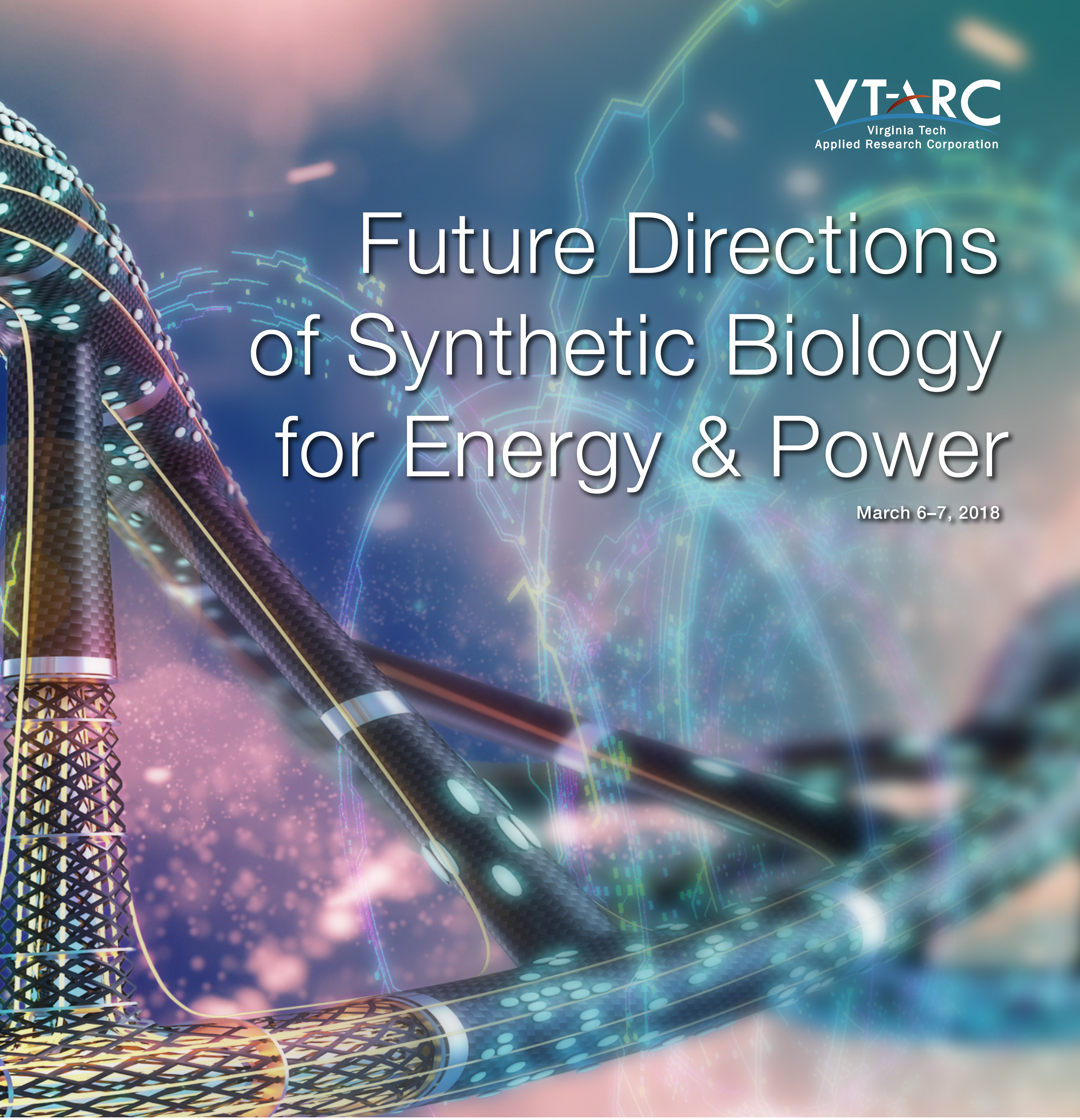

Future Directions of Synthetic Biology for Energy & Power

March 6–7, 2018

Michael C. Jewett, Northwestern University
Yang Shao-Horn, Massachusetts Institute of Technology
Christopher A. Voigt, Massachusetts Institute of Technology

Prepared by: Kate Klemic, VT-ARC
Esha Mathew, AAAS S&T Policy Fellow, OUSD(R&E)

Workshop funded by the Basic Research Office, Office of the Under Secretary of Defense for Research & Engineering. This report does not necessarily reflect the policies or positions of the US Department of Defense

Innovation is the key to the future, but basic research is the key to future innovation.

–Jerome Isaac Friedman,
Nobel Prize Recipient (1990)

Preface

Over the past century, science and technology has brought remarkable new capabilities to all sectors of the economy; from telecommunications, energy, and electronics to medicine, transportation and defense. Technologies that were fantasy decades ago, such as the internet and mobile devices, now inform the way we live, work, and interact with our environment. Key to this technological progress is the capacity of the global basic research community to create new knowledge and to develop new insights in science, technology, and engineering. Understanding the trajectories of this fundamental research, within the context of global challenges, empowers stakeholders to identify and seize potential opportunities.

The Future Directions Workshop series, sponsored by the Basic Research Directorate of the Office of the Under Secretary of Defense for Research and Engineering, seeks to examine emerging research and engineering areas that are most likely to transform future technology capabilities. These workshops gather distinguished academic researchers from around the globe to engage in an interactive dialogue about the promises and challenges of emerging basic research areas and how they could impact future capabilities. Chaired by leaders in the field, these workshops encourage unfettered consideration of the prospects of fundamental science areas from the most talented minds in the research community.

Reports from the Future Directions Workshop series capture these discussions and therefore play a vital role in the discussion of basic research priorities. Each report addresses the following important questions:

- How will the research impact science and technology capabilities of the future?
- What is the trajectory of scientific achievement over the next few decades?
- What are the most fundamental challenges to progress?

This report is the product of a workshop held March 6–7, 2018 at the Virginia Tech Executive Briefing Center in Arlington, VA on the future of Synthetic Biology for Power and Energy research. It is intended as a resource to the S&T community including the broader federal funding community, federal laboratories, domestic industrial base, and academia.

Executive Summary

Energy is a fundamental requirement of all human activity. Global-scale activities such as transportation, manufacturing, and communication require energy to be generated, stored, and delivered on demand and in a use-specific manner. This, combined with the ever-changing technology needs of modern society, means that energy storage and power delivery modalities must also grow and evolve.

As researchers strive to develop ever more sophisticated energy storage and power delivery systems to keep up with demand, the emergence of synthetic biology tools and techniques offers an entirely new design paradigm that harnesses and expands the inherent abilities and chemistries of living systems to transform and store energy. To explore the potential for synthetic biology to address the challenges of energy and power systems, the Office of the Under Secretary of Defense (Research and Engineering) and the United Kingdom Ministry of Defense hosted the Future Directions Workshop in Synthetic Biology for Energy and Power on March 6-7, 2018 at the Virginia Tech Executive Briefing Center in Arlington, VA.

This workshop gathered 26 academic, industry, and government researchers from both the synthetic biology and energy/power communities. To promote more dynamic conversations, participants were split into small groups focused on three conceptual domains in energy and power research that are also central processes in living systems:

- Electrocatalysis
- Electron Storage
- Ion Transport Materials

In each small group, energy/power researchers shared the most pressing research challenges facing energy storage and power delivery. Synthetic biology researchers shared emerging research that could address those challenges. Each working group presented their findings to all workshop participants for a broader discussion and synthesis of ideas. This report summarizes the key findings of the energy/power research challenges most amenable to synthetic biology approaches, the current and future capabilities of synthetic biology to address these challenges, and the research trajectory needed over the next 5, 10 and 20 years to achieve success.

