STANFORD UNIVERSITY

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A Report on Ten Key Technologies and Their Policy Implications

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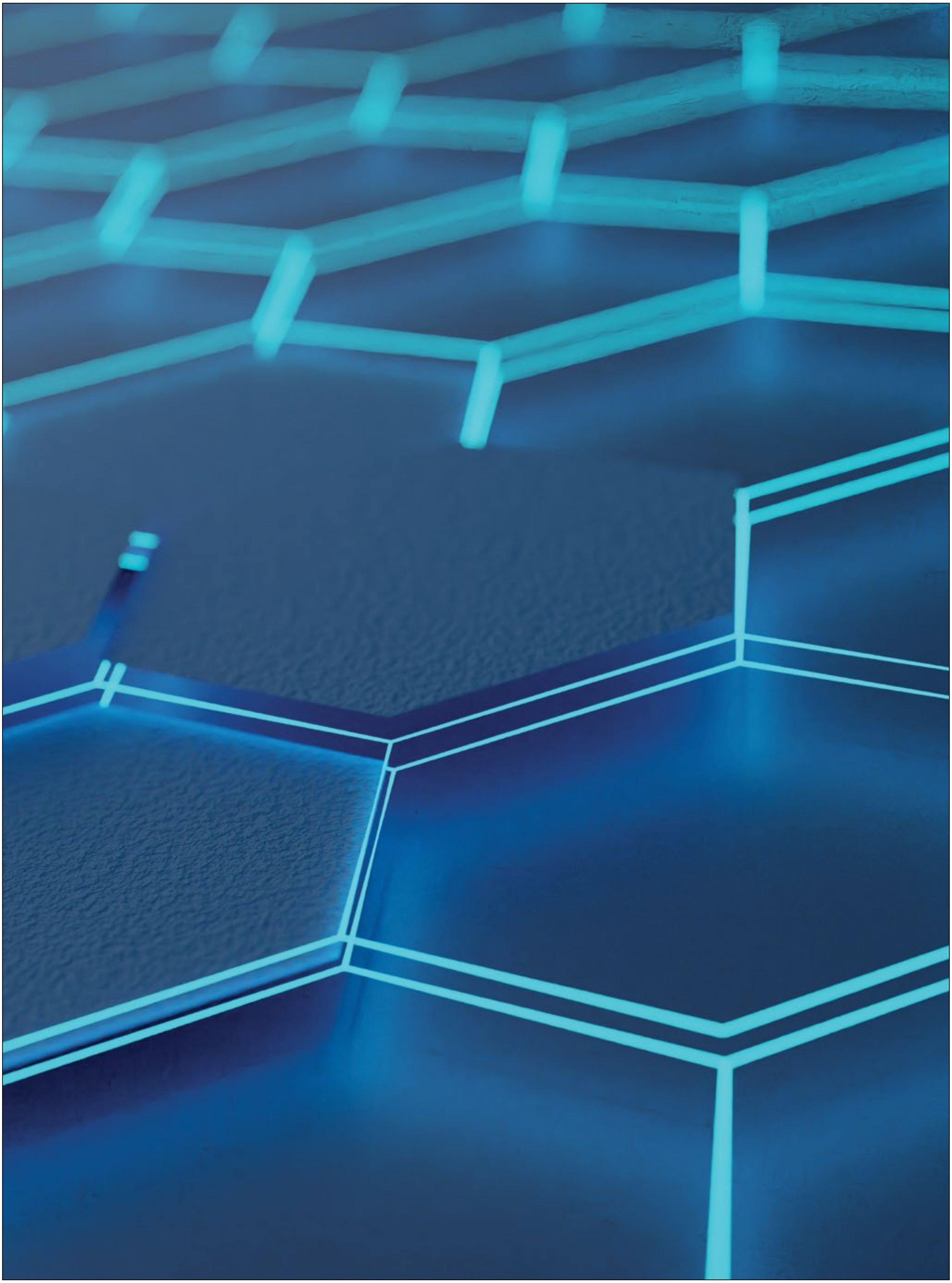

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MATERIALS SCIENCE

KEY TAKEAWAYS

- Materials science is a foundational technology that underlies advances in many other fields, including robotics, space, energy, and synthetic biology.
- Materials science will exploit AI as another promising tool to predict new materials with new properties and identify novel uses for known materials.
- The structure of funding in materials science does not effectively enable transition from innovation to implementation. Materials-based technology that has been thoroughly tested at the bench scale may be too mature to qualify for basic research funding (because the high-level basic science is understood) but not mature enough to be directly commercialized by companies.

