Integration of energy systems

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This article in *MRS Bulletin* and the framework set out in the introductory article articulate a scenario of renewable electrons and electrification of end use appliances and industrial processes as a plausible paradigm to realize a carbon-free energy economy. The subsequent articles cover specific sectoral or chemical applications of those renewable electrons (e.g., for hydrogen, transportation, building use, electrochemical storage, and within the chemical industry). This article addresses the intersections among and across those sectors. We describe the importance of considering integrated systems and systems of systems as we consider pathways to a decarbonized energy economy. Further, we review and summarize key insights into the innovation challenges that reside at the particular integration interfaces among sectors, and highlight the opportunity for advances in materials and processes that will be critical to successful achievement of economy-wide, low-carbon energy systems.

Introduction

An energy system is composed of multiple components that interact to produce, convert, and deliver energy for a specific end-use. Energy systems can be analyzed through both an engineering and economic lens. In the USA, the residential, commercial, industrial, and transportation sectors represent end-use sectors. Traditionally, end-users were purely consumers of energy and converted that energy to useful services or products. Over the past decade, particularly in the power sector, end-consumers have also become independent, self-generators. In some instances, distributed power generators (such as homeowners, or commercial or industrial facilities) have become "prosumers"—those that produce and sell power and other services to the power grid—and consumers.

Figure 1 shows the flow, conversion, and end-use of energy in the USA for 2020. Petroleum, natural gas, and coal comprised 79% of energy production,[1] with nearly all petroleum use in the transportation sector. Coal is nearly completely used for power generation. Natural gas serves power, industry, and transportation. Renewables such as wind, solar and hydropower serve the electric sector.[2] Total energy consumption rose to about 101 quads (107 EJ) in 2018 followed by a drop to 93 quads in 2020 due to COVID-19 impacts—a level of consumption reduction unseen since 1949. The US Energy Information Administration (EIA) attributes this drop to the COVID-19 pandemic that disrupted all energy consuming sectors, with the transportation sector experiencing the largest (15%) drop.

It is noteworthy that more than two-thirds of energy produced in the USA is "rejected." The bulk of rejected energy typically takes the form of waste heat. For example, many coal power plants have overall plant efficiency of 30–40%, while technologies such as natural gas combined cycle and ultra-supercritical coal gasification are approaching 70% efficiencies.[3,4] Much of the US coal fleet is more than 30 years old,[5] with relatively low overall efficiencies. Significant energy is also rejected in the transport and industrial sectors.

Electrification offers the opportunity to rethink not only how (via what energy carrier) energy services are provided, but also scale. For example, we don't need a 1:1 ratio of

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electricity to replace petroleum for transportation. That ratio is more like 1:5. The whole US transportation industry has a net end-use of 5 quads of energy, while it takes 24.3 quads of mostly petroleum to supply that end-use today. Replacing internal combustion with more efficient electric alternatives means we would only need about 6 quads of electricity to serve the same transportation demand.

Global scaling of low-carbon energy under various scenarios

The United Nation's dedicated body for assessing climate change, the Intergovernmental Panel on Climate Change (IPCC), released the report "Global Warming of 1.5°C" to identify the risks and offer mitigation options in the face of a rapidly warming world.[6] With the exception of "overshoot" scenarios as described by the IPCC, 2050 is the definitive year in which net-zero levels of global greenhouse gas (GHG) emissions must be met. Achieving net zero by 2050 implies all fossil fuel consumption needs to be replaced with or converted to zero-carbon energy alternatives. If GHG emissions continued past 2050, as in the overshoot scenarios, billions of tons of carbon dioxide would need to be removed from the atmosphere annually, using technology that has not yet been applied on a global scale.

The pathways with no overshoot or limited 1.5°C overshoot (as previously described) require a rapid, worldwide energy system transition that results in emission reductions across all sectors, including infrastructure, transportation, buildings, and industrial systems. These pathways require pronounced system changes, particularly within the next 20 years.

Other features of energy system pathways with no overshoot or limited overshoot (as previously described) include:

- Faster electrification of energy end-use
- Lower energy use to meet energy service demand (through enhanced energy efficiency)
- Higher share of low-emission energy sources, particularly before 2050
- Greater share (70–85%) of renewable energy-generated electricity in 2050
- Lower shares of gas-generated electricity (8%) and close to zero shares of coal-generated electricity (0–2%)
- Higher shares of nuclear- and fossil fuel-generated electricity with carbon dioxide capture and storage

A more recent analysis by the International Energy Agency (IEA) focused on achieving net-zero energy systems globally, and outlines fundamental transformation of global energy systems.[7] While scenarios of pathways to future net-zero energy economies are derived from a set of assumptions and limited by modeling capabilities, they serve as useful benchmarks to inform decision-making and, in particular, needed innovation. The IEA's path to net-zero emissions outlined is "narrow but achievable," and implies that decisions made within the next decade will have profound impact on that path's trajectory. Per their analysis, and central assumptions, a 40% larger world economy will need to use 7% less energy in 2030, achieved through efficiency measures and significant electrification. Reducing carbon dioxide emissions

