This century will witness a major transformation in how energy is acquired, stored, and utilized globally. The impetus for this change comes from the deep impacts that both developed and developing societies have had on our planet’s environment during the past century, and the projections going forward of what will happen if we do not act transformatively within the next 2 decades. This paper describes the basis for a meeting held in October 2018 on the need for decarbonization in our energy landscape, and specifically the status and challenges of the science that provides the foundation for such technology. Within the realm of decarbonization in energy generation lies the science of solar energy conversion using new or improved photovoltaic materials and artificial photosynthesis for water splitting and other energy-storing reactions. The intimately related issue of renewable energy storage is being addressed with new strategies, materials, and approaches under current investigation and development. The need to improve the interactions between scientists working on these connected but separately considered challenges and on the transition of scientific achievement to practical application was also addressed, with specific efforts enumerated.

Addressing the challenge of carbon-free energy

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This century will witness a major transformation in how energy is acquired, stored, and utilized globally. The impetus for this change comes from the deep impacts that both developed and developing societies have had on our planet’s environment during the past century, and the projections going forward of what will happen if we do not act transformatively within the next 2 decades. This paper describes the basis for a meeting held in October 2018 on the need for decarbonization in our energy landscape, and specifically the status and challenges of the science that provides the foundation for such technology. Within the realm of decarbonization in energy generation lies the science of solar energy conversion using new or improved photovoltaic materials and artificial photosynthesis for water splitting and other energy-storing reactions. The intimately related issue of renewable energy storage is being addressed with new strategies, materials, and approaches under current investigation and development. The need to improve the interactions between scientists working on these connected but separately considered challenges and on the transition of scientific achievement to practical application was also addressed, with specific efforts enumerated.

climate change | decarbonization | energy | solar energy | renewable energy

The current century will witness a major transformation in how energy is acquired, stored, and utilized globally. At this point, nearly one-fifth of the way through the 21st century, changes are clearly discernible but more profound ones are still to come. The challenges we face in carrying out these transformations range from scientific and technological to societal, cultural, and economic in how we live, work, and play. The impetus for these changes comes from the deep impacts that both developed and developing societies have had on our planet’s environment during the past century and the projections going forward of what will happen globally if we do not act. Real and projected urbanization together with growing global population make it clear that we must act now.

The impact of industrialization and modern society on the world-wide environment has been written about and discussed extensively. The bellwether statistics of the amounts of CO₂ in the global atmosphere and the increase in average global temperatures since the dawn of the industrial age coupled with projections of these data under different scenarios by climatologists, environmentalists, and geoscientists have been the basis of debate and have led to suggested paths of action to be undertaken by interconnected parties. In October 2018, the Intergovernmental Panel on Climate Change (IPCC) issued an updated analysis (1) of the worldwide situation with a more dire projection of global warming than it presented earlier (2). In this latest report, the IPCC stressed the need to keep the average temperature increase to less than 1.5 °C over the next 15 y.

Pathways consistent with 1.5 °C of warming above pre-industrial levels can be identified under a range of assumptions about economic growth, technology developments and lifestyles. However, lack of global cooperation, lack of governance of the required energy and land transformation, and increases in resource-intensive consumption are key impediments to achieving 1.5 °C pathways. ... Under emis-
Solar at Scale: A Perspective from the Trenches, Raffi Garabedian, First Solar
Our Chemicals and Liquid Fuels, Karen Goldberg, University of Pennsylvania
Biofuels: Still Needed after All These Years, Lee Lynd, Dartmouth University
Carbon Negative Solar Fertilization and Land Restoration, Daniel Nocera, Harvard University
Pathways for Carbon Dioxide Transformations Using Sunlight, Harry Atwater, California Institute of Technology
Solar Solved—Next, Carbon Negative Technology, Eli Yablonovitch, University of California, Berkeley
Making Solar Fuels, Tom Meyer, University of North Carolina