Overview

Materials are everywhere, from macro features that are visible to the naked eye to microscopic features thousands of times smaller than the diameter of a single human hair. They shape the objects of everyday life and give rise to new possibilities. Materials science cuts across technological areas, contributing to everything from the development of stronger and lighter materials for aircraft to more efficient and less heavy solar cells, better semiconductors, biocompatible materials for medical implants, more stable electrodes for batteries, and easily manufactured and recyclable plastics.

The goal of materials science is to understand how the structure of a material influences its properties and how processing the material can change its structure and therefore its performance. This knowledge can then be used to design new materials with desirable properties for specific uses. The ultimate aspiration, which remains a long way off, is to be able to create materials on demand by specification—put in a request for a material with properties X, Y, and Z, and a 3-D printer produces it for you.

Broadly speaking, materials science and engineering research focuses on four major areas. The first is characterizing the properties of materials. The second is modeling materials, which involves predicting material properties based on atomic principles. The third is synthesizing materials with precise control to verify whether their properties are as predicted. The fourth area is manufacturing and processing materials with well-characterized properties in sufficient quantities for practical applications.

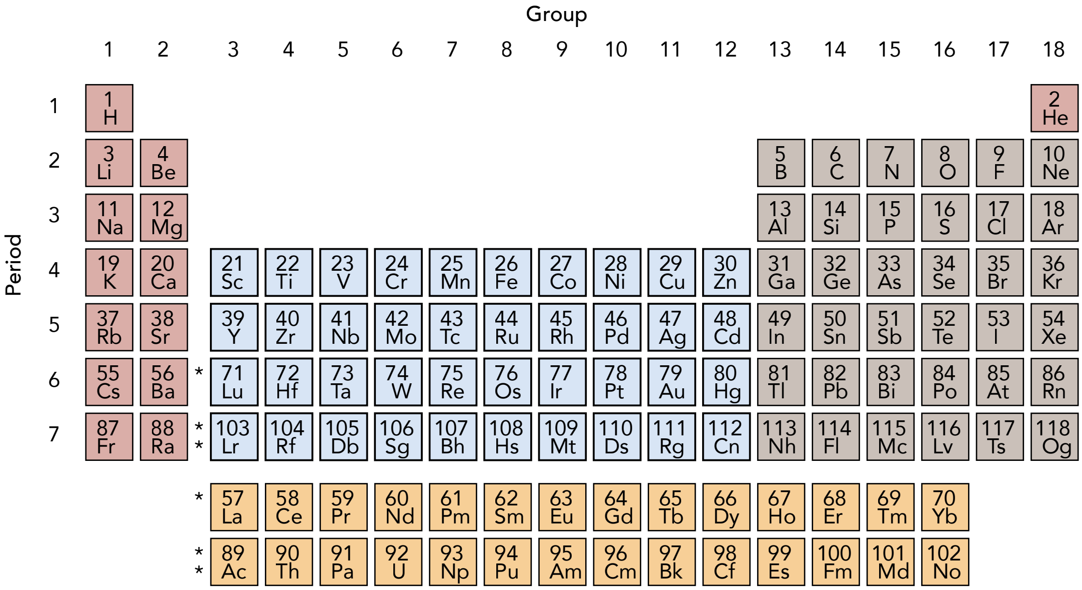
Basics of Materials Science

All materials are composed of atoms. The periodic table of the elements (figure 4.1) lists all the known types of atoms. Certain atoms can be combined into molecules that have vastly different properties than the atoms alone. For example, table salt consists of sodium and chlorine, which are elements. Sodium burns on contact with water, chlorine is a poisonous gas, and yet the table salt we consume every day is a completely different substance.

There are two important points to note about the periodic table. First, there are a lot of elements—ninety-two naturally occurring ones and twenty-six that can be observed only in laboratory conditions. That's a lot of building blocks from which different materials and molecules can be synthesized, and in fact, an astronomically large number of different compounds are possible. The challenge for materials science is to sift through this vast array of possibilities to find the ones that are useful.

The second important point is that the elements in the periodic table are lined up in a certain order. Elements in the same column have properties that are often similar in key ways. This means that insights developed through experimentation or calculation on one element can be transferred, with modifications, to another element above or below it in the periodic table.