The key energy/power research challenges that are amenable to synthetic biology approaches were identified for the three domains as:

Electrocatalysis

- Catalysts that exhibit faster kinetics, improved selectivity, and no requirement for rare elements
- Characterization techniques to interrogate and understand catalytic active sites
- Novel materials and structures that break scaling relationships of reaction intermediates with catalyst surfaces

Electron Storage

- New electrode-electrolyte interfaces with higher stability
- Stable, high capacity battery electrodes
- Discovery of "beyond Lithium Ion (Li-ion)" chemistries and device concepts that enable high energy density and large-scale energy storage

Ion Transport Materials

- Non-flammable electrolytes or systems with high transference numbers
- Solid ceramic electrolytes that are stable with Li-ion battery electrodes
- Polymer electrolytes with ionic conductivity on par with liquid and solid ceramic electrolytes
- Anion (OH^-) conducting membranes with ionic conductivity similar to that of protons in Nafion
- Solid or liquid electrolytes with wide temperature stability windows for safety in military or other demanding applications

Discussions about the potential for synthetic biology approaches to address these challenges focused on the capabilities of four synthetic biology domains:

Bio-inspired Electrocatalysis

Living systems are catalytically diverse and may shed new insights and opportunities for bio-inspired catalytic design or to develop biocatalysts for direct use. The direct coupling of catalysts to electron transport and exergonic processes will enable the efficient production of high-energy chemicals, such as novel rocket fuels. Further, novel biological catalysts may bypass the need for rare earth metals in some manufacturing processes.

Bio-derived Energy Storage Materials

Cellular machinery uses precision synthesis of sequence defined polymers to create exquisite materials that surpasses the abilities of traditional chemical methods. This property can be harnessed to develop new high-performance materials for energy and power platforms. For example, bio-derived conducting polymers could be combined with traditional metal and silicon nanostructures to accelerate battery development, for needs ranging from low-cost/low-environmental impact systems for base operations to miniaturized bio-compatible batteries for medical devices.

Bioprocess Engineering Framework

Successful implementation of synthetic biology for energy and power needs will require new bioprocess engineering frameworks that produce bio-derived materials at scale. These frameworks may also need to include new hybrid chemical/biological processes. In addition, the ability to synthesize materials on demand in resource-limited settings (i.e., decentralized manufacturing) would be transformative.

Biotic/Abiotic Interface

Living systems respond dynamically to their environments. These processes, such as electron transfer between intracellular and extracellular spaces and over long-distances can lead to new solutions for similar processes in energy storage and power delivery platforms. This technology will underlie long-term deployed sensors, powering of autonomous vehicles, and functional materials comprised of living cells.

Participants acknowledged that there is a large gap between the current capabilities of the synthetic biology toolkit and the envisioned capabilities of 10 or 20 years from now. They outlined the most important technical challenges to be:

- Computational frameworks, as well as theory to model and predict biological design of materials
- Analytical tools to characterize interfaces and charge transfer in biological and bio-derived systems
- Bioprocess engineering strategies to enable manufacturing of bio-derived energy materials at appropriate scales
- Strategies to decouple cellular and engineering objectives
- Processes for decentralized, on-demand synthesis
- Biological systems that can scavenge energy from the environment for long-term deployment

They mapped the basic research trajectory for both short- and long-term goals to achieve success as:

Short-term goals

- Training programs that produce researchers proficient in a common vocabulary between physical and life scientists (3 y)
- New theory to model and predict properties of unique materials accessible by engineering biology (5 y)
- Computational frameworks to advance biological design (both of active sites for catalysts, and polymeric materials) (5-7 y)
- New approaches that decouple the production of chemicals/materials from the need to maintain living cells (5 y)
- Technologies for the rapid design of biological materials to the production of sufficient quantities for prototyping in devices (5 y)
- New hybrid chemical/biological syntheses strategies (5 y)
- Incentives to work collaboratively across disciplines: projects, conferences, bio-inspired design of catalytic active sites, new screening targets (5 y)

Long-term goals

- Construction of on-site distributed biomanufacturing capabilities that can derive energy from diverse waste sources (10 y)
- Bioprocess strategies and flexible manufacturing facilities for the rapid scale-up of biomaterials production (15 y)
- Integration of large-scale chemical and biological processing (15 y)
- Integrated design platforms that simplify the design of a material to physical specifications and enable the creation of genetic or bio-catalytic systems at scale (20 y)
- Design integration of scale between the atomic, micro- and macro- domains (20 y)

Workshop participants were generally optimistic about the potential for synthetic biology to create an entirely new design paradigm for energy and power systems. The resulting capabilities will not only enable these systems to keep pace with increasing energy and power demands but also provide new tools that can be used to address future challenges that have not yet been imagined.

Introduction

Biological systems have long been recognized for their ability to transform and store energy, self-repair, and function in and adapt to various external conditions. These capabilities have been recognized and exploited for use in biofuel development as an alternative to fossil fuels. However, the full potential for biology to address energy and power challenges extends well beyond the creation of "drop-in" replacements for conventional energy sources. In particular, the emerging field of synthetic biology offers new tools and techniques for creating an entirely new set of materials and structures that have the potential to transform energy and power systems.

Synthetic biology is the intersection of biology and engineering disciplines, devoted to the rational design and engineering of organisms and their components. It is now possible to both engineer specific functions into living systems and construct entirely new ones. New engineered functionalities can be directed by reading, writing, and editing in the language of DNA, as a computer scientist might program a computer or an electrical engineer would design and assemble electrical circuits. With these new tools of synthetic biology, microorganisms can be used as factories, laboratories, and engineered devices. Inspired by the complexity of the natural world, living organisms are engineered to pattern and produce a wide range of highly-tailored materials and structures with specific desirable properties (Figure 1). While synthetic biology has immediate biomedical applications, there is an opportunity for biological engineering tools to also disrupt non-medical technologies.

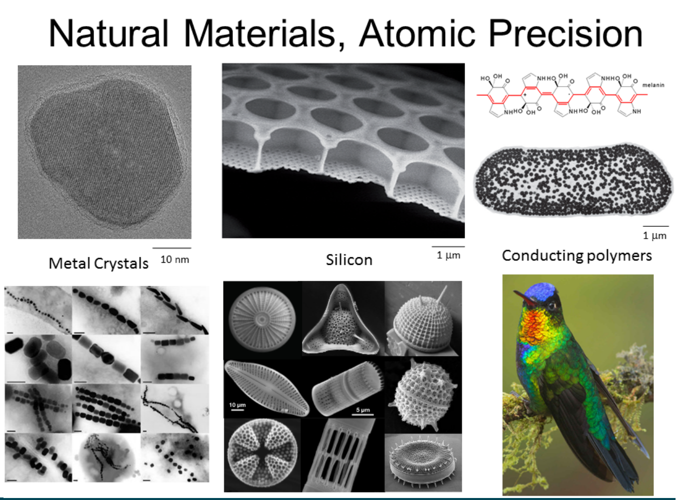

Figure 1 – Biological systems can be used to manufacture a range of materials with atomic-level precision. [Credit: Christopher Voigt, MIT *[1]*]

For energy and power systems, some envisioned applications of synthetic biology include: unmanned aerial vehicles (UAVs) powered by cells and biological materials that scavenge energy from the environment; new rocket fuels formulated with extremely high energy density; new bio-compatible batteries for implantable medical devices; energy generation and storage in transparent materials; and functionalized, self-powering systems that are embedded into textiles, plastics, and 3D printed materials.

There is particular interest in using synthetic biology tools to create energy technologies that are smaller, lighter, and cheaper while having a lower environmental impact and ensuring safety and reliability. Our present energy economy relies heavily on fossil fuels for both energy generation and storage. A significant portion of our electricity is generated from the combustion of coal or natural gas, and our transportation sector relies almost exclusively on gasoline and other petroleum derived fuels to store energy. There has been a recent push to reduce our usage of fossil fuels for power generation and storage. To this end, solar and wind generation have seen great success with new installations that are increasingly cost competitive with other forms of electricity generation, at least in some parts of the world. However, the intermittency of these non-fossil fuel technologies creates a need to store energy either electrochemically or in chemical bonds. These same needs manifest when one considers replacing petroleum-derived fuels to power our transportation sector. Electric or fuel cell vehicles use energy that is stored electrochemically, in batteries or hydrogen, respectively. To realize the promise of battery and fuel cell technologies, their performance, cost, and sustainability must be improved so that they can be widely implemented.