The Sackler Colloquium presentations can be viewed on YouTube (https://www.youtube.com/playlist?list=PLG1mxtXQ0eK3MBVdhrPb/T-RRCNvhQ). Both Moniz and Majumdar helped to frame the current situation and the importance of fundamental research in coordination with a support and funding structure that stimulates innovation and potentially disruptive technologies. It is not just a case of thinking outside the box; rather, it is a structure and culture that encourages being and doing outside the box. The issue of renewable energy storage was analyzed from a number of perspectives including solid-state batteries and electrochemical couples of various types, as well as liquid flow batteries in which 2 solutions of different redox agents flow over a common membrane that is permeable for positive ion migration while electrons proceed through an external circuit at a certain potential to do work. The cost of elements comprising the redox couples in batteries of all types is an important consideration in these different approaches, as are other factors such as electron and ion charge transfer dynamics, component separability, and system durability. All of these issues are being addressed in ongoing research.

A dominant trend in energy storage is the multitude of applications that are emerging as the electricity grid and transportation are transformed to address climate change, increase performance, and reduce cost. Storage applications for battery electric vehicles, renewable electricity integration, distributed energy resources, smart energy management, and electric flight for air taxis, package delivery, and short-haul passenger service were beyond the technology frontier even a decade ago. Conventional lithium-ion batteries have become dominant in the market owing in part to their dramatic drop in price, but they face important cost and performance challenges to fill expanding needs. Increasingly, attention is turning to significant changes in the basic lithium-ion platform such as solid-state electrolytes and anodes based on lithium, magnesium, zinc, or calcium metal, and to even more disruptive innovations such as cathodes based on molecular oxygen or sulfur instead of crystalline transition metal sulfides, oxides, and phosphates or to flow batteries replacing vanadium with more complex and versatile organic redox agents.

One promising advance is a new kind of lithium–oxygen battery capable of 700 cycles that operates in ordinary air (4). The very high theoretical energy density and low materials cost of lithium–oxygen batteries are attractive for many applications including electric vehicles, long-haul freight trucks, and electric flight. The new battery uses nanoflakes of MoS2 as support for the oxygen cathode, a Li2CO3 protective layer on the lithium metal anode, and an ionic liquid as the electrolyte, illustrated in Fig. 2. These novel features address the major challenges of lithium–oxygen batteries: dendrite growth on the lithium metal anode, side reactions of the anode and cathode with moisture, carbon dioxide and nitrogen in air, and dissolution and eventual side reactions of the discharge product Li2O2 in the liquid electrolyte. The new battery operated for more than 700 cycles with no sign of side reaction...
products at the anode or cathode. Extensive density functional theory and molecular dynamics simulations revealed the atomic- and molecular-level origins of the unusual kinetic and thermodynamic stability of the battery.

Aqueous electrolytes are getting renewed attention for their low cost, superior solvation performance, and high ionic mobility, as discussed by Nazar for grid-scale applications (5). Brushett discussed new redox-active organic polymers for flow batteries that can significantly reduce cost and raise performance (6). Flow batteries, while not conceptually new, have stimulated much new research over the past decade for their use in renewable energy storage (Fig. 3). Key questions involve the media in which they operate (aqueous or organic), the solvation environment surrounding the active ions, and the durability of their redox couples. These aspects provide research challenges at a number of levels, all directed to cost-effective energy storage at scale (7). Both the mass and volume energy densities of flow batteries render them more suitable for stationary energy storage than mobile applications based on electric vehicles.

Chemical stability of organic flow batteries in which the redox active couples are reversible 1-electron agents such as viologens and 2-electron pairs such as quinone/hydroquinone systems represents a genuine challenge, but one that offers new possibilities for eventual implementation (8, 9). There was also discussion of related fuel cells based on H2 by Haile and a new long-duration flow battery by Chiang based on inexpensive, Earth-abundant S, O2, and water (10, 11). The low materials cost of this battery enables storage of large amounts of energy for long-duration discharge economically feasible (Fig. 4).