FIGURE 4.1 Periodic table of the elements



Group

Period	1	2		3	4	5	6	7	8	9	10	11	12	13	14	15	16	17	18
1	1 H																		2 He
2	3 Li	4 Be												5 B	6 C	7 N	8 O	9 F	10 Ne
3	11 Na	12 Mg												13 Al	14 Si	15 P	16 S	17 Cl	18 Ar
4	19 K	20 Ca		21 Sc	22 Ti	23 V	24 Cr	25 Mn	26 Fe	27 Co	28 Ni	29 Cu	30 Zn	31 Ga	32 Ge	33 As	34 Se	35 Br	36 Kr
5	37 Rb	38 Sr		39 Y	40 Zr	41 Nb	42 Mo	43 Tc	44 Ru	45 Rh	46 Pd	47 Ag	48 Cd	49 In	50 Sn	51 Sb	52 Te	53 I	54 Xe
6	55 Cs	56 Ba	*	71 Lu	72 Hf	73 Ta	74 W	75 Re	76 Os	77 Ir	78 Pt	79 Au	80 Hg	81 Tl	82 Pb	83 Bi	84 Po	85 At	86 Rn
7	87 Fr	88 Ra	* *	103 Lr	104 Rf	105 Db	106 Sg	107 Bh	108 Hs	109 Mt	110 Ds	111 Rg	112 Cn	113 Nh	114 Fl	115 Mc	116 Lv	117 Ts	118 Og
			*	57 La	58 Ce	59 Pr	60 Nd	61 Pm	62 Sm	63 Eu	64 Gd	65 Tb	66 Dy	67 Ho	68 Er	69 Tm	70 Yb		
			* *	89 Ac	90 Th	91 Pa	92 U	93 Np	94 Pu	95 Am	96 Cm	97 Bk	98 Cf	99 Es	100 Fm	101 Md	102 No		

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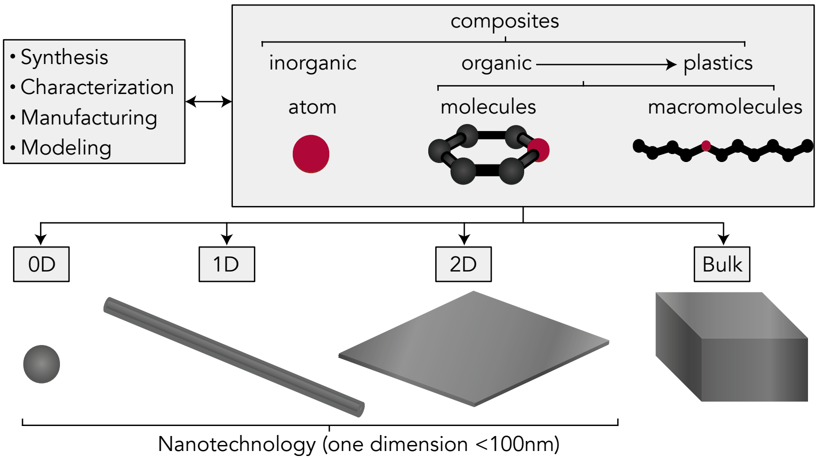
FIGURE 4.2 The basic layout of materials science



Atoms can be arranged spatially in various ways. A crystal, for example, is the result of arranging atoms in a periodically repeating lattice. The silicon wafer at the heart of the semiconductor industry is one such crystal; more precisely, it's a slice of a single silicon crystal.

Molecules, in turn, can be linked together into structures called macromolecules (see figure 4.2). These can occur naturally, such as proteins, DNAs, and cellulose, or can be synthesized artificially, resulting in polymers/plastics, for example. Plastics are particularly useful because the long chains of macromolecules are often more flexible. Research on new macromolecular structures can be used to develop plastic materials that are easier to recycle or that hold advantageous mechanical properties while weighing less than metals.

Key Developments

Present-Day Applications

Some interesting applications from studying materials science include:

Biomedical applications Wearable electronic devices made from flexible materials conform to skin or tissues and serve specific sensing or actuating functions. More specifically, wearable electronic devices or "e-skin" can sense external stimuli such as temperature and pressure and encode these stimuli into electrical signals.[1] For example, a "smart bandage" with integrated sensors and simulators can accelerate healing of chronic wounds by 25 percent.[2]

Novel and recyclable plastics Researchers are developing new sustainable methods to couple molecules into polymers for deconstructable plastics that are easier to recycle.[3] New electrically conductive polymers are also a focus of study. Electrical conductivity in flexible materials such as plastics can be achieved by inserting specific bonds between individual atoms that make up the material backbone. This allows for the fabrication of flexible electronic devices such as wearable sensors and foldable screens for mobile devices.