There are three high-level energy and power challenges for which synthetic biology is well-suited: *(1) electromobility and grid independence, (2) recycling and sustainability, and (3) precision materials synthesis.*

1. Electromobility and Grid Independence

Today, the cost of electricity from newly installed wind and solar sources is approaching 10¢/kWh *[1]*, which is cost competitive with conventional forms of electricity generation based on fossil fuels. If we can store this renewably generated electricity in chemical bonds (electrochemical energy storage), then we can significantly reduce our reliance on fossil fuels. Moreover, on demand use of clean energy has the potential to transform how we travel and live by promoting electromobility and grid independence. Affordable, lightweight, and reliable batteries would enable more universal adoption of electric vehicles across all transportation sectors and would permit decentralized, distributed energy generation such as smart buildings powered by wind and solar. These technologies for grid independence are especially important to national defense efforts to enable quiet and self-contained energy systems in a range of off-grid circumstances, like humanitarian and first responder efforts.

Recent research efforts to facilitate energy storage via electrochemistry with low cost and earth abundant elements are well-suited to synthetic biology methods. One example is research into reliable and consistent energy scavenging from local surroundings. Living systems perform bioenergetic functions in a variety of external conditions, from terrestrial to aqueous, high to low pressures and temperatures, and everything in between. They also synthesize the structural matrices inside which they perform these activities. As biology elucidates the mechanisms by which these processes occur, the synthetic biology toolkit can engineer microorganisms that can quickly synthesize their own matrices and harness materials from their surroundings, whether it be sunlight, urine, or even meals ready to eat (MREs), to generate electricity. These abilities can achieve low, consistent power densities that reduce the need to tie into existing power grids.

2. Recycling and Sustainability

As more and more batteries are removed from service, recycling their component materials to recover rare or expensive elements such as cobalt or copper will become critical. Current battery recycling is limited by high costs, energy-intensiveness, and harsh processing requirements. Although the use of these technologies may be environmentally friendly, the continued need for raw materials sourcing, manufacture, and disposal still has tremendous environmental impact. New methods to recover valuable materials without the need for high temperatures and harsh chemicals can improve the environmental footprint of energy storage technologies and provide domestic security in the materials supply chain.

The utility of microorganisms has already been demonstrated in this space with biomining. In the copper mining industry, microorganisms naturally present at the mining site are used to extract copper from ore and have reduced the energy requirements compared to conventional mining methods. Aside from copper, microorganisms are also used to extract uranium, gold, cobalt, nickel, and rare earth elements. New methods to modify microorganisms or cell-free systems could enable improved recycling processes for energy storage technologies across a diverse array of chemistries. This in turn could change the paradigm of power and energy platforms to rely on sustainability and recycling of materials. These approaches could also represent new sources of energetic materials, such as uranium extraction for nuclear power.

3. Precision Materials Synthesis

High performance materials are key to achieving small, lightweight, and cheap energy devices, be they batteries, fuel cells, electrolyzers, solar cells, or capacitors. Improved materials will require innovative synthesis techniques and research efforts in theory, computation, and simulation to screen and predict new high-performance materials.

Living systems can synthesize a wide range of functional structures far more complex than man-made methods, and in a renewable and low-cost manner. From DNA and RNA that encode information to proteins and carbohydrates that perform chemical and structural functions, nature shows a remarkable diversity of polymeric structures. For example, proteins self-assemble into highly structured environments. Comprised of sequences of amino acids, they provide a unique template for environmental control of chemical and physical space at the nanoscale. For example, the primary sequence of amino acids in proteins determines function and hierarchical structure formation (secondary and tertiary structure). Important contributions arise from the rotational flexibility along the peptide backbone, as well as the chemical diversity of amino acid monomers. Remarkably, biopolymers achieve a broad range of potent functionalities and higher-order structures from a small pool of relatively simple monomers (e.g., ~20 monomers in proteins).

Living systems are also capable of precision synthesis down to the nanometer scale, which enables bonds and structures not accessible by chemical means. Furthermore, a subset of microorganisms, called extremophiles, that are capable of surviving in extreme environmental conditions (temperature, chemical condition, alkalinity, and acidity) can drive new materials capabilities. **The ability to harness and engineer this robust cellular machinery can lead to new catalytic, ion transport, and energy storage materials with unique functions.** Ongoing work in synthetic biology to improve circuit design *[2]*, further control polymer sequence and synthesis, and possibly include natural and non-natural elements (e.g., expanding genetically encoded chemistry using parallel and independent translation systems *[3]* *[4]*) could have a transformative impact on materials for challenges in the energy/power space.

This report summarizes the findings of the Future Directions in Synthetic Biology for Energy and Power workshop held on March 6–7, 2018, to explore the potential for synthetic biology to address energy and power challenges. The workshop gathered a truly multidisciplinary group of synthetic biologists, chemists, materials scientists, and engineers to share the current state of research in each domain, identify the opportunities for synthetic biology approaches in energy/power research, and map the trajectory of research over the next twenty years that is needed to realize those opportunities. An ancillary benefit of this workshop is that it opened a dialogue between the two communities that have been generally unaware of the needs, challenges and opportunities in the other domain.

Energy and Power Research Challenges

As our energy landscape evolves to address issues of sustainability, cost, and security, novel technologies are needed to meet these new demands. Sustainable and low-cost storage technologies are especially critical to bridge energy demand with generation from renewable sources. Lithium ion (Li-ion) batteries often serve as the workhorse for energy storage needs for consumer electronics, electric vehicles and increasingly for military and aerospace applications. However, lithium ion batteries are expensive, require rare elements, and pose significant safety hazards due to toxic and flammable components. The cost of lithium ion batteries is very high (~$300/kWh) compared to wholesale electricity from solar and wind (~10¢/kWh), which means that these electrochemical energy storage devices need to be cycled 10,000+ times in order for the stored electricity to compare with the cost of electricity directly from solar and wind (Figure 2).

New chemical processes and new materials are essential to enable sustainable, low-cost storage technologies such as batteries, fuel cells, flow batteries, and yet-to-be invented devices. **Specific near-term challenges include developing materials that rely on elements that are more earth abundant than cobalt and nickel (Figure 3), improving the catalytic kinetics of chemical transformations for making H_2, NH_3, and alkali metal oxides (Figure 4), stabilizing electrochemical interfaces with reversible ion and electron transport, and identifying polymers that are fast ion conductors at room temperature.**

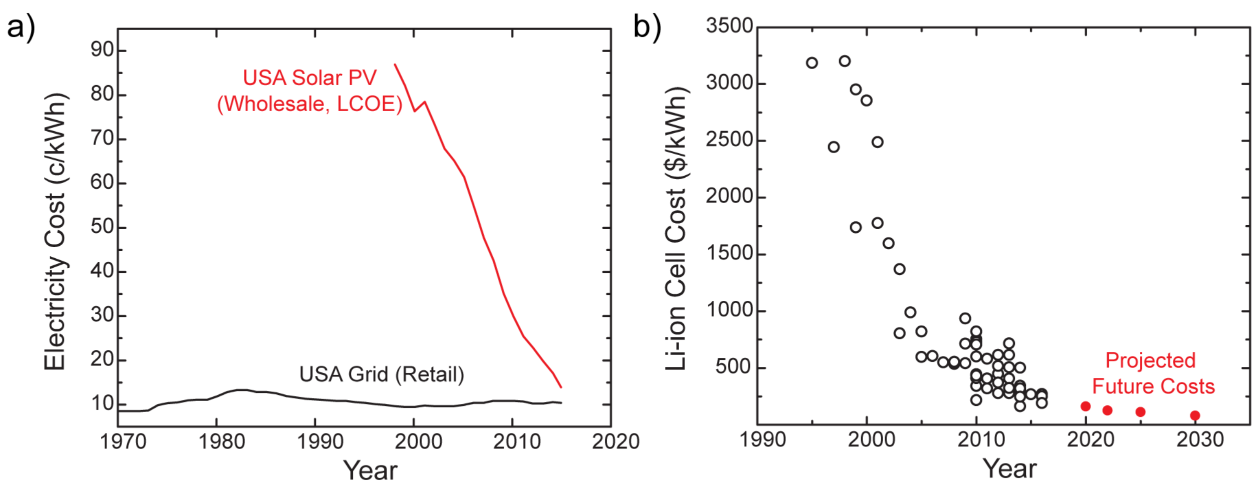

Figure 2 – (a) The cost of US solar energy has dropped significantly compared to the overall US grid and fossil fuel wholesale generation *[5] [6]*. (b) Cost of lithium ion batteries over time. Red dots represent predicted future costs. Adapted from ref *[7]*.