Following the first day of lectures, there was a wide-ranging panel discussion on the subject of renewable energy storage that included the scientific, materials, and technology challenges that must be met to enable the widespread integration of variable wind and solar electricity on the grid and of battery and fuel cell vehicles in transportation. The urgency to achieve aggressive decarbonization goals in the next 15 y was central to these discussions.

During the second day of the meeting, the focus shifted to solar energy conversion into electricity directly using PV materials and assemblies, or into stored chemical energy via photosynthesis. The growth of photovoltaic installations during the past decade has been enormous, while price points per kilowatt hour have become competitive with electrical energy obtained from fossil fuels. The technological key to this result has been the ability to produce PV-grade silicon in huge quantities, mainly in China. Thin-film PVs composed of coatings containing copper–indium–gallium–seLENide and GaAs have the promise of substantially greater efficiency but are also at this time more expensive to produce. Talks by Garrabedian of First Solar and Atwater of the Department of Energy’s Joint Center for Artificial Photosynthesis indicated that such systems are approaching the theoretical Shockley–Queser limit for the conversion of light into electrical energy in a single junction system (12, 13). Yablonovich, whose work on thin-film GaAs is also notable (14), considers that with such a construct in hand the fundamental scientific challenge associated with widespread use of PV materials may have been met, although cost remains a key problem.

While natural photosynthesis ultimately into stored chemical energy in the form of carbohydrates, it is the reduction of protons together with the generation of oxygen from water that provides stored chemical potential. Whereas other possible light-driven energy-storing reactions exist under the rubric of artificial photosynthesis, it is light-driven water splitting into hydrogen and oxygen that is the main focus of current research. Even in natural photosynthesis, energy storage involves the key steps of water oxidation to O2 and proton reduction (in the conversion of NADP+ to NADPH). Subsequent CO2 reduction occurs through dark reactions proceeding by thermodynamically favorable chemistry, meaning that light is not required for CO2 incorporation into carbohydrate products once reducing equivalents in the form of NADPH have been generated. While other energy-storing reactions have been proposed and examined for artificial photosynthesis, none has been found to have the qualities and utility of water splitting for energy storage. This is especially true if the energy-releasing reaction is
carried out employing hydrogen fuel cell technology (discussed below).

The main challenge with light-driven water splitting arises in the catalysis of both half-reactions—H₂ formation from water and water oxidation to O₂—that can be deleterious to catalyst stability over the long run. For the water oxidation half-reaction, the process may involve generation of reactive oxygen species that can attack the catalyst to render it inactive. In their lectures, Meyer described his efforts on the subject using photoelectrosynthetic cells (Fig. 5; refs. 15 and 16), while Nocera recounted briefly his research on the artificial leaf that generates H₂ and O₂ employing a Si-based light absorber with the necessary reducing and oxidizing equivalents (17). However, in artificial leaf research it was found that cost and stability factors for the light absorber are too high for translation into practical technology at this time.

The dye-sensitized photoelectrosynthesis cell illustrated in Fig. 5 integrates high-bandgap, nanoparticle oxide semiconductors with the light-absorbing and catalytic properties of designed chromophore–catalyst assemblies to give water splitting. Additional modification to the cathodic compartment of the cell to employ the reducing equivalents of H₂ for the conversion of CO₂ into organic oxygenate fuels are also being conducted (16). It is worth noting that while efforts to use anthropogenically produced carbon dioxide for materials and polymers are in progress, the amounts of CO₂ produced in the course of energy production is far greater than is needed in materials and polymer applications.

Another approach, which was presented by Jaramillo, follows a path in which the efficiency of current and near-future PV technology is coupled with separate water electrolyzers for H₂ and O₂ generation, rather than via a single integrated light absorber–catalytic system (18). This would combine the necessity of large-area PV light absorbers for relatively diffuse solar energy with the efficiency of a more centralized electrochemical reactor for making H₂ and O₂. With PV prices declining rapidly, the challenge then becomes the cost and efficiency of the water electrolyzer.