Energy materials Materials design and processing is integral to decarbonization efforts through the electrification of transportation and industry. Some challenges persist, however, including storing energy from intermittent energy sources, such as solar and

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wind, in batteries. Therefore, designing batteries with materials and architectures that enable quick recharging and long stability while reducing costs will be crucial. Important discoveries in engineering battery electrode materials have been made.[4] Studying the electrolyte-electrode interface in batteries has also led to higher performing and more stable electrolytes in batteries.[5]

Additive Manufacturing

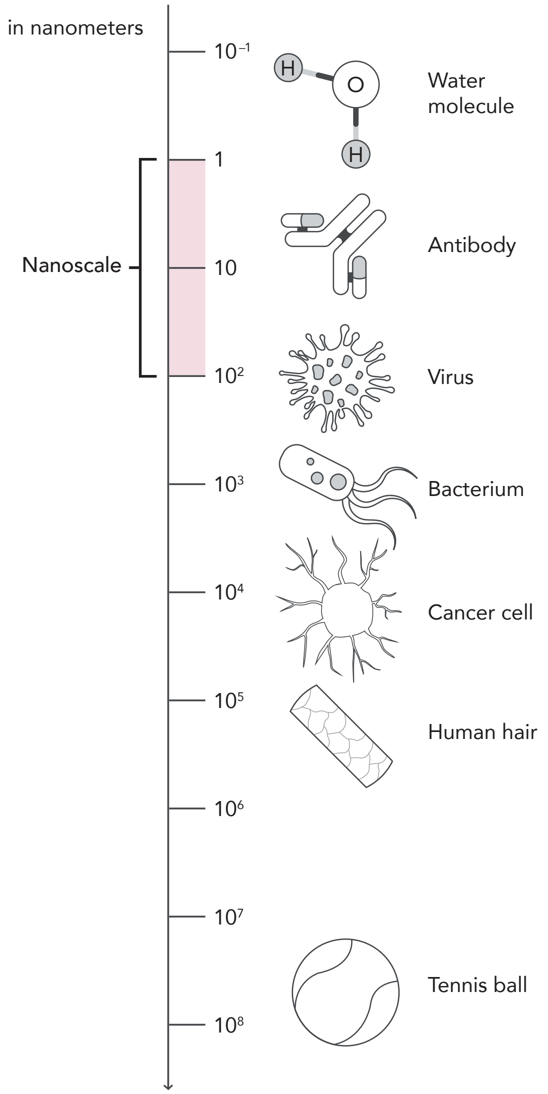
One promising advance in materials processing over the past fifteen years is additive manufacturing, or 3-D printing. A novel method termed continuous liquid interface production (CLIP) has been established that uses directed ultraviolet light to pattern structures from a polymer resin.[6]

This technology has been used to make customized football helmet liners,[7] and a number of companies have sprung up to commercialize and scale up additive manufacturing both by producing stand-alone products and by collaborating with multinational companies. More recent active research in 3-D printing includes scaling down 3-D printable feature sizes and exploring methods to 3-D print with conductive materials and artifacts using multiple materials at once.

Nanotechnology

Nanotechnology is a large and growing subfield of materials science. Size has a profound impact on the properties of a material. Figure 4.3 shows different length scales compared to a water molecule (which is below a nanometer), a human hair (roughly

FIGURE 4.3 The size of nanoscale objects



10^5 nanometers), and a tennis ball (at 10^8 nanometers). A structure is typically referred to as nanoscale if at least one dimension is in the 1–100 nanometer range.

In the past twenty years, nanoscience and nanotechnology have attracted enormous interest, for two reasons. First, many significant biological organisms (such as viruses and proteins) are nanoscale in size. Second, it turns out that the properties of nanoscale materials—including their electronic, optical, magnetic, thermal, and mechanical properties—are often very different from the same material in bulk form.[8] Materials that are smaller than about 100 nanometers in one dimension, two dimensions, or in all dimensions are called nanosheets, nanowires, and nanoparticles, respectively.