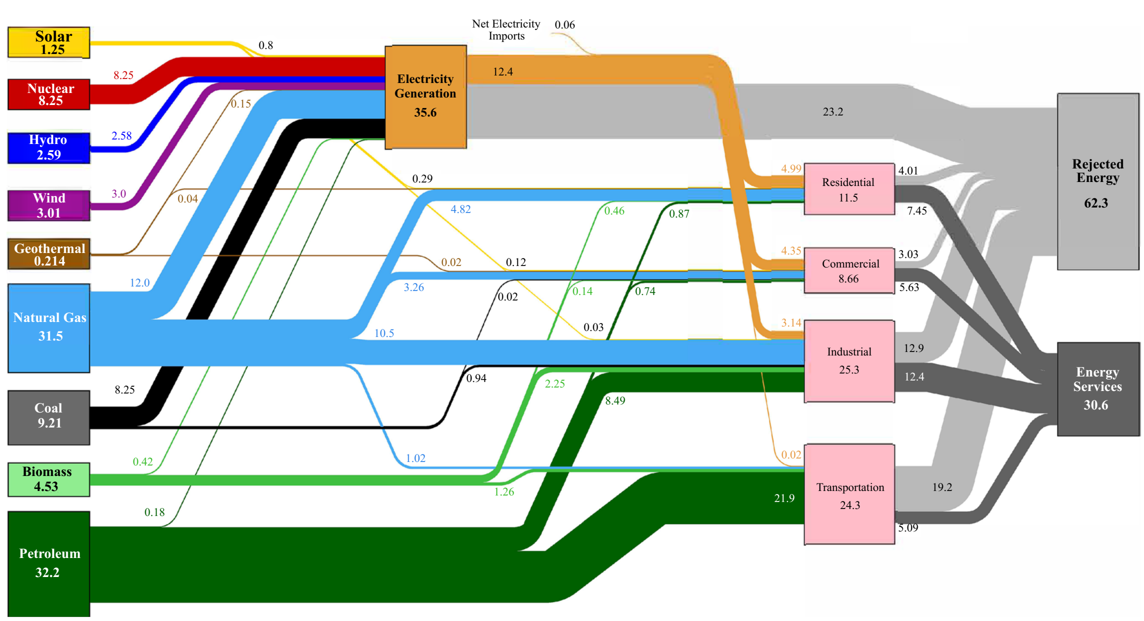

Figure 1. Estimated US energy consumption in 2020.[2] Source: Lawrence Livermore National Laboratory.

would be complemented by a 75% drop in fossil fuel-driven methane emissions; deploying renewable energy technologies plays a key role in this systemic transformation as shown in **Figure 2**. By 2025, coal would be globally displaced by renewable energy sources (e.g., hydro, wind, solar PV, bioenergy, geothermal) as the dominant electricity provider. By 2030, renewable energy would provide nearly 40% of electricity supply and meet 80% of global electricity demand.[8]

Cheaper renewable energy technologies and a cleaner electricity sector position electrification as the key tool to reduce emissions, dramatically displacing fossil fuels. Electric vehicles will comprise more than 60% of global car sales by 2030, with all new sales of internal combustion engine cars ceasing by 2035. Other sectors previously dominated by fossil fuel dependence will also electrify their technologies, including heat pumps in buildings and electric furnaces for steel production. All coal and oil power plants without emissions abatement measures in place will be phased out by 2040.

Today's hydropower and nuclear energy sectors serve as essential foundations for future transitions; solar and wind sectors see the greatest demand for rapidly scaled integration. Solar photovoltaics (PV) and wind-generated energy will need to be integrated into the global energy system at a rate of 630 GW and 390 GW, respectively, on an annual basis up to 2030—a quadrupled rate of integration than the records set in those sectors in 2020. With these 2030 targets in place, the pathway to 2050 leads to an energy sector based mostly on renewable energy; renewable resources will generate 90% of the world's electricity. Solar PV and wind comprise nearly 70% of supply combined, leveraging their increased capacities of 20-fold and 11-fold, respectively.

Decarbonizing power may include carbon capture utilization and storage (CCUS), advanced nuclear and renewable generation. According to the IEA, the key to unlock the power of these decarbonized domains is an 80% increase in electricity network capacity—two million km of transmission lines and 14 million km of distribution lines—over the next decade.[8]

Understanding integrated energy systems: Definitions; the framework from materials, to components, to devices to "products" to system solutions

A flexible energy system will be paramount if we want to maintain energy reliability and competitiveness while simultaneously deploying renewable energy resources. **Figure 3** illustrates how flexibility is contingent on energy sources and carriers linked and coordinated across infrastructures, with institutional coordination facilitating energy market adjustments and increased market footprints to accommodate customers.[9]

An integrated energy system (IES) provides the flexibility needed to accommodate rapidly scaling energy sources across geographic regions. Temporal and geographic coordination of individual system components enables the system to dynamically optimize energy output, thereby enabling system-wide delivery of reliable and cost-effective energy services. A departure from a one-size-fits-all energy system toward a flexible IES that accommodates local and regional energy nuances has the potential to bring with it lower and reliable energy costs, reduced risk associated with environmental impacts, and better stewardship of natural resources.[10]

The opportunity space among IESs is defined by the design impacts of each component within the system—from the molecular composition of materials and their influence on component performance, to the manufacturing process of products and their successful delivery and integration into a larger energy network.

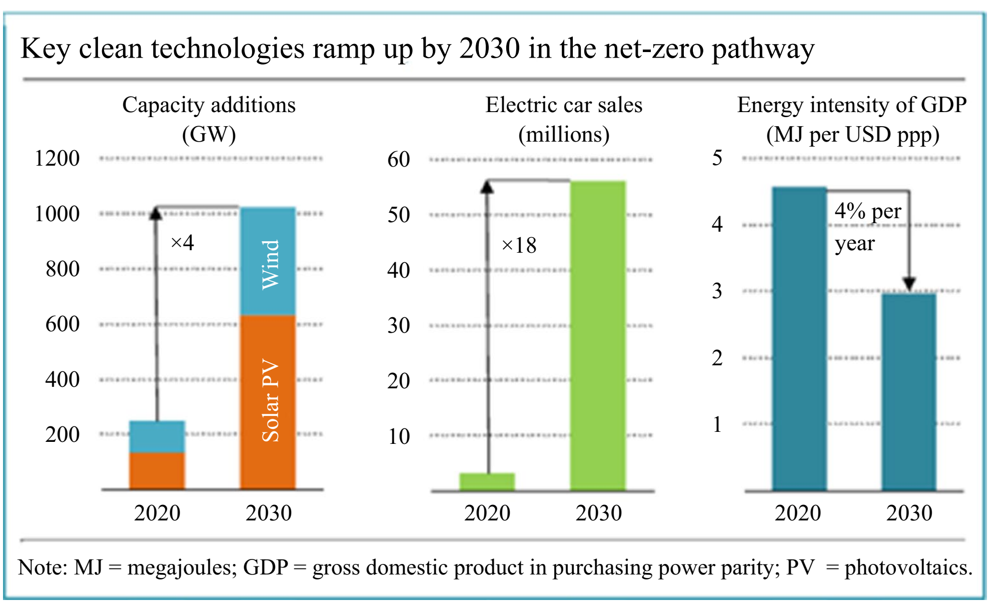

Figure 2. Anticipated changes in renewable power, electric vehicles, and energy intensity of GDP for the International Energy Agency (IEA) net-zero scenario.[7] Source: IEA.

Human behavior is the ultimate variable in IESs, influencing the system's ability to anticipate and respond to demand at the individual and component levels within and among IESs.

There is no singular system design for IESs; design variations have been and will be shaped around the community needs, energy sources and their various output mechanisms.

