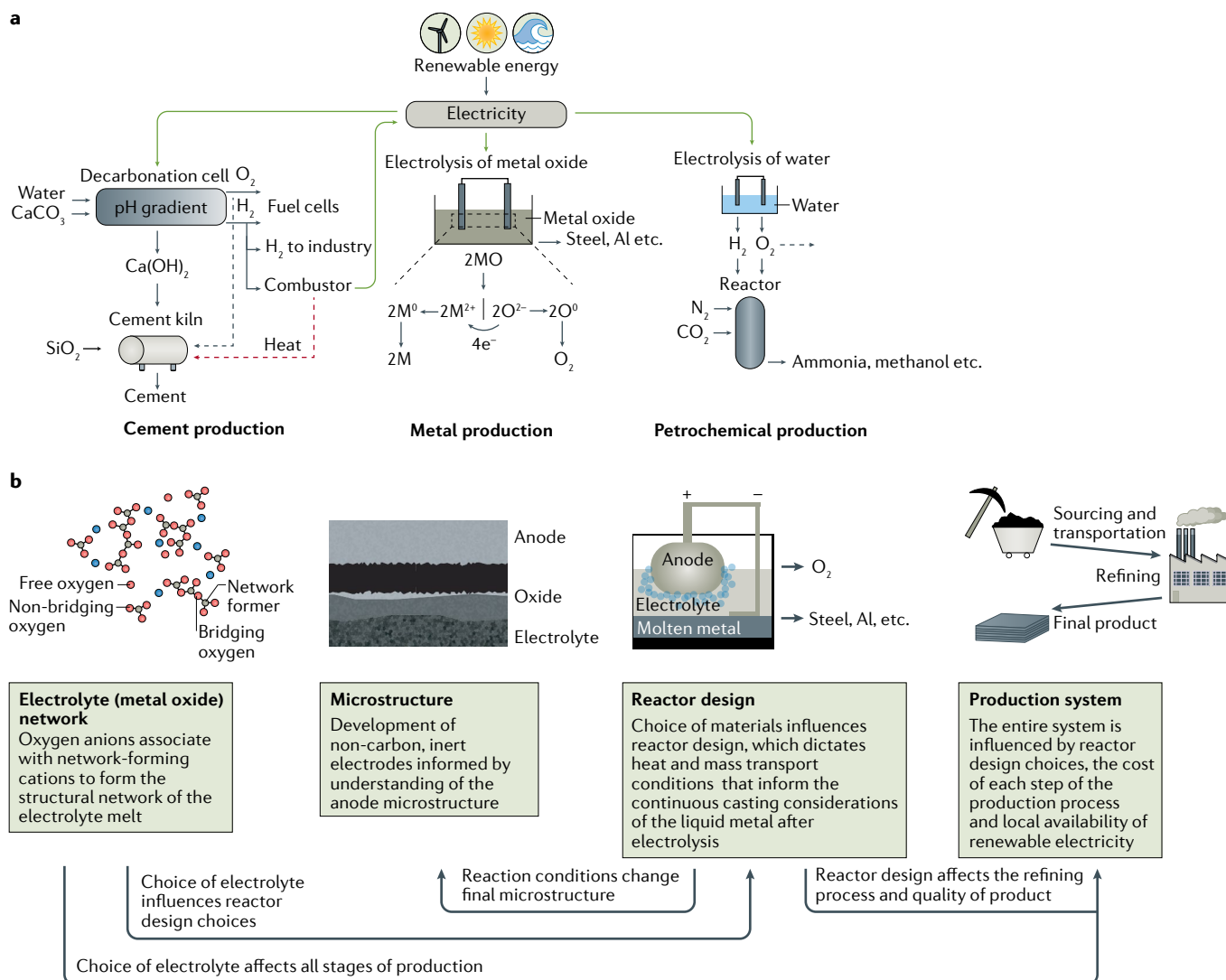
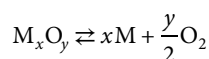