Quantum dots—for which the Nobel Prize in Chemistry was awarded in 2023—have garnered public attention through their use in televisions. Quantum dots are metallic, carbonaceous, or semiconductor spherical nanocrystals that emit bright monochromatic light in response to excitation by a light source with a higher energy, such as blue light from the back panel in a display.[9] Quantum dots are a model example of variable material properties due to scale as their optoelectronic properties differ from those of the same bulk material. The diameter of quantum dots shifts the color of light that they emit, with larger quantum dots emitting longer wavelengths. This allows for tunable light emission based on the desired application.

Some current applications of quantum dots include:

Medical imaging Quantum dots are being used to improve the contrast of biomedical imaging, for example, as in fluorescent markers to allow selective labeling of biological structures in vitro and in vivo.[10] Additionally, biocompatible nanomaterials can be employed as optical probes to sense mechanical forces and electrical fields in biological organisms, thus circumventing specialized and bulky equipment, opening the possibility of new experiments.[11]

Solar cells Quantum dots can improve the efficiency of solar cells. Their ability to absorb different frequencies of light means they can potentially capture more of the solar spectrum, boosting the performance of solar panels.[12]

Sensors Quantum dots and plasmonic nanoparticles can be used in sensors for detecting chemicals and biological substances.[13]

Anticounterfeiting Quantum dots can be embedded in labels to defend against counterfeiting[14.]

Some examples of applications of other nanomaterials include:

Pharmaceutical delivery An injectable polymer-nanoparticle hydrogel, for example, was developed so the delivery of drugs, proteins, and cells can be precisely controlled, enabling months-long release of entrapped cargo.[15] The efficacy of insulin administration can also be improved through this research.[16] Nanoparticles can be engineered to permeate the blood–brain barrier, delivering drugs to treat neurodegenerative diseases.[17]

Vaccine stabilization Nanoassemblies can be used to stabilize certain types of vaccines, notably mRNA vaccines, by encapsulating them.[18] In this form, it is easier to inject the vaccine into the human body and to release it over time inside the body in a controlled manner.

Smart windows Silver nanowires arranged into a thin film on a window become a transparent conductive film rather than the familiar reflective mirror from silver behind the window. Running a current through the film can then change the opacity of the window electrically.[19]

2-D semiconductors, graphene, carbon nanotubes, and nanoscale materials These are at the forefront of the next generation of high-tech electronic devices. Active research efforts are dedicated to designing new methods to integrate 2-D or carbon nanotube semiconductors into electronics that are currently silicon based to increase their energy efficiency and heat management.[20]

Higher-capacity batteries High-performance lithium battery anodes have been developed by integrating silicon nanowires as an anode material. When bulk silicon is used as an anode, it undergoes significant changes in volume as the battery charges and discharges, often leading to mechanical failure. Use of silicon nanowires bypasses this problem and increases battery capacity by a factor of ten.[21]

Catalysis Catalysts are used to accelerate chemical reactions, and nanomaterials are well suited for this role.[22] Nanoparticles are particularly well suited for this task, as they contain a high number of active sites per unit mass and can be chemically architected to catalyze various chemical reactions. Advances have been made in converting CO_2 to value-added chemicals using electrified nanoparticle catalysts and in employing palladium catalysts for the combustion of methane, which could improve the efficiency of electricity generation from methane.[23] Nanocatalysts have also been used to improve the rate at which hydrogen can be produced from water through electrolysis.[24] The challenges include developing catalysts that are sufficiently active, stable, and low in cost to produce hydrogen in large quantities and inexpensively.[25]

Over the Horizon

Impact of New Technologies

LOW-CARBON STEEL AND CEMENT PRODUCTION

As an example of how materials science could have impact on a large scale, note that steel and concrete are critical building materials. World production of concrete is some 30 billion tons per year. For comparison, the weight of all the concrete in New York City is around 750 million tons, according to the US Geological Survey.[26] The Hoover Dam involves about 10 million tons of concrete.

Cement production is an extremely carbon-intensive activity, contributing to 8 percent of CO_2 emissions. Limestone is burned to produce lime, thereby releasing CO_2. A number of approaches have potential for reducing the CO_2 footprint of cement production. One focuses on using different material inputs in the production process that release less CO_2. These inputs are the basis for "supplementary cementitious materials," which are formulated differently than traditional Portland cement but nevertheless can substitute for Portland cement in many cases. Another approach incorporates captured CO_2 into concrete during the curing process.[27]

These techniques are all well proven, but further research is needed to make them economically competitive with traditional CO_2-intensive methods of production.