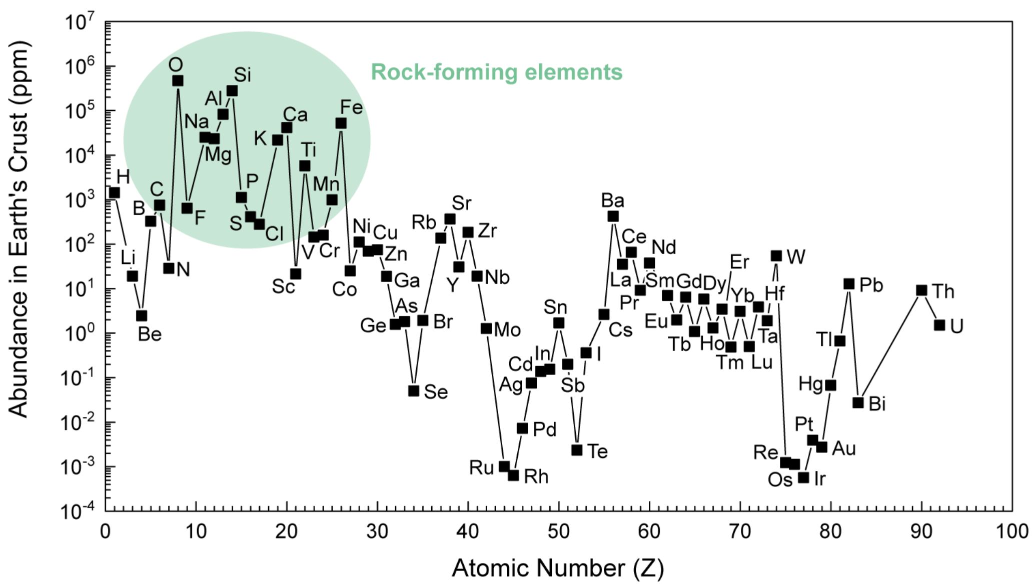

Figure 3 – (a) Abundance in the earth's crust of chemical elements reported on a log scale in ppm. Common rock forming elements are highlighted. Note that Co, Ni, and Li are all relatively rare elements. [Credit: Yang Shao-Horn, MIT]

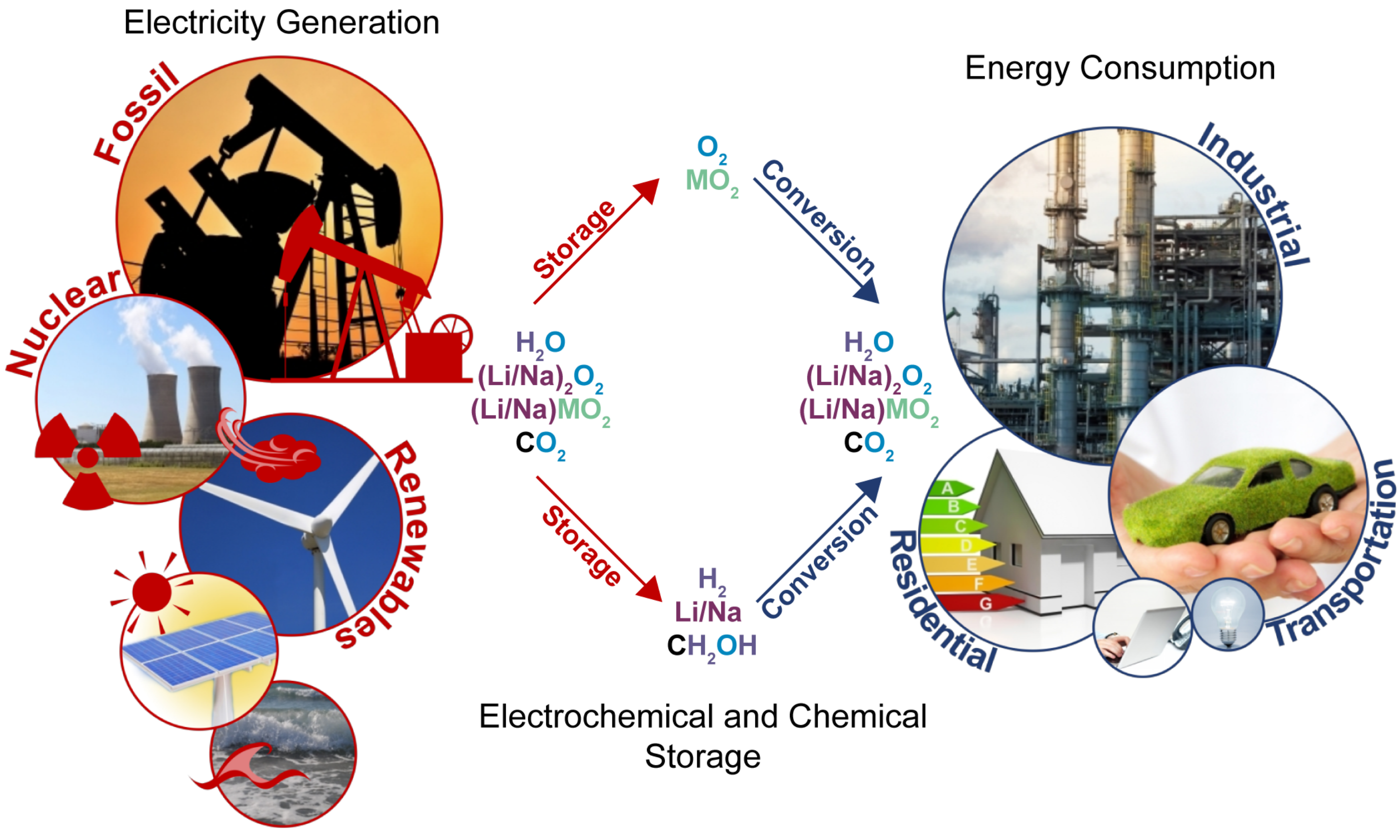

Figure 4 – Schematic of a future energy landscape that relies on electrochemical energy conversion including splitting water in to H_2 and O_2, alkali metal (Li and Na) – air batteries, lithium and sodium ion technologies (M = Ni, Mn, and/or Co), and the reduction of CO_2 into chemical fuels. These technologies will transform the way we power our vehicles and buildings and enable highly distributed energy systems. [Credit: Yang Shao-Horn, MIT]

Generally, electrochemical devices consist of two electrodes that convert electronic currents to ion currents at the electrified interface (electrode-electrolyte interface). These electrodes are separated by an ionically conductive but electronically insulating electrolyte material as shown in Figure 5. In order to convert electrical energy into chemical energy, electrons must be transferred at the electrified interface and either stored in chemical bonds (such as hydrogen in fuel cells or metal oxide bonds in Li-ion battery electrodes (e.g. $LiMO_2$, where M = cobalt)), stored on the surface of active materials through the formation of an electrical double layer capacitance, or though Faradaic reactions (pseudocapacitance) near the surface. In devices like electrochemical capacitors, this surface storage mechanism yields high reaction rates and power capability but lower gravimetric energies. Storing energy chemically in the bulk of active materials can be done through lithium intercalation and de-intercalation into/from host structures. Lithium metal oxides and graphite in Li-ion batteries offer high gravimetric energies and reasonably high rate capability (power). These chemistries are used in the current Li-ion devices that are dominating the markets of portable electronics, hybrid and electric vehicles, and stationary storage (Figure 6). The stored energy density of Li-ion technology is limited to storing one electron with each cobalt or nickel metal center in the positive electrode, which limits the wide use of these batteries for future electromobility and grid technologies due to the limited availability of Co and Ni in the earth's crust. **Therefore, it is of critical importance to develop new chemistries and materials for electron storage using elements in the air, water, or rock-forming elements for sustainable and scalable development of electrochemical energy storage technologies.** Furthermore, as shown in Figure 6, storing energy in chemical bonds using chemical transformation to form energy carriers can provide significantly greater stored energy than Li-ion chemistries.