Sector examples of integrated energy systems

Power systems

The traditional structure of the US power system relies on large generators of energy (e.g., power plants) providing one-way power flow to end-users via an interconnected network (i.e., grid) of electricity substations, transformers, and power lines. Local grids are connected to form larger grid networks to enable coordination of electricity supply across the nation.[11] This traditional structure relies on energy utilities to coordinate grid operations in real time to manage fluctuating load demands (i.e., how much energy end-users need based on various factors such as time of day, seasonal changes, and extreme weather events and disruptions).

Fossil fuels, nuclear energy, and renewable energy comprise the "energy mix" in the USA; fossil fuels, especially natural gas and coal, have remained the dominant source of electricity generation for US end-users (**Figure 4**) until recent declines in coal power generation. Natural gas accounted for 40% of electricity generation in 2020—a historic year in which for the first time in the last 70 years, renewables produced more energy than either coal or nuclear.[12]

Though fossil fuels comprise most of the energy generation, renewable energy (e.g., biomass, geothermal, hydroelectric, solar, wind) has experienced marked growth in its share of the energy mix within the past decade. Renewables generated 20% of total US electricity in 2020, with wind and hydropower comprising 43% and 37%, respectively, of that renewable share (**Figure 5**).

Distributed energy systems—Emergence of PV in particular, now batteries w/PV

Transitioning from a centralized model of power generation and delivery to a decentralized model that supports multiple actors and energy sources entails the build out of distributed energy systems (DESs).[13] In the residential sector, solar PV panels, small wind turbines, and fuel cells are common components of a DES. A more diverse DES portfolio is common in the commercial and industrial sectors, which may include the addition of hydropower, biomass, municipal solid waste, and energy storage. The growing availability of these renewable energy options, paired with smart metering technologies and regulations to better monitor and manage consumption, will facilitate transitions to DESs across these sectors.[13]

DESs are growing in the USA for a variety of reasons, including:

- Affordability: More homeowners and businesses are attracted to renewable technologies, such as solar panels, as these technologies continue to become more affordable at point-of-sale and demonstrate long-term cost savings.
- Resiliency: DESs can provide electricity during power outages and high-energy demand days.
- Efficiency: By relying on local energy generation, DESs reduce "line loss" (i.e., wasted energy) that occurs in the traditional grid's transmission and distribution processes.

As traditional generation systems are replaced with DESs, new challenges emerge for consideration. Their footprint and proximity to end-users impacts the visual esthetics of a community. Some DES system processes—such as incineration or combustion—require steam or cooling provided by local water resources. DESs are subject to a variety of local, state, and federal regulations, which can impact the financial incentives to implement them.[14]

DESs not only begin the transition to more autonomous energy generation at the local level, but also support the end-user's transition from traditional consumer to prosumer—one who produces their own energy for consumption. Solar power continues to be the most popular renewable choice for US households, with total capacity reaching 97 GW in 2020, enough to power 18 million homes (**Figure 6**).[15] Industry

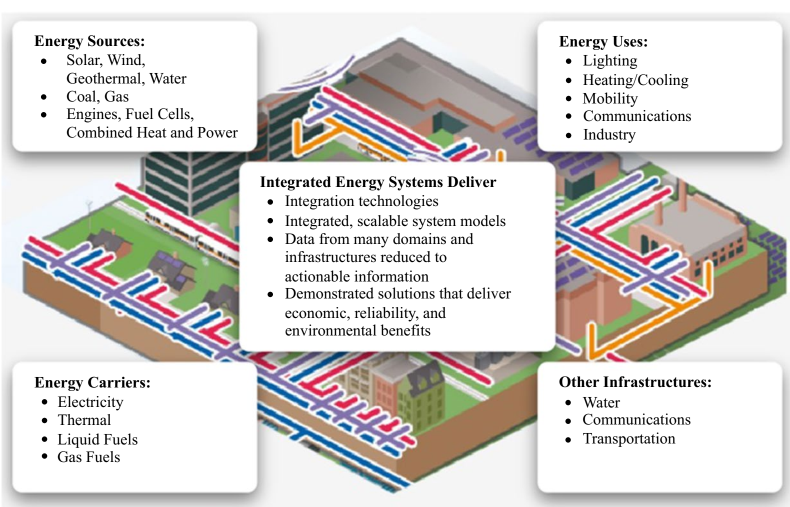

Figure 3. Example of an integrated energy system scaling energy vectors and infrastructures at the customer, city, and regional levels.[9] Source: M. O'Malley et al.

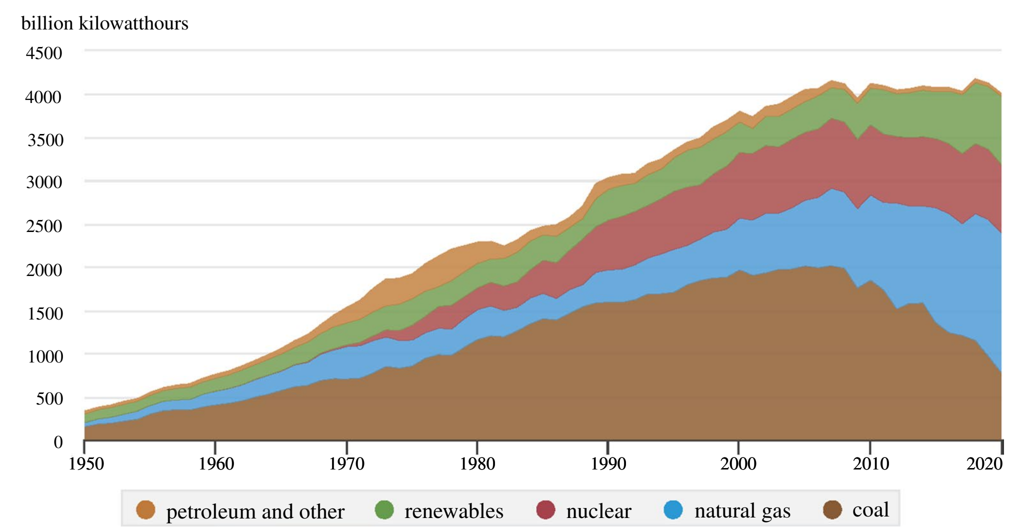

Figure 4. US electricity generation by energy source.[12] Source: EIA.

infrastructures will benefit from minigrid deployment to provide 40% capacity necessary for universal access to electricity by 2030.[17]