Fig. 5 | **Electrification of materials production.** **a** | The electrolytic production of cement, metal and petrochemicals could lead to a substantial decrease in greenhouse gas emissions<sup>163,169,174</sup>. **b** | For electrolytic steel production, links have been established between the molten oxide electrolyte network, microstructure of the anode, reactor design and requirements of production systems. These links across different physical length scales have effected progress and reveal promising avenues for further development. M, metal. Panel **b** (scanning electron microscope micrograph) adapted from REF.<sup>169</sup>, Springer Nature Limited.

requiring fewer process steps and enabling impurities to be separated as desired for a given application. In molten oxide electrolysis, the feed oxide is dissolved in a molten oxide electrolyte, and its decomposition into  $O_2$  and metal (M) occurs through



Overall, electrolytic processes are particularly exciting for the possibility to flexibly handle lower-grade, more complex ores in fewer process steps. With lower capital costs and smaller footprints compared with pyrometallurgical routes<sup>165</sup>, electrolysis cells could be deployed close to mines, powered by renewable energy and the tonnes of molten melts could be used for energy storage, offering opportunity to coordinate with variable energy generation.

The average global  $CO_2$  intensity of electrolytic aluminium production could be decreased by 70% as the grid decarbonizes, resulting in huge mitigation potential (FIG. 2b, left). The production of aluminium through the Hall–Héroult process provides some insight into how iron production might be transformed, given that both are high-production-volume materials (FIG. 5). However, there are some limitations to this comparison, as iron would require higher processing temperatures than those for aluminium,  $>1,583^\circ C$ , which accelerates corrosion, making electrode development challenging<sup>166</sup>. The Hall–Héroult process also uses a carbon anode, such that  $CO_2$  emissions are inherent, and the development of an inert anode to fully decouple  $CO_2$  emissions from aluminium production remains challenging. The multiple valence states of iron lead to a low faradaic yield, as electron transfer between the valence states leads to electronic



current flow. Thus, electrolyte design must maximize ionic conductivity (along with high solubility for the feedstock and chemical and thermal stability)<sup>167</sup>. Molten oxides contain oxygen anions in different coordination environments that associate with network-forming cations to form the structural network of the electrolyte melt. Identifying resistances governed by the oxidation of Fe(II) in the melt and the reaction kinetics within the network structure of the electrolyte<sup>168</sup> is key to elucidating process operating conditions. These innovations at the ion scale inform electrolyte design, which then guides the choice of electrode materials, both of which dictate the physical arrangement of the cell and operating parameters. At the microscale, understanding of anode microstructure has informed the development of non-carbon, inert anodes. For example, anodes made from chromium-based alloys showed high stability in molten oxide electrolytes; investigation of the microstructure uncovered the role of a solid solution of chromium and aluminium oxides covered by a  $\text{MgCr}_2\text{O}_4$  spinel layer that forms slowly during electrolysis and protects the anode in these aggressive melts<sup>169,170</sup>. This insight can facilitate development of resilient anodes through understanding of how the diffusivity of species changes with microstructure evolution and how the film forms. Further innovation could come through the development of ceramic anodes, which may be the most cost-effective option, but their limited electronic conductivity requires the toolbox of materials engineering to make viable. Electrode design must also be optimized for gas production and recovery at high temperature. The choice of electrode and electrolyte materials subsequently influences reactor design, which dictates the heat and mass transport conditions that inform the continuous casting considerations of the liquid metal after electrolysis. This last point influences materials throughput and, therefore, the cost, which is also influenced by the current density, temperature and voltage.

These innovations for iron oxide have inspired progress in the electrolysis of other ores, including sulfides. The production of liquid copper and gaseous sulfur was demonstrated at high current density using a molten sulfide electrolyte comprising  $\text{Cu}_2\text{S}$  and  $\text{BaS}$  (REF.<sup>171</sup>). Direct, elemental decomposition of the ore by electrolysis not only averts noxious by-products that arise from conventional production (such as  $\text{SO}_2$ ) but may enable enhanced control over impurities. Selective recovery of rhenium, molybdenum and copper present in a sulfide-based molten electrolyte has been achieved, and the approach could be extended to a wide range of valuable impurity elements in copper ore<sup>172</sup>.