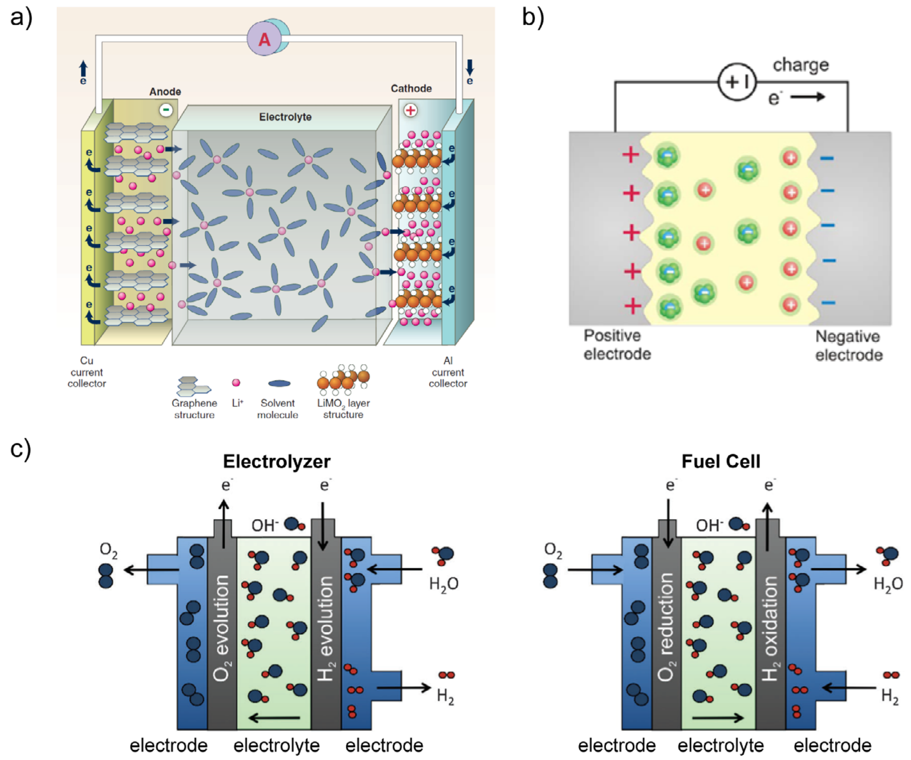

Figure 5 – Diagrams of energy storage devices including a) a Li-ion battery *[8]*, b) a supercapacitor *[9]*, and c) an electrolyzer/fuel cell *[10]*. Each of these devices contains two electrified electrodes separated by an electronically insulating ion conductor. [Credit: Yang Shao-Horn, MIT]

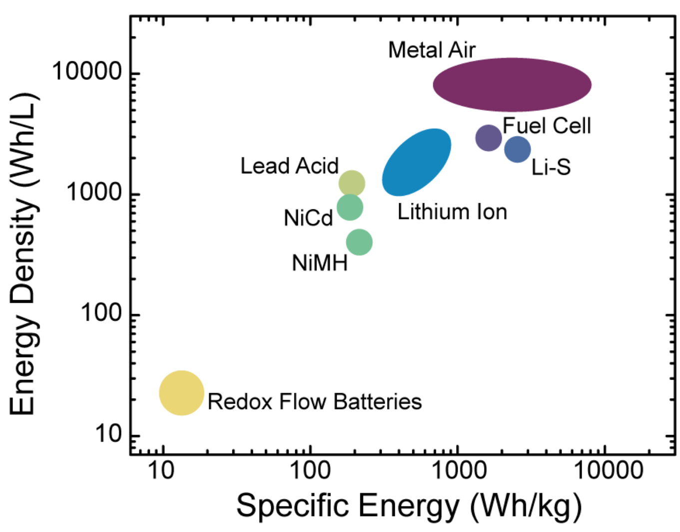

Figure 6 – Plot comparing the maximum theoretical specific energy and energy density of different energy storage technologies. These values are calculated using only the mass and density of the active materials in the electrode and represent the theoretical maximum achievable values. The calculations are based on whichever state (charged or discharged) volume per charge and weight per charge is larger respectively. [Credit: Yang Shao-Horn, MIT]

Despite the scope and difficulty in developing of new energy materials, significant progress continues to be made, which has translated to improved performance of commercial devices. Over just the last 10 years, Li-ion battery prices have fallen by a factor of 10 and are predicted to continue decreasing due to continued development and optimization of materials and fabrication processes (Figure 2b).

This workshop identified conceptual challenges and opportunities that cut across multiple technologies and are most amenable to synthetic biology approaches. This section highlights those challenges, organized around three areas: Electrocatalysis, Electron Storage, and Ion Transport.

Electrocatalysis

Catalysts increase the rate of a chemical reaction by lowering the energetic barrier to form the intermediate species. They are therefore critical to the transition away from fossil fuels to a renewables-based energy economy. Unfortunately, the kinetics of oxygen reduction and evolution, which is needed universally for making these energy carriers, are slow. These slow kinetics limit the efficiency of such devices to be much lower than that of Li-ion batteries. In addition, the kinetics of both carbon dioxide (CO_2) and nitrogen (N_2) reduction to ammonia are even more sluggish than oxygen reduction and oxygen evolution, which further decreases device efficiency. *[11]* *[12]* Therefore, more active catalysts are needed to increase the reaction kinetics. However, there are theoretical and technical challenges to developing new catalysts.

For CO_2 reduction reactions, copper is presently the best-known catalyst. However, its performance suffers from unwanted hydrogen production which can suppress the yield of the desired products. Furthermore, poor understanding of how to promote certain pathways over others makes it difficult to control the selective production of the desired CO_2 reduction products. *[13]*

For ammonia production, *[14]* the challenge is to develop catalysts that work at low temperature and pressure to replace the current Haber-Bosch process that is energy intensive and requires both high temperature and pressure.

In fuel cell/electrolyzers, the overpotential associated with oxygen reduction and oxygen evolution catalysis (ORR/OER) and the availability of catalyst materials are the key challenges for catalyst development. The ORR/OER reactions are not as efficient as the hydrogen evolution/hydrogen oxidation (HOR/HER) counterpart reactions on the opposite electrode (Figure 7). Furthermore, the best catalysts for the oxygen reactions are based on rare precious metals like ruthenium and iridium, which have limited global supply. If H_2 is to be used as an energy storage medium for future energy infrastructure, the discovery of new non-precious metal ORR and OER catalysts with low overpotentials will be critical.

Development of new catalyst materials and structures is currently underway to improve catalytic activities by modifying the energetics of the metal catalyst site through inductive effects from the chemistry around the active site [15]. But before these new catalyst materials can be developed, key hurdles must be overcome. First, in-situ characterization of the active sites will be needed to ensure better understanding of how reactants, intermediates, and products bind to the surface. This is essential to guide rational design of new materials. A second challenge is to minimize the correlated scaling of the binding energies of reaction intermediates, as it prevents the free tuning of the reaction energetics to achieve lower overpotentials [16].