Some developing countries that lack national energy infrastructure have modeled successful minigrid and microgrid implementation in rural and remote communities. These minigrids have typically leveraged an energy mix of solar PV, diesel fuel, and batteries; increasingly this energy mix has shifted away from diesel to incorporate more renewable energy sources like small wind and small or micro hydroelectric energy. Further, minigrids have increasingly become connected to the main grid, as seen in countries like Cambodia, Indonesia, Nepal, and Sri Lanka.[18]

has taken note of this trend, and has begun to incentivize US households toward more prosumer choices; some companies now bundle solar panels with battery systems and electric vehicle chargers.[16]

Minigrids

Minigrids, though modest energy generators (10 kW–10 MW),[17] are also expanding, particularly for large installations such as campuses and bases, and are poised to play a larger role in global energy transition plans. More than one billion people still lack access to a form of modern electricity, according to the US Agency for International Development, and the vast majority of those (80%) live in rural communities.[17] A global transition away from traditional energy

Transformation of power systems

There is a massive transformation of the power system occurring around the globe (**Figure 7**). Succinctly, the left diagram articulates the historical traditional power system in which large power stations, often remotely located, are connected to a one-way transmission grid that delivers power to end-users. The right diagram shows the increased use of DESs, and the evolution of two-way power flow (represented by bidirectional arrows) indicating a much more heterogenous (e.g., technology, size, spatial, temporal) mix of power generators. Those DES systems may include PV, batteries, wind, hydrogen, diesel, or other energy sources, to serve local loads and provide services to the power system (under the appropriate market and regulatory conditions). As this evolution advances, incorporating renewable energy sources into larger energy grids poses challenges to grid operators. The variable nature of wind and sunlight as energy sources—while manageable with advanced forecasting systems in combination with increased DESs—remains a challenge for grid

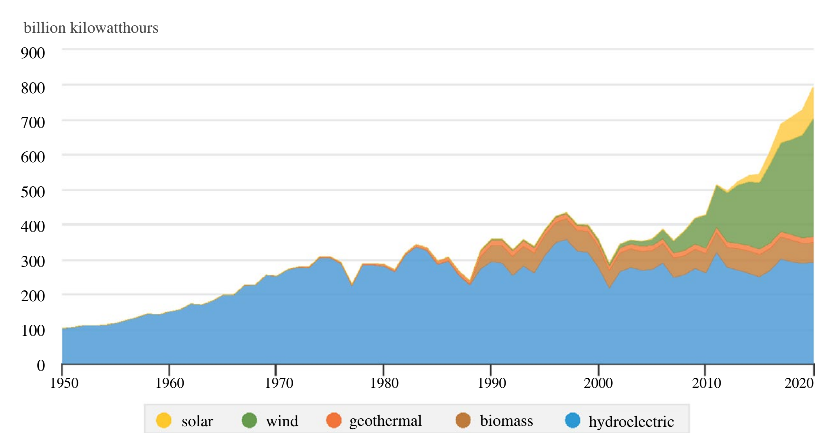

Figure 5. US electricity generation from renewable energy sources, 1950–2020.[12] Source: EIA.

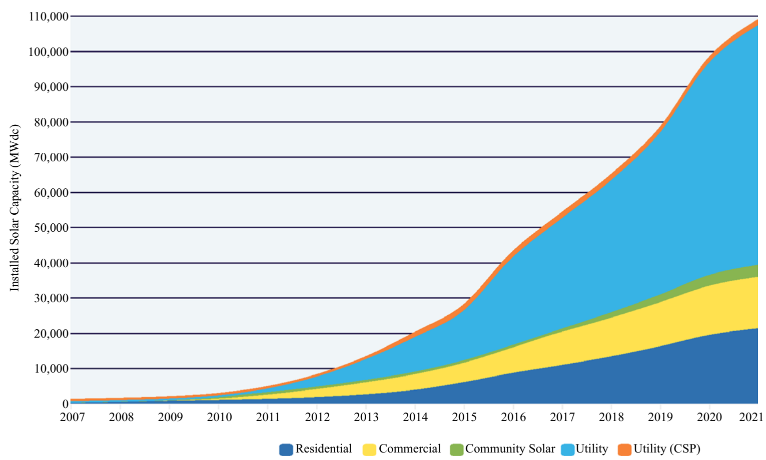

Figure 6. Cumulative US solar installations, 2007–2021.[15] Source: Solar Energy Industries Association.

operators attempting to anticipate future energy supply, demand, and loads.

Controllable and responsive loads are an opportunity to better match the variability of wind and solar PV generation. Controllable loads can be turned off by the utility when the total load in a region exceeds the energy available (e.g., when the wind is not blowing and the sun is not shining). Responsive loads are similar, but they automatically respond to price signals to reduce loads when the prices are high (e.g., when demand is close to exceeding supply). At a large scale, opportunities include water electrolysis to produce hydrogen that can be used as energy storage for the grid or for many applications, as well as water desalination and pumping. At a more distributed scale, electric water heaters and electric heating and cooling for buildings have inherent storage and thus can be shut off at times without impacting building occupants.

DESs can provide a degree of energy autonomy at the local—even household—level by enabling self-generated energy and bulk power and storage. Energy storage balances fluctuations in solar and wind availability, allowing users to capitalize on high-generation days by capturing and storing energy for future use during high-demand periods. Energy autonomy provides a degree of resilience and reliability; when power flow to the grid is disrupted by weather or natural disasters, the ability to disconnect from the impacted regions enables energy continuity. Conversely, as energy production increasingly becomes decentralized and empowers end-users to create their own energy, the opportunity emerges for multiple power flow pathways; energy prosumers may sell energy (and other services) to their grid.

Energy meters (on homes and businesses), sensors (on transmission lines), and synchrophasors (on grids) form a smart grid system that can monitor supply, demand, and flow of electricity in real time, which allows for system-wide management, more economic efficiency, and increases in system reliability. Distribution management systems can be used in conjunction with synchrophasor data to better predict and avoid those disruptions by adjusting grid controls. This smart, tailored response mechanism means energy consumption is based on more accurate demands, with potential to reduce energy costs. Industrial facilities benefit from the additional sources of energy that DESs provide, reducing their energy consumption costs as well.