Although hydrogen as a fuel has many positive attributes—it generates the most energy of any chemical fuel per unit mass on oxidation and its supply would be limitless—there are aspects to its use that represent obstacles and challenges. One challenge is storage of H₂ since it is not a readily condensible gas. In the process of liquefaction of H₂, which is currently done in industry for convenient and inexpensive delivery, approximately one-third of its value as a fuel is consumed (19). A second challenge is the distribution of hydrogen to filling stations for transportation, which is a larger consumer of energy than electricity generation. Fuel cell electric vehicles (FCEVs) running on hydrogen need filling stations delivering H₂ at 70 MPa pressure. As of 2018, there are ~50 such fueling stations in California to support a limited number of...
FCEVs as a pilot project for their use in carbon-free transportation. It should be noted that Japan has undertaken a major long-term commitment to FCEVs with projected numbers of cars and fueling stations over the next 8 y of 800,000 and 2,000, respectively (20). There are also commuter scale fuel-cell electric trains made by Alstom operating in Germany (21, 22). All of these efforts are in addition to the rapidly growing electric vehicles sector which is based on batteries rather than fuel cells for operation—once H2 can be generated by PV-driven water electrolyzers, it can replace the hydrogen now used in industry and produced by reforming natural gas (with attendant CO2 generation). The largest industrial process using hydrogen is Haber–Bosch ammonia synthesis; it produces 4.5 × 109 kg of NH3 for agriculture and food production, with global consumption of 3 to 5% of natural gas annually. The process is critically important in making nitrogen biologically available on the scale needed to feed the planet’s inhabitants. The role that ammonia plays in today’s world may also expand greatly in the energy landscape of the future as a source of “stored” hydrogen (23). Ammonia as a possible fuel has long been recognized (although not widely used) and the thermodynamics of its formation support its possible role as a stored hydrogen source. In view of the fact that the handling of CO2. In other talks, Lynd and Nocera considered a strategy of carrying this solution to completion would be to bury the generated CO2, allowing CO2 reduction to produce fuels that upon oxidation—using modified organisms to reduce CO2 to carbohydrate levels of chemical potential so that such compounds could be used as energy sources. In that way, the use of such fuels would be carbon-neutral—allowing CO2 reduction to produce fuels that upon oxidation regenerate the same amount of CO2. A system from the Nocera laboratory is shown in Fig. 6 in which hydrogen produced from water splitting is consumed by Ralstonia eutropha to grow and produce biomass, or for more highly engineered versions to produce liquid fuels such as isopropanol (25, 26).

The interconversion of compounds from carbon oxygenates to carbohydrates and other reduced carbon compounds was discussed by Goldberg in terms of challenges in catalysis of such CO2 reduction reactions and how these transformations could be conducted through the development of new selective catalysts. Details can be found in their respective talks available at the Colloquium website.

A distinguishing feature of the Sackler Colloquium was the presence of 2 panel discussions at the end of the presentations each day during which questions, comments, and opinions could be far-ranging and proceed beyond the scope of usual discussions at scientific meetings. Each panel discussion created lively interaction between the audience and speakers. One provocative topic was the outlook for achieving decarbonization in the short time scale needed to prevent critical climate change. The goal of long-duration energy storage is a significant barrier to decarbonization of the electricity grid. Li-ion battery technologies in the planning stage typically have a 4–h discharge time, enough to shift afternoon solar electricity into the evening, or to cover a calm afternoon when the wind may not blow. However, much longer duration storage is needed to bridge the weekday–weekend demand disparity, the daily and weekly weather patterns of calm, cloudy or inclement days, outages from extreme weather damage, and seasonal variations in heating and cooling demand (10).