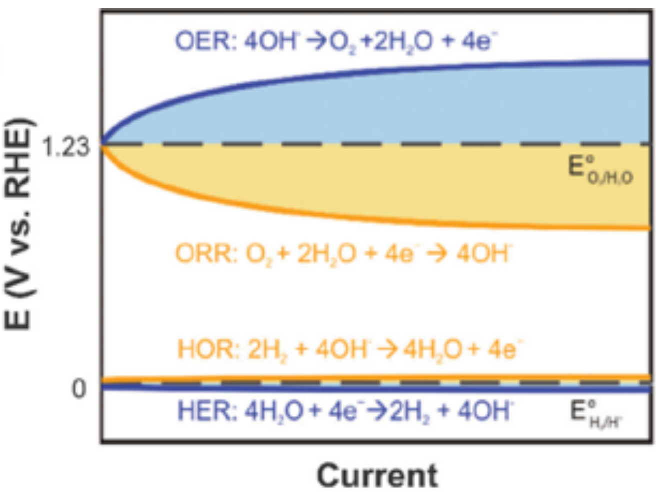

Figure 7 – Plot of the overpotentials for oxygen and hydrogen electrocatalysis. Oxygen reactions severely limit the energy efficiency of fuel cells and electrolyzers due to the large overpotentials required to drive the reactions, even when using the best catalysts [10].

In summary, the key electrocatalysis research challenges that are amenable to synthetic biology approaches are:

- Development of catalysts that exhibit faster kinetics for ORR/OER reactions, CO_2 reduction, and N_2 reduction
- Improvement to the selectivity of catalysts for the reduction of CO_2 into high value products without H_2 evolution
- Synthesis of non-precious metal catalysts for oxygen reduction/evolution with low overpotential
- Development of techniques to better identify and understand active sites for catalytic reactions
- Design and fabrication of novel materials and structures to break scaling relationships of reaction intermediates with catalyst surfaces

Electron Storage

Electron storage discussions focused on batteries and the materials used for electrochemical energy storage. Much of the research on battery materials is focused on lithium ion technology due to its high energy density compared to other electrochemical energy storage technologies (Figure 6). While technologies based on alternative chemistries, such as sodium and magnesium, may improve sustainability and safety, they have lower energy densities and operating voltages than lithium [17]. Zinc, which is far more abundant than lithium in the Earth's crust, has better safety and energy density, but is hindered by the lack of reversibility [18].

Numerous design strategies have been pursued to stabilize the interface between the lithium metal and the electrolyte and potentially replace the graphite layers with lithium for Li-ion batteries. This would essentially double the energy density as lithium metal is the ideal negative electrode due to its low potential and high capacity. But issues of safety, due to dendrite formation that can short circuit the cell, and cyclability, due to low efficiency of the Li plating and stripping and side reactions, have prevented commercialization thus far. For the positive electrode, new metal oxides with a reduced amount of cobalt are being studied, but the cycling stability is low for these systems due to irreversible oxygen loss at higher potentials. Understanding how to control this oxygen redox will open the door to new materials with greatly increased capacity. New materials are continually being reported that take advantage of this effect. Looking beyond metal oxide cathodes, sulfur has the potential to enable high energy density batteries due to its extremely high capacity, which is almost seven times that of metal oxide cathodes. The polysulfide species that form during this conversion reaction are soluble in the liquid electrolyte and this dissolution prevents stable cycling.

In addition to improvements to lithium ion technologies, researchers are studying new battery concepts such as liquid based flow batteries and battery systems based on sodium, magnesium, and zinc ions. New organic molecules are also being studied as interesting alternatives to metal-based compounds and have been particularly attractive as active materials in flow and sodium-ion batteries [19].

In summary, the key electron storage research challenges that are amenable to synthetic biology approaches are:

- Design of electrode-electrolyte interface stability
- Stabilizing high capacity battery electrodes including lithium metal and ligand redox (e.g. sulfur)
- Discovery of "beyond Li-ion" chemistries and device concepts that enable high energy density and large-scale energy storage

Ion Transport Materials

Ion transport across different interfaces and through electrode materials or bulk electrolyte is a key process in electrochemical energy storage. Efforts to improve transport must overcome numerous challenges including: selectivity; chemical, mechanical, and thermal stability; and performance. Workshop participants discussed the research challenges in the pursuit of optimized ion transport materials, especially for battery applications.

Presently, batteries include porous polymer separators that are filled with organic liquid electrolytes, having ionic conductivity values of ~10^{2} S/cm at room temperature. However, these organic solvents are highly flammable, and the porous separators have limited ability to prevent thermal runaway, the primary cause of the well-known issue of fires and explosions in these batteries. The safety of Li-ion and other battery devices is of critical concern for both civilian and military applications, so new non-flammable electrolytes are needed. Additionally, liquid electrolytes typically have low selectivity to cation (Li^+ or Na^+) transport with typical values for the transference number (the fraction of the total electrical current carried in an electrolyte by a given ionic species) around 0.2. This leads to polarization in the cell and prevents high rate capability.

Solid electrolytes made from both ceramic and polymer materials are a promising replacement for organic liquid electrolytes as they have reduced flammability (Figure 8). Ceramic solid electrolytes like $Li_{10}GeP_2S_{12}$ have ionic conductivity that is equal to that of liquid electrolytes, but many of these ceramic materials have very small electrochemical stability windows, so they react with electrode active materials during cycling, thus limiting the lifetime of the battery *[20]*. New chemistries or strategies must be developed to stabilize the interfaces of the electrolyte with the battery electrodes. The development of "superionic" conductors with ionic conductivities exceeding that of liquid electrolytes would transform energy storage technology.

Polymer electrolyte materials are based almost entirely on poly (ethylene oxide) (PEO) and are limited in conductivity to ~10^{-5} S/cm at room temperature. Small molecule and ceramic additives can allow for systems to reach ~10^{-3} S/cm, but generally the mechanical or electrochemical stability is sacrificed. Polymer electrolytes also have similarly low transference numbers to liquid electrolytes. Therefore, polymer designs other than PEO are needed to enable higher ionic conductivity at room temperature and selective cation transport through the polymer. Hydrated polymers are also commonly used as electrolytes for fuel cells, and Nafion is the gold standard for proton (H^+) transport in acidic cells. To date, there has been no material developed with similarly fast anion (OH^-) conductivity for fuel cells and electrolyzers operating in basic conditions. The development of an anion exchange membrane that has similar conductivity to Nafion is needed to enable catalysts that function in basic medium.

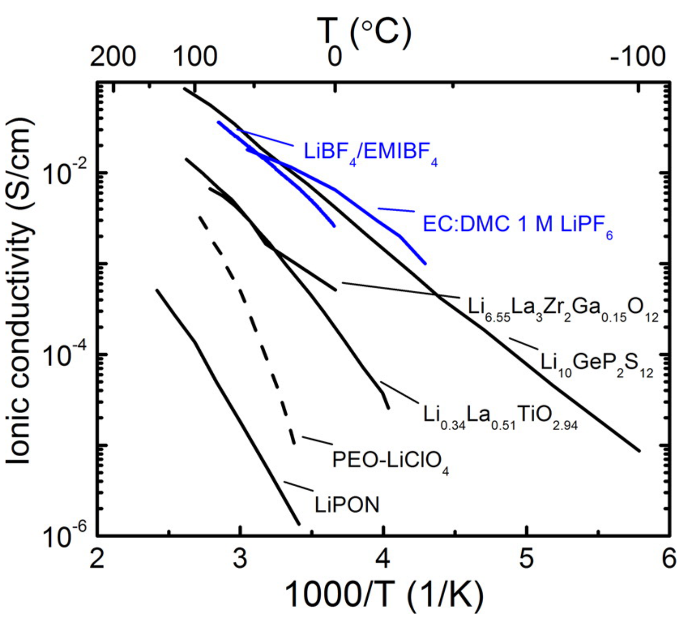

Figure 8 – Ionic conductivity values reported as a function of temperature for liquid electrolyte (blue), polymer electrolytes (dashed), and inorganic solid electrolytes (solid lines). Some solid electrolytes have demonstrated ionic conductivity on par with that of liquid electrolytes (LGPS) *[20]*.