As millions of DESs are deployed at customer locations—and new methods of control are needed to successfully manage such a large number of distributed assets—a concept called autonomous energy grids (AEGs) could be used to enable resilient, reliable, and economic optimization.[19] The security and

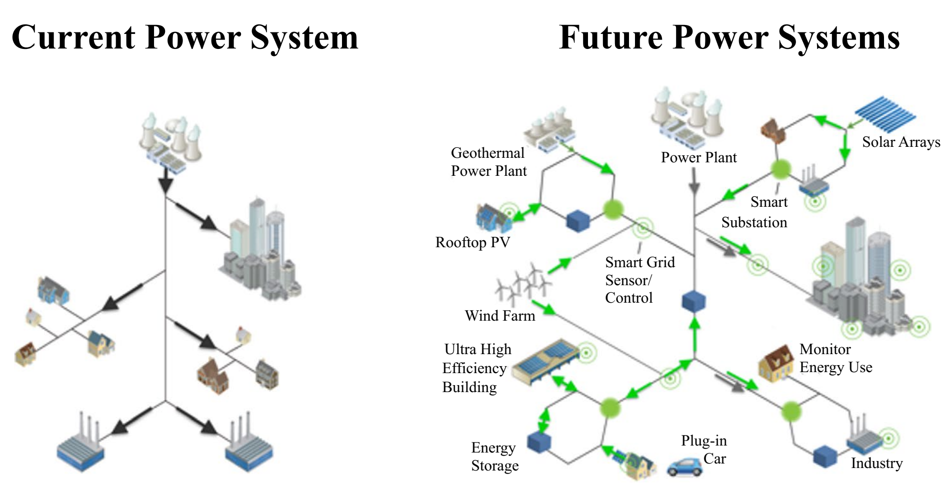

Figure 7. Conceptual contrast of traditional power system configuration (left) with one-way power flow, compared to evolving system with distributed resources, managed loads, and two-way power flow (right). Source: National Renewable Energy Laboratory. Figure by David Hicks, National Renewable Energy Laboratory. PV = photovoltaics.

resilience of AEGs lies in their scalable, reconfigurable, and self-organizing control infrastructure, providing an ability to self-optimize and operate either in isolation or as part of a larger, interconnected grid.

Growing dependence on digitalized energy systems will require an unparalleled demand for high-performance computing that is robust enough to store and process data, sophisticated enough to forecast and anticipate energy demands at scale, and resilient enough to cyber attacks. The US Government Accountability Office warns that industrial control centers managing grid generation and distribution have remained mostly unchanged since the 1970s and thus are at great risk to cyber attacks. The USA has already experienced these cyber intrusions—a grid attack in 2019, followed by a ransomware attack on an oil pipeline in 2021.[20]

Buildings

Electrifying energy production must be complemented by electrified energy consumption processes in order to fully realize an IES. Also known as "sector coupling,"[21] linking the electricity and gas sectors on the energy supply side with major energy consuming sectors on the demand side—such as transportation, buildings, and households—will yield its own challenges for efficient energy storage and distribution solutions, especially in urban centers with more diverse building types at higher densities. In the USA, office buildings consume the most energy in the commercial building sector, with consumption dominated by heating, ventilation, and air conditioning (HVAC), and lighting; whereas health care buildings such as hospitals that provide life-saving services do not consume as much energy.[22] Societal values (such as cost of carbon or other traditionally categorized "externalities") placed on private organizations and public services will also shape how energy consumption is prioritized in a decentralized IES.

Energy-efficient building design can contribute to a more effective energy system transition. Infrastructure projects present opportunities to apply innovative materials and technologies to retrofit and optimize new building components (e.g., HVAC, doors, windows, controls, insulation, lighting).

Households

Space heating and air conditioning are the most demanding energy consumption activities in US households, which vary on a seasonal basis based on factors such as geographical location and home size and structure. Year-round energy consumption by water heating, lighting, and refrigeration account for less than half of a household's total energy consumption.[23]

Demand-side load management opportunities will continue to grow. As households switch to rooftop solar panels, electric vehicles, home batteries and heat pumps, they can operate as self-contained energy supply and demand units capable of enabling more grid flexibility.[24]

Behavioral changes are the hardest to anticipate, and will remain one of the unique challenges for successful energy transformation. System flexibility will remain a critical characteristic in order to accommodate shifting priorities and preferences of households. To date, demand management has shown to add value for peak reduction and peak shifting, nearly always within a given day. Upcoming innovations exploring longer-duration (>24 h) load shifting would add new sources of flexibility.[25] Further, insights into peer-to-peer/neighbor influences on renewable energy adoption continue to offer new insights to expand adoption and are being included in increasingly sophisticated energy models.[26] Diverse choices in DES adoption can benefit the system as a whole, depending on community resources rather than requiring a robust portfolio for each individual household.

Moving from sector systems to economy-wide integrated systems of systems

Decarbonizing the way we produce, transport, store, and consume energy is the critical foundation needed to facilitate a sustainable and long-term energy transition to a net-zero energy economy. Fossil fuels—the dominant energy source through which we produce electricity—are being replaced by renewables, but some modes of transportation and industrial sectors will be harder to decarbonize. Additionally, decarbonizing our energy processes must be complemented by decarbonized materials to create not just operational/logistical change, but set the stage for a circular economy where clean energy is used to create goods and services that are also inherently clean and can remain a part of the energy life cycle in perpetuity.

Energy-dense fuels for aviation and marine

Airplanes need energy-dense fuel to carry heavy loads across long distances without refueling. This has resulted in a concerted focus on biofuels. The contents (i.e., blend ratios) of jet fuel are highly regulated, but biofuels can meet those thresholds through sustainable aviation fuel (SAF). In 2020, the US Department of Energy (DOE) released a report on SAF, which summarized the key learnings from three DOE-supported workshops and outlined a research and development (R&D) strategy to meet this growing demand.[27] A key takeaway from this report is the need to reduce the cost of SAF and optimize the value proposition to accelerate deployment; the authors note that the key cost drivers are feedstock costs, yields, and plant capital recovery. R&D is needed for food waste and wet waste processes to produce SAF that can both fuel present-day jet engines and also cancel out the very carbon those engines produce. The GHG emissions that are removed or diverted during this SAF production process cancel out the emissions produced during jet engine combustion. But, we must be cognizant of not simply transferring one problem in one domain to another; producing biofuels may require considerable arable land for feedstock, and other industries will compete for biofuels. Fuels made from crop waste or municipal waste alleviate stressors placed on exhausted land resources, but supply of these wastes is limited.[28]

A similar scenario exists in marine shipping. Approximately 80% of global trade by volume is carried by sea, with global shipping accounting for more than 2% of total global carbon dioxide emissions.[29] The International Maritime Organization has mandated at least a 50% reduction in GHG emissions by 2050 (as compared to 2008 levels), which will require low-carbon, energy-dense fuels.[30] Activities are ongoing to develop and deploy these low-carbon, energy-dense fuels for marine use, including low-carbon ammonia, hydrogen, methanol, biofuels, and liquefied natural gas (LNG) with CCUS or renewable gas LNG.[31–33]