Discussion on the relative merits of batteries vis-a-vis storage of hydrogen produced via artificial photosynthesis or PV-driven electrolysis illustrated not only the scientific challenges but also the importance of low cost in driving widespread deployment. While batteries and PVs are the poster children for rapid cost-driven deployment, each was enabled by long incubation periods required to understand the fundamental materials and phenomena. The importance of such discovery periods is seen in other sectors such as fracking and light-emitting diodes that exhibited widespread deployment following rapid cost reductions. In various ways, although artificial photosynthesis and electrocatalysis are still in their fundamental science and discovery modes, shorter timelines to practical implementation need to be achieved.

The importance of strong cross-disciplinary interaction to facilitate progress was highlighted frequently. The fundamental electrochemistry that underpins research in batteries, fuel cells, catalysis, and photosynthesis provides a common connection among scientists pursuing different approaches in energy decarbonization research. We all agreed that finding ways to share information and ideas across fields is critical to advancing the pace of discovery and innovation. One platform for sharing information and stimulating ideas is numerical simulation of molecules and materials before they are made in the laboratory. There are now many extensive databases of equilibrium properties of materials and molecules such as crystal, molecular, electronic, and magnetic structures, formation
energies, ionization potentials, and electron affinities (27–29). These databases enable fast screening of thousands of materials or molecules for the most promising candidates for a given application.

Materials simulations can be taken to the next level with 2 game-changing advances. The first is a single interactive search engine that can access the many separate databases created and maintained by distinct research groups. Google is a prime example: It collects data from far-flung sources and sorts and presents information in seconds in response to a search request. A Google-style search engine able to access all of the specialized materials and molecular databases and sort the search results quickly would accelerate the generation of new ideas and allow them to be evaluated on much shorter time scales than is now possible.

The second advance for materials simulations is moving beyond equilibrium properties of perfect materials and molecules to embrace defects, disorder, doping, dynamics, mobility, excited states, metastable phases, and chemical reactions. These are all critical features of realistic systems that are mostly beyond the reach of existing high-throughput simulations. Given large-enough computers, some of these properties, such as defects, disorder, and doping, can be simulated now. Others, such as dynamics, excited states, metastable phases, and chemical reactions, require formulation of new computational approaches to become mainstream. Machine learning and artificial intelligence, long used for drug discovery but only now being applied to materials for energy, can reveal hidden correlations among materials and properties for which there is no good first-principles understanding, such as excited states and nonequilibrium dynamics (30). Simulations beyond equilibrium properties, now imaginable but not yet reduced to practice, would greatly accelerate the discovery of new materials and phenomena for decarbonization and help drive the cost reductions needed for widespread deployment.

In an article for the World Economic Forum entitled “Who Will Our Energy Come from in 2030 and How Green Will It Be?” Katherine Hamilton, director of the Project for Clean Energy and Innovation and cochair of the Global Future Council on the Future of Energy, stated the following (31):

The energy sector is already changing very rapidly. It is transitioning, we hope, towards greater ability to meet the energy needs of a growing global population with reduced use of carbon, supporting continued economic growth in an environmentally sustainable way. But that transition will not necessarily happen on its own. We need to get key players in the same room who can bring different experiences and perspectives, and collectively come up with better ideas than any of us could on our own—and then work out how to implement those ideas. Hence the need for this Global Future Council.

Who are the key players that need to be involved?

The incumbents are important, of course—the large energy companies who own and control the infrastructure, especially in industrialized countries. They are often criticized as being part of the problem, but they also have to be part of the solution. In addition, we need the innovators—entrepreneurs who are coming up with ideas to disrupt the sector. And we need input from energy consumers, including large corporations and municipalities.

Representatives of the financial sector are important—experts in bonds, risk, and insurance. There is plenty of capital out there looking for good project risk. Finally, a common concern of investors is the assurance that these projects will find a market. Creating certainty is one important thing politicians and policymakers can do to help—and it is they who, ultimately, will need the vision to define goals for the energy sector and devise policies to achieve them.