In summary, the key ion transport materials research challenges that are amenable to synthetic biology approaches are:

- Non-flammable electrolytes or systems to prevent thermal runaway
- Electrolytes with high transference numbers for cations used in energy storage devices (Li+ and Na+)
- Solid ceramic electrolytes that are stable with Li-ion battery electrodes
- Polymer electrolytes with ionic conductivity on par with liquid and solid ceramic electrolytes
- Anion (OH^-) conducting membranes with ionic conductivity similar to that of protons in Nafion
- Solid or liquid electrolytes with wide temperature stability windows for safety in military or other demanding applications

Recent Advances and Future Opportunities for Synthetic Biology

Synthetic biology aims to use engineering principles to improve upon the existing processes of a living system or create new ones. In its early years, biologists studied a particular gene, modified it, and used it to perform a desired function. More recently, the dramatic increase in the ability to read, write, and edit in DNA has allowed an unprecedented level of control over the information flow in biological systems. For example, the cost of DNA synthesis is at an all-time low, at less than ten cents per DNA nucleotide; these costs only continue to decrease (Figure 9). The increased modification capability and reduced costs drives our ability to design and build both existing and novel DNA elements, which in turn enables *de novo* creation of biological systems in ways never before possible. This has opened up opportunities to create sophisticated genetic programs and functions with applicability across multiple sectors. Current capabilities include the creation of programming languages in cells through computer-written genetic codes subsequently synthesized in DNA for a desired function. The ability to genomically recode organisms has expanded their repertoire of biological functions. These capabilities will continue to grow as additional study of living systems elucidates novel cellular functions and their underlying mechanisms.

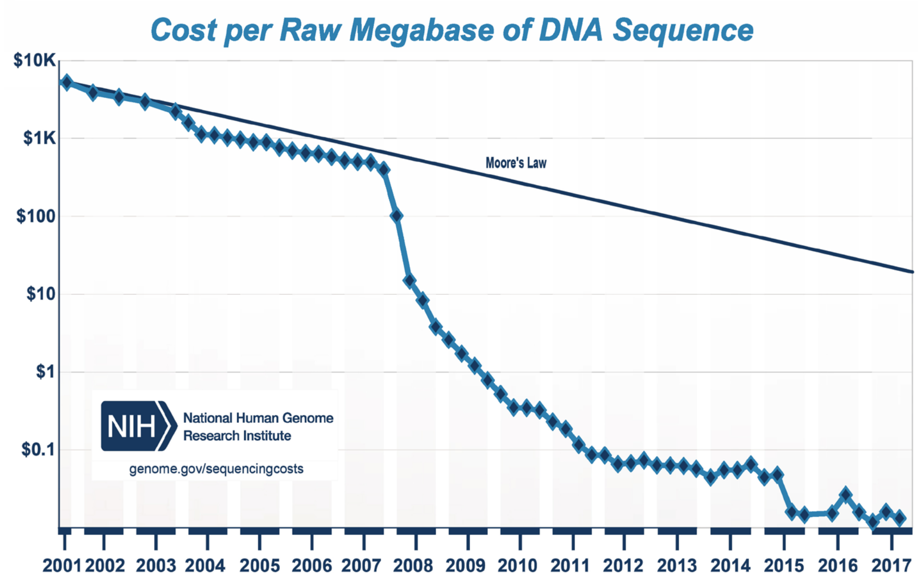

Figure 9 – Costs associated with DNA sequencing performed at the sequencing centers funded by the National Human Genome Research Institute (NHGRI) *[21]*.

These advances in tools for genetic design and manipulation are increasingly coupled with automated screening technologies to create an agile and robust Design-Build-Test cycle (Figure 10).

Over time, the synthetic biology toolkit has expanded to include biological parts including DNA, RNA, protein, and carbohydrate elements, as well as the design rules necessary to implement them into coherent biological systems for desired functions. DNA regulatory elements including promoters, ribosome binding sites, and terminators are characterized, standardized, and cataloged to provide confidence in the parts that exist for engineering *[22]*. In addition, tools to predict DNA, RNA, and protein structure and function, while in their infancy, are beginning to inform biological systems design. Cell-free systems, along with high-throughput and automated cellular engineering platforms, are now coming online as ways to prototype and test synthetic biological parts and systems as a whole. Taken together, the synthetic biology toolkit has enabled efforts to manipulate biochemical transformations, create novel cellular devices and therapies, and expand the chemistry of life by introducing non-canonical amino acids and nucleobases into traditional biological systems. Recent efforts in chemical synthesis of bacterial genomes and interest in artificial cellular systems represent another avenue with great potential in the coming years.

The speed at which the field of synthetic biology has evolved mimics that of the computer industry, illustrating the rapid increase in opportunities to synergize with the traditional approaches to address energy and power challenges. From enzymatic catalysis to small molecule and material synthesis, synthetic biology is poised to address grand challenges relevant to generating and storing energy through the creation of new biological systems.

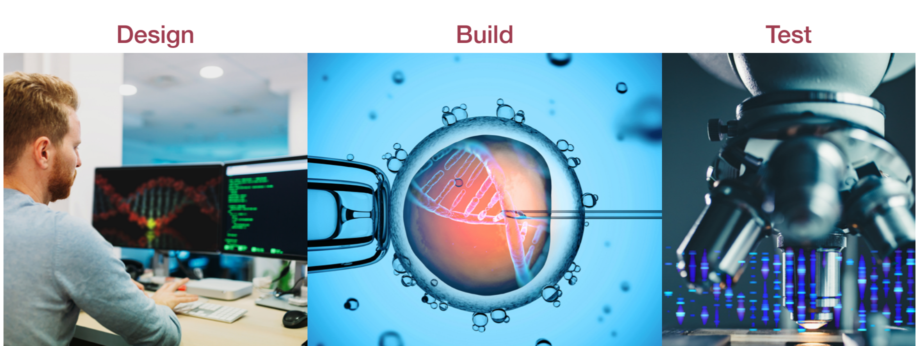

Figure 10 – Advances in synthetic biology tools has enabled an efficient Design—Build—Test cycle.

Workshop participants reviewed the current and future synthetic biology capabilities that were most likely to have an impact on energy/power research efforts. This section presents those discussions as three topics:

- Synthetic Biology for Catalysis
- Biosynthesis of Materials
- Microorganisms at the Biotic/Abiotic Interface

Synthetic Biology for Catalysis

Nature has evolved its own set of biological catalysts, called enzymes, to accelerate chemical reactions. These proteins have high catalytic density with high selectivity and efficacy under ambient conditions. Isolating enzymes from thermophilic and pH-tolerant organisms can enable catalysts with robust stabilities. The wide variety of catalogued genome sequences provides a rich resource of enzymatic diversity to identify biological catalysts for desired functions (Figure 11).

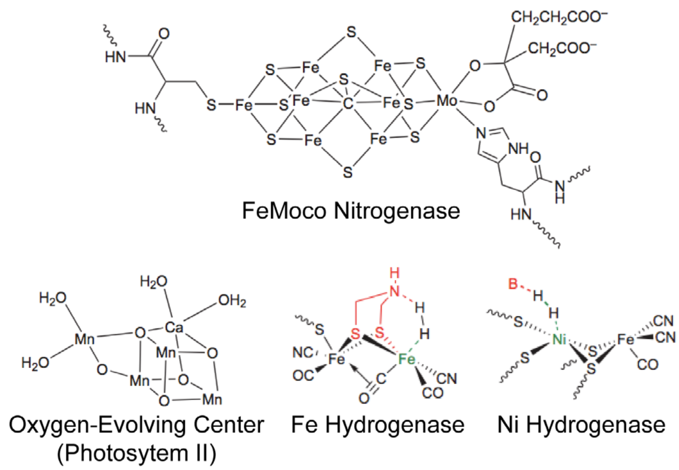

Figure 11 – Examples of catalytic centers from biological systems. [Credit: adapted from *[23]*]

Thus, there is a significant opportunity for synthetic biology to draw upon these properties to improve catalysis for energy applications. The participants discussed these opportunities along two main avenues:

1. Enzymes as a design guide for catalysis

Both computational and experimental methods to design and optimize catalysts are an area of active research. Enzymes have evolved over millions of years to perform reliably, safely, and selectively, and can be integrated into these current methods to identify design principles for desired catalytic reactions. While there are numerous individual enzymes, these can be broadly categorized into families that share common conformations and conserved amino acid residues that provide insight into structure-function links. Structure-function relationships for energy catalysis could thus be enabled by high-throughput design-build-test-learn cycles, and any learned rules can subsequently inform the design of minimal (e.g. single atom) catalysts that have a smaller footprint and higher stability than whole enzymes. Such minimal catalysts might also be able to avoid the use of rare earth metals.