Industrial-Chemicals

The chemicals industry in the USA consumes more than 3000 trillion Btus per year to produce more than 70,000 products, with large-volume chemicals (e.g., ammonia, ethylene, propylene, methanol, benzene, toluene, and xylene) accounting for the majority of this energy demand.[34–36] While it is a vast and diverse industry, decarbonization strategies are targeted at electrification (for heat input and reactant conversion), energy efficiency improvements, and alternative, low-carbon (renewable and recycleable) feedstocks. Considering energy efficiency improvements, more than 80% of industrial chemical processes require a catalyst, providing an avenue for energy savings through materials advancements. It has been estimated that catalyst and related process improvements could save as much as 13 EJ and 1 Gt of carbon dioxide equivalent per year by 2050 versus a "business-as-usual" scenario.[34] When considering electrification and low-carbon feedstocks, there has been a marked rise in pursuit of synthesizing chemical products from carbon dioxide, water (as a hydrogen source), and nitrogen, with electricity as the primary energy input.[37,38] Utilizing carbon dioxide and water as feedstocks has the potential to decouple chemical production (of carbon-based chemicals) from fossil resources; however, a recent study reported that it will require significant production capacity of renewable electricity, on the order of 18 PWh, which corresponds to more than 55% of the projected global electricity production in 2030.[36] It is also important to note that low-carbon hydrogen is an enabler of this decarbonization strategy as it is a heavily utilized feedstock in the chemicals industry.[39–41]This low-carbon hydrogen can be generated through water electrolysis with renewable electricity, but also through steam methane reforming of natural gas combined with CCS, biomass gasification with CCS, and methane pyrolysis.

Industrial—Steel and concrete

Steel furnaces and cement kilns reach very high temperatures (in excess of 1000°C) during their respective manufacturing processes by burning fossil fuels[28] and often entail chemical processes that generate additional carbon dioxide.

Steel production using electric arc furnaces that convert recycled steel can reduce emissions if carbon-free power is used in them. However, steel products are limited by contaminants, thus fresh steel has been traditionally produced using blast furnaces. Historically, that process has required coke as a reducing agent, but direct reduction of iron processes are being developed that use natural gas and/or hydrogen as the reducing agent. H2 Green Steel, a steel manufacturing company based in Sweden, has created a fossil-free manufacturing plant; it integrates a new carbon-free energy process that replaces the traditional blast furnace with direct reduction reactors, and manages its waste byproducts. The process utilizes renewable-produced hydrogen and relies on electrification of every process, an example of highly integrated system of systems for low-carbon processes and products.[42]

Concrete is another high-GHG-content material that is prevalent worldwide. About half of concrete's emissions come from producing "clinker," a binding agent created by heating ground-up limestone in giant kilns; burning fossil fuels (usually coal) heats the kilns, and the heating process releases carbon dioxide from the limestone.[43]

Replacing coal with biomass or municipal waste products is also a viable alternative, but most recent projects have focused on reducing the amount of clinker needed for concrete, or the need for concrete at all:[44]

- A blend of limestone and calcined clay developed by the Swiss Federal Institute of Technology in Lausanne, or EPFL, has been used to create a type of cement capable of reducing its carbon footprint by 40 percent.[45]
- An adjustment to the ratio of calcium to silica in concrete developed by a Massachusetts Institute of Technology team has produced a stronger version of the material, thereby reducing cement volume and its carbon emissions by up to 50 percent.[46]

In heavy industry where viable fossil fuel replacements have yet to emerge, carbon emissions can be captured, injected deep underground, or used in a secondary process.[28]

Overcoming the material limits of concrete is edging closer to resolution, with solutions on the market or close to commercialization.[47] Other approaches include entirely new, bacteria-based building materials that live and multiply; a self-generating brick as strong as cement can remove carbon dioxide from the air.[48]

Implications for innovation

We have previously outlined key aspects of IESs, spanning material systems through integrated power/heat/chemical/mobility/built environment "systems of systems." Achieving GHG goals as outlined by the IPCC requires economy-wide solutions. Not only must solutions address direct emissions but also the emissions associated with materials and processes and end-uses across an entire economy. Achieving such bold ambitions demands new innovations in technologies and system solutions for decarbonized power as well as the power-to-X processes to decarbonize the most difficult-to-decarbonize energy services and materials.

The integrated systems nature of our energy economy is depicted in **Figure 8**. Decarbonized power is the backbone of the system, which relies on renewables, nuclear, and fossil with CCUS. Power then is critical to industrial processes for hydrogen, ammonia, and synthetic fuels. Achieving a reliable, affordable, resilient, and secure decarbonized energy economy will require significant innovations—in power systems, integrated systems, and use of power (and other energy sources) for the creation, manipulation, and formation of low-carbon chemicals and fuels. Carbon management, through the selective use of biofuels, carbon capture, land use and forestry, agriculture and ocean/air management will also be increasingly important to realizing such a vision.

In addition to low-carbon electricity, net-zero energy economies will require electrified substitutes for most fuel-using devices; alternative materials and manufacturing processes, including CCUS for structural materials; and carbon–neutral fuels for the parts of the economy that are not easily electrified. The innovation landscape is both broad and deep, as only a finite number of technology choices exist today for each functional role. Achieving a robust, reliable, affordable, net-zero emissions energy economy requires researching, developing, demonstrating, and deploying those candidate technologies at a speed and scale that is unprecedented.

Furthermore, while the IPCC, IEA, EIA, and related academic literature articulate possible pathways to decarbonized power systems and broader energy economies, it is important that the tools used to evaluate the pathways, economics, and policy options incorporate as much detail as possible within the modeling environment, and the analytic teams work to incorporate the most recent and best knowledge of technology options. However, most energy technologies are characterized by cost and performance with limited technical details. Such limited technical parameterizations are less reasonable as electricity markets become more diverse and dynamic, and energy ecosystems become increasingly cross-coupled. For example, at a fundamental level, including details of technologies that span the time scales governing power system operations—sub-second (for power system stability) to minutes, days, and seasons (for hydropower and maintenance scheduling)—is limited to very few power system modeling tools. Looking deeper across the energy economy, increasing challenges arise considering coupling of building loads (including on site generation, electric vehicle charging, occupancy dynamics, and occupant behaviors), mobility loads from electric vehicles, trains, trucks; power to chemical or other industrial processes, power generation, and heat supply. In addition, most modeling approaches and nearly all the integrated assessment models (IAMs) incorporate only commercially available and well characterized (with regard to cost and performance) technologies, which hinder transparent evaluation of new technologies.