Integrated electrochemical routes for ammonia production are at the forefront of the effort to electrify the petrochemical industry. The electrochemical synthesis of ammonia from water-split  $\text{H}_2$  and air-separated  $\text{N}_2$  is thermodynamically feasible, with high pressures replaced by moderate voltages that can be carbon-free if the grid is decarbonized. Various technologies have been proposed<sup>173</sup>: from liquid and polymer electrolyte systems that operate near room temperature to molten salt, composite, ceramic and other solid electrolyte systems at higher temperatures (400–800 °C).

As the reaction is exothermic, lower temperatures are favourable, but ammonia production rates are quite low ( $10^{-13}$ – $10^{-8}$  mol cm<sup>-2</sup> s<sup>-1</sup>), owing to slow transport to and slow reaction kinetics at the ammonia-production electrode–electrolyte interface<sup>173</sup>. Higher temperatures accelerate kinetics and increase the  $\text{H}^+$  flux, but also lead to a higher ammonia dissociation rate and decreased faradaic efficiency. Another proposed avenue involves forgoing water splitting and combining this step with synthesis to directly react  $\text{H}_2\text{O}$  with  $\text{N}_2$ ; its thermodynamic feasibility at ambient temperature and pressure requires an electric potential of  $\geq 1.17$  V (REF.<sup>174</sup>). Without the need for high temperatures or pressures, modular production can be economically viable, and theoretical studies suggest that this modularity reduces GHG emissions from ammonia synthesis by ~50%<sup>175</sup>. Many catalysts have been proposed for this reaction, including noble metals; metal oxides, nitrides and sulfides<sup>176</sup>; and lithium metal<sup>177</sup>. Research into direct electrochemical routes for the production of methanol, ethylene and propylene is lacking.

### Output

Production outputs are driven by the demand for services, such as housing, transportation, manufacturing equipment and packaging. These applications require different property profiles, which determine the performance of the product and its usable lifetime (if discarded owing to material degradation, rather than replacement). Most materials research is motivated by the prospect of enhancing materials properties, acknowledging that high-performance materials may lead to emissions reductions. For example, high-performance structural metal alloys are pursued to enable energy-efficient products, weight reduction in transportation, increased alloy longevity through corrosion protection, or damage tolerance and repairability for longer product use<sup>178</sup>. For cement, performance could be enhanced through mechanism-based (or performance-based) approaches that focus on the mechanisms behind concrete setting and durability, and, thus, rigorously describe and exploit complex composition–processing–property relationships<sup>179,180</sup>. For both metals and cement, strict specifications are set on the composition of the product to ensure safety and uniformity. These specifications can be restrictive, as inputs and processing shift to support decarbonization; thus, research and policy activity are needed to promote the adoption of property-based specifications.

The use of a material is not, however, solely determined by its property profile. Materials interface with human needs, and the multitude of technical and non-technical reasons why materials are used and discarded must be appreciated. Research into materials efficiency has revealed diverse strategies to cut  $\text{CO}_2$  emissions associated with material production<sup>181,182</sup>. Steel products are often discarded before any notable material degradation<sup>183</sup>. Steel structures, in particular, could have much longer lifetimes and be directly reused at end of life<sup>184</sup>, while the amount of steel used in buildings could be halved by avoiding ‘overdesign’<sup>185</sup>. Reducing steel demand is one of the most promising decarbonization

solutions for the metals industry (FIG. 2b). Similarly, concrete structures are often overdesigned and demolished for reasons unrelated to degradation. Prestressed structures, which are thinner and lighter, require less concrete for the same service, whereas precasting enables more complex, optimized forms. In the petrochemical sector, nitrogen fertilizers could be used more efficiently and plastic demand could be greatly reduced by reusing and recycling packaging. While technically readily available, these material-efficiency strategies are challenging to implement, owing to regulatory requirements, lack of knowledge or cost-saving (often material cost versus labour cost trade-offs) reasons, and require changes in industry practice and consumer behaviour. Nevertheless, materials engineers can make materials and design choices that minimize emissions over a product's lifetime, using material-selection approaches<sup>186,187</sup>.