The final points made by Hamilton are similar to ones raised by Moniz and Majumdar in establishing a structure to support and promote innovation. However, there was a conspicuous absence of “scientists” in Hamilton’s key players. Such individuals are the researchers who discover and develop promising new materials and methods for energy conversion and storage on which future energy technology will be built. The science presented in the Sackler Colloquium included discoveries of more efficient materials for light absorption, membranes for separation of oxidation and reduction sides of energy-storing reactions, insight into the photophysics and photochemistry that leads to electrical current and/or stored chemical potential, and methodologies and systems for reversibly storing and converting energy into useful work. These are the kinds of things that led to the great clean-energy advances like the low-cost silicon solar cell. How can we get the next generation of clean-energy advances without financing the science to support them? The scientific advances are often driven by visions for large-scale implementation of carbon-free energy. The research presented in the Sackler Colloquium highlighted the need for a vision for carbon-free energy by 2050.

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1. IPCC, “Summary for policy makers” in Global Warming of 1.5°C. An IPCC special report on the impacts of global warming of 1.5°C above pre-industrial levels and related global greenhouse gas emission pathways, in the context of strengthening the global response to the threat of climate change, sustainable development, and efforts to eradicate poverty, by Masson-Delmotte et al., Eds. (Intergovernmental Panel on Climate Change, 2018), https://www.ipcc.ch/sr15/.
2. IPCC, Climate change 2014: Synthesis report. Contribution of Working Groups I, II and III to the Fifth Assessment Report of the Intergovernmental Panel on Climate Change, Core Writing Team, R. K. Pachauri, and L. A. Meyer, Eds. (Intergovernmental Panel on Climate Change, 2014), https://www.ipcc.ch/report/syrcl/
3. C. Figueiras et al., Emissions are still rising: Ramp up the cuts. Nature 564, 27–30 (2018).
4. M. Asadi et al., A lithium-oxygen battery with a long cycle life in an air-like atmosphere. Nature 555, 502–506 (2018).
5. D. Kundu et al., Aqueous vs. nonaqueous Zn-ion batteries: Consequences of the desolvation penalty at the interface. Energy Environ. Sci. 11, 881–892 (2018).
6. D. R. Nevers, F. R. Brushett, D. R. Wheeler, Engineering radical polymer electrodes for electrochemical energy storage. J. Power Sources 352, 226–244 (2017).
7. C. C. Zhang et al., Progress and prospects of next-generation redox flow batteries. Energy Storage Mater. 15, 324–350 (2018).
8. M. J. Baran et al., Designing redox-active oligomers for crossover-free, nonaqueous redox-flow batteries with high volumetric energy density. Chem. Mater. 30, 3861–3866 (2018).
9. D. G. Kviatkovskiy, A. A. Wong, M. J. Aziz, Rational evaluation and cycle life improvement of quinone-based aqueous flow batteries guided by in-line optical spectrophotometry. J. Electrochem. Soc. 165, A1770–A1776 (2018).
10. Z. Li et al., Air-breathing aqueous sulfur flow battery for ultralow-cost long-duration electrical storage. Joule 1, 306–327 (2017).
11. Y.-M. Chiang, L. Su, S. M. Pari, Z. Li, Lowering the bar on battery cost. Joule 1, 121–219 (2017).
12. N. M. Haegele et al., Terawatt-scale photovoltaics: Trajectories and challenges. Science 356, 141–143 (2017).
13. D. J. Sarkhel, A. R. Dayevey, J. Wong, H. A. Atwater, Van der Waals materials for atomically-thin photovoltaics: Promise and outlook. ACS Photonics 4, 2962–2970 (2017).
14. O. D. Miller, E. Yablonovitch, S. R. Kurtz, Strong internal and external luminescence as solar cells approach the Shockley–Queisser limit. IEEE Journal of Photovoltaics 2, 303–311 (2012).
15. L. Wu et al., Stable molecular surface modification of nanostructured, mesoporous metal oxide photoanodes by slane and click chemistry. ACS Appl. Mater. Interfaces 11, 4560–4567 (2019).
16. M. K. Brenneman et al., Finding the way to solar fuels with dye-sensitized photoelectrosynthesis cells. J. Am. Chem. Soc. 138, 10385–10312 (2016).
17. D. G. Nocera, Solar fuels and solar chemical industries. Acc. Chem. Res. 50, 616–619 (2017).
18. L. A. King, T. R. Hellistern, J. Park, R. Sinclair, T. J. Jaramillo, Highly stable molybdenum disulfide protected silicon photocathodes for photovoltaelectrochemical water splitting. ACS Appl. Mater. Interfaces 9, 37652–37678 (2017).
19. H. Azam, S. Oh, M. Ghadiri, Advanced energy and exergoeconomic analyses of a hydrogen liquefaction plant equipped with mixed refrigerant system. J. Clean. Prod. 144, 248–259 (2017).