A conceptual figure for this modeling architecture is shown in **Figure 9**. As shown in Figure 9a, core aspects of the framework include an appropriate physics-based representation of critical processes and systems, both of physical infrastructure and earth systems, and appropriately capturing the appropriate characterization of human and institutional dynamics in the economic representation. Further, building off the successful

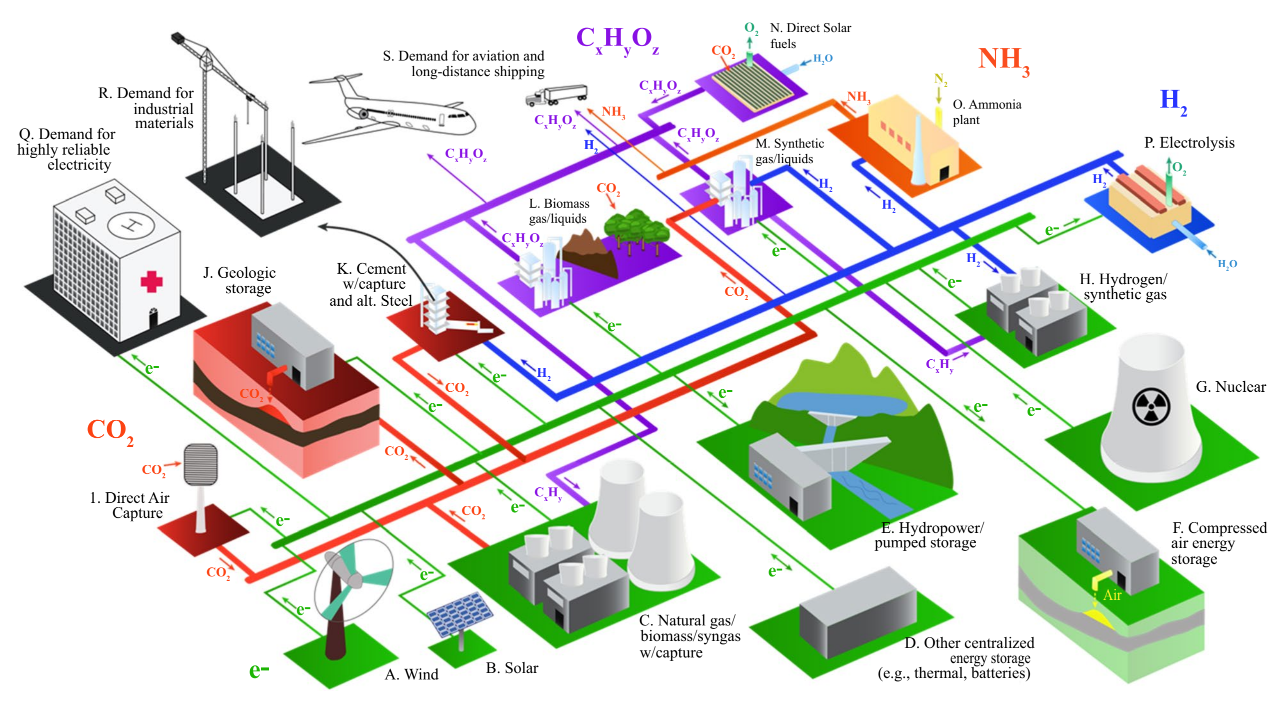

Figure 8. Net-zero energy systems.[49] Source: S. J. Davis et al. Reprinted with permission from AAAS.

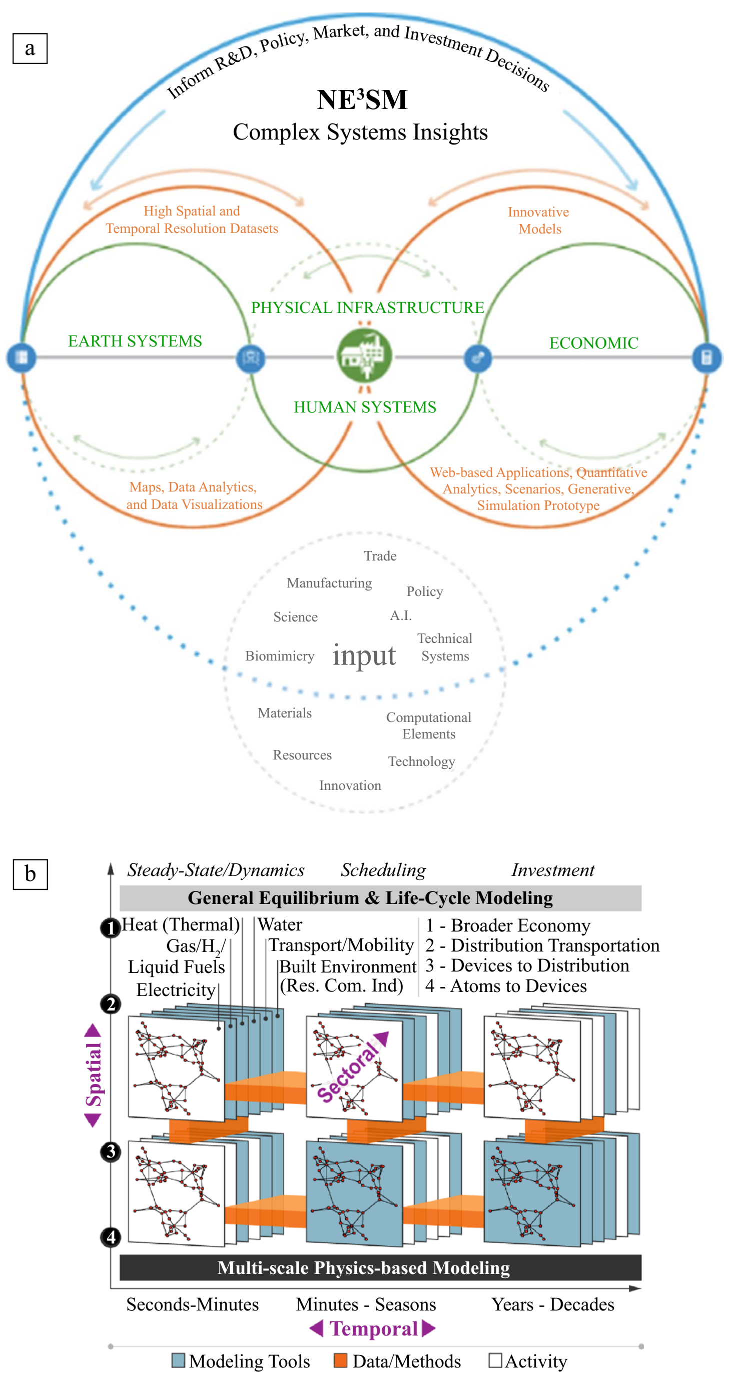

Figure 9. (a) Conceptual Model of National Energy-Economic-Environmental System Model (NE3SM) Community Platform. Source: National Renewable Energy Laboratory (NREL). Figure by Stacy Buchanan, NREL. (b) Architecture of Scalable Integrated Infrastructure Platform, developed by NREL for co-optimization with Julia, across sectors, spatial, and temporal scales to effectively incorporate physics into energy-economic modeling as appropriate. Source: NREL. Figure by Alfred Hicks, NREL. A.I. = artificial intelligence.