The area in which research aligns least well with GHG emissions reduction in outputs is in designing for recovery across the materials of interest; therefore, we focus attention on this area. For cement, there is also the potential for CO<sub>2</sub> uptake during product use.

### **Design for recovery in metals and polymers**

Designing products and alloys with recycling in mind, by avoiding combinations of metals that are difficult to separate during refining, can minimize recycling losses and contamination. Modelling tools that account for the thermodynamic distribution tendencies of alloying elements in metals can be used in product design to help flag which metal combinations are problematic<sup>188</sup>. Another approach is designing 'recycling-friendly' alloys — that is, alloys that can accommodate more scrap in their manufacture and require little or no compositional modifications while meeting functionality requirements<sup>189</sup>. The design of recycling-friendly aluminium alloys is a rich research topic, and alloys that can tolerate higher amounts of copper, iron and silicon while achieving the same corrosion resistance, formability and toughness as existing alloys are being developed. Strategies include the development of universal alloys, or 'unalloys', that meet performance requirements of multiple applications<sup>189</sup> and optimizing compositional variations through modelling<sup>190</sup>, without compromising on performance. Other innovative strategies include defining criteria such as the 'shredding criticality potential indicator' to compare scrap quality and, thereby, inform product design<sup>191</sup>.

The secondary production of 160 Mt of plastics per year by 2050 can be achieved only by redesigning the composition of polymers and their use in products. Average use lifetime of commercial polymers is often low<sup>192</sup>, largely owing to single-use plastic products that are thrown away because of product design, rather than property degradation. One study<sup>193</sup> estimates that up to 20% of plastic packaging can be redesigned for reuse with innovative delivery models that could decrease the use of primary material for packaging by 80–90%. Plastic products have not only grown considerably in volume over the past five decades (with an 8.4% compound annual growth rate, corresponding to ~2.5 times the global gross domestic product growth)<sup>192</sup> but they have also diversified,

with myriad resin types and chemical compositions, additives and formats. Although this diversity allows for custom-tailored properties for varied applications, it also hinders recyclability at end of life. The current recycling infrastructure is limited by uneconomical collection volumes<sup>194</sup>, mixing and contamination of plastic waste<sup>195</sup>, expensive sorting and separation measures<sup>196</sup>, and a volatile and often ill-defined market<sup>197</sup>. Many of the problems associated with recycling stem from upstream choices. Resin and product design practices that do not include end-of-life considerations lead to plastic products that are incompatible with each other or the recycling process. Notable among these are challenges associated with multi-material and multi-polymer films<sup>198</sup>. The quality of recyclates is compromised<sup>199</sup>, even when products of the same resin type are recycled together, indicating additive and processing differences<sup>200</sup> that create materials that are incompatible for closed-loop recycling. Efforts to harmonize resin and product design are needed to improve the quality of recyclates, while also finding applications for low-quality recyclates that cannot be upgraded using appropriate compatibilization<sup>201</sup> techniques. For polymers that degrade in quality over time due to wear and tear, mendable polymers<sup>202</sup> based on dynamic covalent networks with reversible crosslinks are being explored for autonomous life cycle control<sup>203</sup> and increasing lifetimes. New bio-based polymers are also being explored that can emulate properties of fossil-derived polymers but are also biodegradable or chemically recyclable. Aliphatic polyesters such as PLA, polyglycolic acid, poly( $\gamma$ -butyrolactone), polybutylene succinate, aliphatic polycarbonates and polyhydroxyalkanoates are most susceptible to depolymerization by enzymes and microbial systems<sup>204</sup>. Many of these polymers currently find applications in biomedical applications, but their enzymatic biodegradability comes at the cost of durability, strength and chemical resistance, making them unsuitable for large-scale commodity applications that encounter a wide range of environmental conditions. Chemically recyclable polymers are also being investigated; thermoplastic polyesters with degradable linkages<sup>205</sup> and depolymerizable poly( $\gamma$ -butyrolactone)s<sup>133</sup> and their derivatives with low ceiling temperatures are some candidates for the transformation to a circular plastics economy.