Eisenberg et al.
20. M. Nagashima, Japan’s hydrogen strategy and its economic and geopolitical implications. Études d’Ifri (2018). https://www.ifri.org/en/publications/etudes-difi/japans-hydrogen-strategy-and-its-economic-and-geopolitical-implications. Accessed 21 September 2019.
21. Anonymous, Germany launches world’s first hydrogen-powered train. The Guardian (2018). https://www.theguardian.com/environment/2018/sep/17/germany-launches-worlds-first-hydrogen-powered-train. Accessed 21 September 2019.
22. C. English, S. Miller, Alstom’s hydrogen fuel cell train wins 2018 GreenTec Mobility Award (Alstom, 2018). https://www.alstom.com/press-releases-news/2018/5/alstoms-hydrogen-fuel-cell-train-wins-2018-greentec-mobility-award. Accessed 21 September 2019.
23. A. Valera-Medina, H. Xiao, M. Owen-Jones, W. I. F. David, P. J. Bowen, Ammonia for power. Prog. Energy Combust. 69, 63–102 (2018).
24. M. Bui et al., Carbon capture and storage (CCS): The way forward. Energy Environ. Sci. 11, 1062–1176 (2018).
25. J. P. Torella et al., Efficient solar-to-fuels production from a hybrid microbial-water-splitting catalyst system. Proc. Natl. Acad. Sci. U.S.A. 112, E1507 (2015). Erratum in: Proc. Natl. Acad. Sci. U.S.A. 112, 2337–2342 (2015).
26. C. Liu, B. E. Colon, P. A. Silver, D. G. Nocera, Solar-powered CO2 reduction by a hybrid biological vertical bar inorganic system. J. Photoch. Photobio. A 358, 411–415 (2018).
27. Bassman L, et al., Active learning for accelerated design of layered materials. NPJ Comput. Mater. 4, 74 (2018).
28. X. Zhang, Computational screening of 2D materials and rational design of heterojunctions for water splitting photocatalysts. Small Methods 3, 1700359 (2018).
29. P. Canepa et al., Odyssey of multivalent cathode materials: Open questions and future challenges. Chem. Rev. 117, 4287–4341 (2017).
30. J. Jung, J. I. Yoon, H. K. Park, J. Y. Kim, H. S. Kim, An efficient machine learning approach to establish structure-property linkages. Comput. Mater. Sci. 156, 17–25 (2019).
31. K. Hamilton, “Where will our energy come from in 2030, and how green will it be?” (2018). https://www.weforum.org/agenda/2016/11/where-will-our-energy-come-from-in-2030/. Accessed 21 September 2019.
32. C. Le Quéré et al., Global carbon budget 2017. Earth Syst. Sci. Data, 10, 405–448 (2018).