THE APPLICATION OF AI TO MATERIALS SCIENCE

An interesting topic today is whether AI machine learning and modeling will be useful in predicting properties of new materials based on what is known about existing materials.[28] Success has been seen with less complicated materials, but much is to be done and more data are needed for complex materials.

Challenges of Innovation and Implementation

The materials science research infrastructure does not adequately support the transition from research to real-world applications at scale. Such transitions generally require construction of a small-scale pilot project to demonstrate feasibility of potential large-scale manufacturing. At this point, the technology is too mature to qualify for most research funding—because the basic science questions do not address issues related to scaling up—but not mature enough to be commercialized into actual companies. Neither government nor venture capital investors are particularly enthusiastic about funding pilot projects, so different forms of funding are required to bridge this gap between bench-scale research and company-level investment. The support could even go one step further and establish national rapid prototyping centers, where academic researchers find the help and tools necessary to build prototypes and pilot plants for their technology.

Research processes born in the past are also ill suited to the rapid transitions to real-world application. Such processes emphasize sequential steps. The standard process has been to characterize a material and then proceed to a simple demonstration of how it might be used. Today, addressing big society challenges calls for a more scalable system-level approach that involves extensive rapid prototyping and reliable demonstrations to provide feedback on and fill in gaps of knowledge.

Current infrastructure makes this difficult. For example, in collaborations with a medical school, it is often necessary to bring almost-finished products to clinical tests to validate the true impact of a new medical device. With typically less than a thirty-minute window to place a device on a patient and gather data, any malfunction, such as a sudden equipment failure or a loose wire, can jeopardize the entire experiment and potentially halt future patient interactions. The laboratory-assembled devices may not meet this standard of reliability, even if they do demonstrate the value of the underlying science.

Policy, Legal, and Regulatory Issues

REGULATION OF PRODUCTS INCORPORATING NANOMATERIALS

As with regulation in other areas of technology, concerns arise about the appropriate balance between promoting public safety from possible downside risks and the imperatives of innovation to move quickly and leapfrog possible competitors. In the biomedical space, the FDA created a Nanotechnology Regulatory Science Research Plan in 2013.[29] Today, FDA regulation and review of nanotechnology is governed by Executive Order 13563.[30] Outside of biomedicine, regulation and infrastructure for nanomaterials research from the government side is largely based in agencies of the National Nanotechnology Initiative, which include the Department of Energy, the National Cancer Institute, the National Institutes of Health (NIH) more broadly, the National Institute for Standards and Technology (NIST) in the Department of Commerce, and the National Science Foundation (NSF).

TOXICITY AND ENVIRONMENTAL ISSUES

Nanoparticles raise particular concerns because their small size may enable them to pass through various biological borders such as cell membranes or the blood–brain barrier and could affect biological systems in harmful ways. Nanoscale particles inhaled into the lungs, for example, may lodge themselves permanently, causing severe health outcomes, including pulmonary inflammation, lung cancer, and penetration into the brain and skin.[31]

Furthermore, because engineered nanoparticles are, by definition, new to the natural environment, they pose unknown dangers to humans and the environment. There are concerns about incorporating nanomaterials into products that enter that environment at the end of their life cycles. As nanomaterials are employed in and considered for electronic and energy products, it is paramount that those materials safely degrade or can be recycled at the end of a product's life. Policy will be particularly important in shaping responsible end-of-life solutions for products incorporating nanomaterials.

FOREIGN COLLABORATION AND COMPETITION

Historically, the United States has led the world in nanotechnology, but the gap between the United

States and China has narrowed. Notably, in 2016, the president of the Chinese Academy of Sciences openly announced Beijing's ambition to compete in the field of nanotechnology.[32]

As great power competition intensifies, many researchers are concerned that fundamental research could now be considered export controlled. Policy ambiguity can inadvertently hinder innovation by creating obstacles for non-US researchers wishing to contribute to work in the United States and by deterring international collaborations, allies, and partners who are important for advancing the field. In nanomaterials, for example, researchers in Korea are making significant strides with biomedical applications and consumer electronics. There is an urgent need for clarification of these policies, particularly delineating fundamental research and export-controlled research.

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