### **In-use opportunities for cement**

The uptake of CO<sub>2</sub> in concrete during its life through carbonation (BOX 2) has the potential to reabsorb the emissions generated during calcination in the cement production process. Indeed, estimates indicate that 43% of the CO<sub>2</sub> emissions (4.5 Gt) from cement production from 1930 to 2013 has been sequestered in cement materials that are in-use or discarded<sup>206</sup>. The projected cumulative CO<sub>2</sub> uptake of ~100 Gt during the period 2015–2100 in carbonating cement materials corresponds to ~30% of the expected process and energy CO<sub>2</sub> emissions arising from the global cement cycle over the same period assuming business as usual<sup>207</sup>. Although these figures are significant, the carbonation process is extremely slow (complete carbonation can take decades) and rates depend on climate, concrete composition, amount of concrete exposed and disposal method

## Box 2 | Carbon capture in cement and concrete

In the carbon cycle of cement and concrete, CO<sub>2</sub> is emitted when limestone is transformed into clinker through calcination and is then reabsorbed over the course of the concrete's use through carbonation<sup>88,204</sup>. Cementitious materials are, therefore, amenable to the process of mineralization, which transforms captured CO<sub>2</sub> mixed with an alkaline reactant into construction materials, including aggregates, binders and concrete. Captured carbon is already being used in small quantities in the curing of conventional concrete mixes with ordinary Portland cement, while carbonatable calcium silicate clinker is an example of a binder designed to be cured with CO<sub>2</sub> (REF.<sup>225</sup>). The considerable interest in mineral carbonation is because of its potential to permanently sequester carbon from industrial sources into construction products, which are used in large quantities<sup>225–227</sup>. The Center for Climate and Energy Solutions estimated the global market size in 2030 for use of captured carbon in concrete and aggregates to be US\$400 billion and \$150 billion, respectively, and the greenhouse gas mitigation potential to be 1.4 and 3.6 billion tonnes of CO<sub>2</sub>, respectively. To realize this mitigation potential, the National Academies of Sciences, Engineering, and Medicine has identified several research needs, including accelerating the mineralization process, furthering understanding of the process and its products, and increasing adoption of the products in construction<sup>225</sup>.

(crushing concrete at end of life increases surface area and, therefore, carbonation rates)<sup>208,209</sup>. Moreover, carbonation could lead to corrosion in the reinforcing steel bars used in prestressed concrete. Thus, the aim is to maximize carbonation in concrete mixtures (for example, with higher calcium contents) while limiting the risk of durability issues, which will depend on the specific applications in a given climate. This approach may be more feasible in applications in which reinforcing steel is not used, which constitutes ~75% of all cement usage<sup>89</sup>.

### Conclusion and outlook

Considerable opportunities exist to decarbonize cement, metals and petrochemical production.

Within cement, first and foremost, structures are often demolished for reasons other than material degradation; therefore, engaging with policymakers and architects to design adaptable infrastructure is a powerful pathway to reduce demand. On the materials side, using a mechanism-based approach to advance understanding of the processes underpinning cement production, concrete setting and durability would drive towards emissions reductions. Such mastery would enable optimized concrete mixing, depending on the local context and properties required, advancing from the current 'one-bag-fits-all' approach of Portland cement. The proportion of low-carbon alternative cementitious binders could be increased, while adapting to cost, performance and materials availability constraints. This knowledge would aid the development and use of high-performance concrete for greater materials efficiency. Finally, there is the opportunity to reabsorb CO<sub>2</sub> during concrete use and at end of life. To promote carbonation, models that incorporate concrete composition, surface exposure, local climate and durability requirements must be developed.