model of the community earth system modeling platform, researchers from across the USA, Europe, and a few other regions have begun to create an Energy-Economic-Engineering-Environmental Community Platform through efforts such as OpenMod, Hierarchical Engine for Large-Scale Infrastructure Co-Simulation (HELICS), and Scalable Integrated Infrastructure Platform (SIIP).[50]

However, significant hurdles must be overcome to achieve the concept modeling architecture illustrated in Figure 9b, which shows the breadth of temporal, spatial, and sectoral scales to address. Misalignment of the temporal or spatial scales that govern the operation of different sectors, complex and complementary interactions between sectors, and mismatching mathematical modeling paradigms are just a few of the fundamental challenges faced by the community developing high-fidelity, multisector models. Recent advancements in high-performance computing, mathematical programming solution techniques, and other fields show promise for tackling these challenges, but significant advances are still required. Furthermore, inconsistencies in data and modeling assumptions across sectors exacerbate challenges representing multisector interactions, such that in many cases fundamentally new modeling capabilities must be developed to represent well-established representations within a coherent framework. These issues underscore a need for a community-based modeling framework with appropriate abstractions so that modelers with expertise in different sectors, mathematical modeling paradigms, and computational techniques can contribute to the benefit of the entire community.

Materials and process innovations

Accelerating the deployment of next-generation energy systems is inextricably linked to materials and process innovation across areas of production, conversion, delivery, and sustainability. Some recent notable advancements in these areas include the development of power-to-X processes enabling the conversion of low-cost intermittent electricity to chemical products via waste feedstocks,[51,52] physical and chemical sorbents enabling the efficient capture of waste carbon dioxide,[53] wind turbine blade design,[54]

Table I. Key energy carriers and conversion interfaces for a net-zero energy economy.[49] Source: S.J. Davis et al. Reprinted with permission from AAAS.

From	To			
e^-	e^-	H_2	$C_xO_yH_z$	NH_3
		Electrolysis ($5 to $6/kg H_2)	Electrolysis + methanation	Electrolysis + Haber–Bosch
		Electrolysis + Fischer–Tropsch		
H_2	Combustion		Methanation ($0.07 to $0.57/$m^3$ CH_4)	Haber–Bosch ($0.50 to $0.60/kg NH_3)
	Oxidation via fuel cell		Fischer–Tropsch ($4.40 to $15/gallon of gasoline-equivalent)	
$C_xO_yH_z$	Combustion	Steam reforming ($1.29 to $1.50/kg H_2)		Steam reforming + Haber–Bosch
	Biomass gasification ($4.80 to $5.40/kg H_2)			
NH_3	Combustion	Metal catalysts (~ $3/kg H_2)	Metal catalysts + methanation/Fischer–Tropsch	
	Sodium amide			

solar PV,[55] advances in batteries,[56] phase change materials,[57] and metal complexes for high-temperature gas turbines.[58] The latter innovations allow such turbines to burn fuels ranging from natural gas to pure hydrogen, enabling significant infrastructure to transition away from GHG-emitting processes toward an effective and valuable role in a decarbonized energy economy.

As outlined in Davis et al.,[49] there are multiple critical conversions for a net-zero economy. **Table I** outlines multiple approaches to cross power to core chemicals for a decarbonized energy economy, and lists known approaches.

The core materials/chemistry is well understood for nearly 100 years for many of these, but the opportunity presents itself to rethink approaches. That is, the application of advanced artificial intelligence methods to evaluate new materials for catalysts—considering computational capabilities available today—combined with multiple activation methods (e.g., heat, light, vibration, etc.), as well as evaluating design for purpose materials. Further, advanced synthetic methodologies will be needed to access these next-generation materials, especially given the emphasis on multifunctionality and precise control over material properties at the atomic-, nano-, and mesoscales.[59] More importantly, as power systems evolve to incorporate significantly more variable renewables, the technologies for power-to-chemicals must also evolve to not only efficiently and cost effectively conduct their primary purpose, but also to be a value-added element of the broader energy system. One of the major strategies to maximize value requires fundamentally rethinking materials and processes for lowest possible capital costs and flexible (e.g., dynamic versus static) operations in order to efficiently and cost effectively operate while providing value-added services for the power system and taking advantage of low-cost electrons during times of high generation.[60,61]

Conclusions

Realizing a decarbonized energy economy poses an inspiring set of challenges, particularly from a materials and process perspective and when considering IESs. Looking across the energy economy, strategies based on decarbonized power as the backbone of the energy economy pose fundamental strategic differences from history. Separate sectors, particularly petrochemicals, power, and mobility are becoming increasingly integrated. The forthcoming deeper sector integration implies the need not only for reassessing the historical approaches to materials for energy systems and processes, but also for rethinking our innovation ecosystem. That is, traditionally, fundamental research in materials has been performed by teams independent from the device and process development engineers. Given the time constraints to innovate and scale to commercially viable projects at sufficient scale to achieve deep decarbonization by 2050, creating multidisciplinary teams spanning fundamental science, computational sciences, and engineering, with behavioral scientists and business managers from across multiple sectors, will be increasingly important. These cross-functional teams will hopefully accelerate the time from fundamental innovation to commercial viability and roll out.

Disclaimer

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Conflict of interest

On behalf of all authors, the corresponding author states that there is no conflict of interest.

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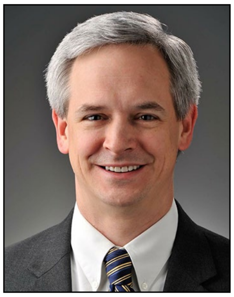

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