For the near-term reduction of emissions from the metals industry, it is imperative to increase production from secondary sources, which can occur only with enhanced alloy and contaminant management. High-throughput sensing is needed to accurately grade

scrap and, thus, incentivize and enable more efficient recycling. The development of targeted refining technologies will prevent certain types of scrap accumulating in surplus. Transformative decarbonization options exist for the sizable fraction of steel demand that must be met with primary production. Direct electrolysis of iron oxide ore using renewable energy supports iron production with oxygen as the only by-product, but electrolytic cells must be engineered to withstand highly corrosive conditions and compete with the remarkable productivity of traditional blast furnaces. Aluminium production is already electrified; thus, for the next 20–30 years, opportunities for significant mitigation are in the continued decarbonization of the electricity grid, as well as in production, in the form of operational efficiencies (for example, continuous strip casting and oxy-fuel combustion), and improving yield ratios during forming and fabrication. Full decarbonization of aluminium production can only be realized through the development of an inert anode.

Decoupling the chemical industry from fossil feedstock use is a crucial challenge for the materials community in pursuit of decarbonization. Using alternative feedstocks from bio-based sources is a key strategy to mitigate fossil demand. However, the economic success of the petrochemical industry is not easy to surpass, and innovative catalytic pathways that use lignocellulosic wastes to make platform chemicals with high yields and reduced costs will be needed to sustainably divorce non-renewable resources. Initial opportunities might be in bio-based by-product streams, particularly for use in low-volume products, so that success in scaling could be demonstrated while reducing concerns relating to competing land use. The chemical industry could also use captured CO<sub>2</sub> as an alternative feedstock. Besides the development of large-scale capture technologies, this strategy requires further mechanistic understanding of CO<sub>2</sub> reduction and conversion pathways. Activating a relatively unreactive molecule such as CO<sub>2</sub> is impossible without modern catalytic prowess; the design of efficient and economical catalysts with stable catalytic activity and minimized coke deposition remains a challenge. Last, electrification of the chemical industry would not only minimize the industry's dependence on fossil fuels for high-temperature and high-pressure processes but also provides the enticing possibility of overcoming the intermittency of renewable electricity and developing modularized electrochemical production. However, despite thermodynamic feasibility at ambient conditions, kinetic limitations and stability considerations point to a need for improved understanding and design of electrocatalytic systems.

The interdisciplinary nature of the materials community is uniquely positioned to rapidly scale innovation in high-volume and complex industries to achieve impactful reductions in GHG emissions associated with materials production. The cement, metals and petrochemical industries must undertake similar endeavours: expanding and deepening understanding of composition–processing–property relationships for greater use of alternative low-carbon feedstocks or end-of-life scrap; investigating the thermodynamics

and kinetics underlying electrified processes to design robust, high-throughput reactors; and designing materials to support product efficiency, longer lifetimes and recyclability at end of life. Thus, transfer of knowledge and predictive tools are needed not only within but across the main materials industries. The strongest materials innovations towards decarbonization described herein link theoretical underpinnings of the materials domain at the atomistic scale to industrial implementation. We invite the materials community to link knowledge within the materials domain to the systems-level processes and environmental implications to develop comprehensive strategies to meet global

climate targets. Our analysis reveals a considerable gap between the known decarbonization technologies that might be applied in 2050 and the climate targets for the cement, metals and petrochemicals industries. The wide decarbonization landscape must be mapped and navigated with a rigorous understanding of physical phenomena and constraints. We must pursue new approaches to bridge the emissions gap that couple creative, cross-disciplinary research with policy-engaged implementation strategies to address the societal needs driving material demand.

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## Author contributions

E.A.O. and K.D. discussed the content of the article. K.D., R.B. and J.G. researched data for the article. All authors contributed to the writing of the article, and K.D., J.G., V.S. and E.A.O. edited the manuscript prior to submission.

## Competing interests

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