Enzymatic reactions and metabolic pathways also provide an opportunity for the design of multistep cascade reactions. Within any given cell, hundreds of reactions proceed simultaneously drawing from a common set of precursors. Despite the heterogeneous mixture of catalysts and reactants, natural biosynthetic pathways produce chemicals on-demand and with high specificity. This is made possible by compartmentalization and confinement strategies, and by assembling enzymes into well-defined architectures that promote the efficient use of reactants and drive flux down a desired pathway. **Analogous to the structure-function relationships between enzymes and their catalytic activity, design rules for multistep and cascade reactions can be learned from evolved metabolic pathways and translated to new catalytic processes.** These processes include not only multi-enzyme reactions but also chemical cascade reactions comprised of heterogeneous and homogenous catalysts or hybrid cascades that combine two or more catalytic modalities.

2. Enzymes used directly for catalysis

Enzymes, just as they are in nature, can be used directly for energy/power catalytic purposes. Synthetic biology can improve upon them further by creating more streamlined enzymes with smaller footprints. Further, while many enzymes have novel functionalities, they can also be inefficient. This can be overcome by engineering enzymes without catalytically unnecessary structures in stable and active conformations. Given the molecular diversity and density inside a cell, enzymes are extremely selective, a property than can be further engineered to improve upon chemical catalysis. Aside from optimizing already-existing catalysis, the tools of synthetic biology can also expand the repertoire of enzymatic functions to include non-natural chemistries. For example, *de novo* enzyme design is emerging as an approach to evaluate new enzymes via computer simulation. Given a set of enzymes necessary for a desired molecular transformation, cascades of enzymes can be constructed in cells and cell-free systems to both generate and store energy.

Importantly, enzymes provide unique opportunities to identify and harness chemistries that may not exist or are difficult synthetically. For example, France Arnold's laboratory at the California Institute of Technology has created new enzymes that catalyze non-biological reactions with high efficiencies and selectivities with sulfur-carbon iron sites, iron-carbenes and carbocycles *[24]*. They also provide a direct mechanism to link electron transport chains, ATP usage to drive endergonic reactions, and the direct coupling of energy sources (e.g., solar) to catalysis.

Looking forward, a particularly tantalizing future direction is the multistep enzymatic synthesis of complex biomolecules composed of elements derived from both metabolic pathways and chemical synthesis.

Biosynthesis of Materials

Critical energetic processes occur in extremely short timescales and involve changes at the atom and electron level. Thus, harvesting and storing energy from renewable resources requires materials with nanoscale resolution and atomic-level functionality to achieve higher performance levels. **From silk proteins as membrane separators to eggshell-inspired piezoelectric materials, nature is filled with unique, self-assembling materials that can be useful in energy technologies.** With the capacity to synthesize materials with nanometer-level precision, biological machinery also offers a pathway to create tailored polymers or their monomeric units.

Participants discussed several opportunities for synthetic biology to improve current methods using combinatorial design and synthesis and the proper high-throughput screens to enable selection of desired functional properties. This coupled with the natural ability of living systems to evolve could enable powerful tools for new material and structural discovery. Precision synthesis could enable new functional materials such as high ionic conductivity polymers and ion transport materials that have transport energy built into the construct.

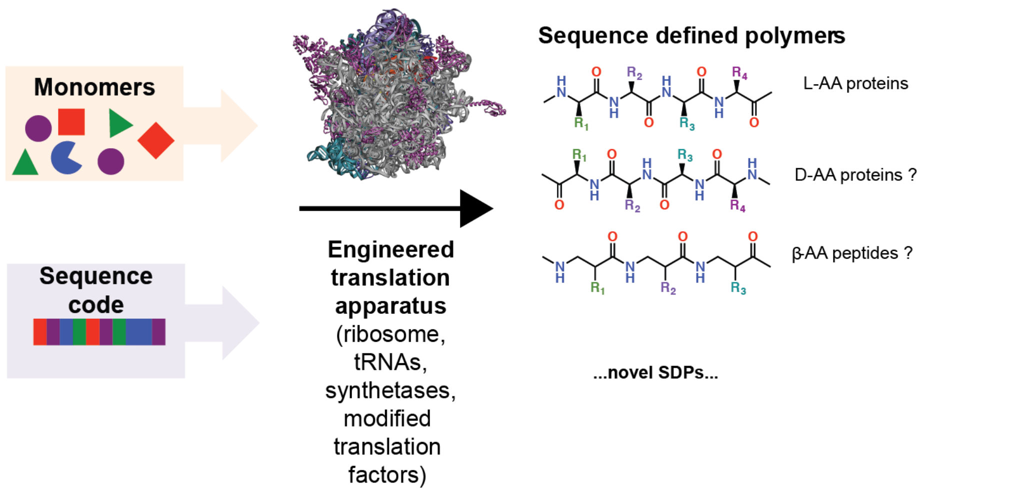

Figure 12 – Engineering the translation apparatus to manufacture sequence-defined polymers. Expanding the repertoire of ribosome substrates and functions has the potential for making polymers with even greater functional breadth, but this potential remains underexploited. By repurposing ribosomes, the field seeks to open up new areas of research in materials science, medicine, and synthetic biology. [Credit: Michael Jewett, Northwestern University]

Bio-derived polymers can be used as electrolyte materials in lithium ion and other battery chemistries. The use of the synthetic biology toolkit was also discussed as a potential way to engineer the electrode-electrolyte interface in batteries. Stabilizing this interface is critical to enabling high efficiency and long cycling stability of LIBs. Using biology to create materials with improved selectivity to lithium cation transport may also be possible by studying how selective ion channels in cell membranes function and translating these design concepts to solid polymer electrolytes.

One exciting example of polymers discussed was the synthesis of sequence defined polymers (SDPs). SDPs are macromolecules whose chemical and physical properties can be programmed with atomic-scale resolution. To date, it has been very difficult to produce finely tailored non-natural SDPs (i.e., materials of defined atomic sequence, exact monodisperse length, and programmed stereochemistry), yet the development of synthetic routes toward these molecules promises technological breakthroughs in advanced functional materials, nanotechnology, power, electronics, and beyond. One approach to address this need is to engineer and repurpose the translation apparatus (including the ribosome and the associated factors needed for polymerization) to produce new classes of SDPs (Figure 12). Indeed, repurposing the translation apparatus holds promise to eclipse the level of compositional control previously achieved by chemical synthesis approaches, allowing us to develop empirical and perhaps even model-based connections between polymer sequence, polymer composition, and polymer function using an evolved translation apparatus. This would allow new materials to be designed in a knowledge-based way. It will also harness one of the most salient features of biology, its ability to evolve, in search of new material forms.

In addition to polymers synthesized by cellular polymerases, biological materials produced by cells exhibit similar monomeric precision and provide platforms for energetic systems. Organic polymers, such as melanin and other pigments, have precise monomeric units and self-assemble into three-dimensional structures (e.g., an insulating sheath around a conducting core). These materials provide electron, proton, and ion conducting amorphous semiconductors that can be incorporated into batteries (Figure 13). Further, they absorb UV and radiation by converting it to heat, which can form the basis for protecting components in extreme environments, including nuclear reactors and space-based energy systems.

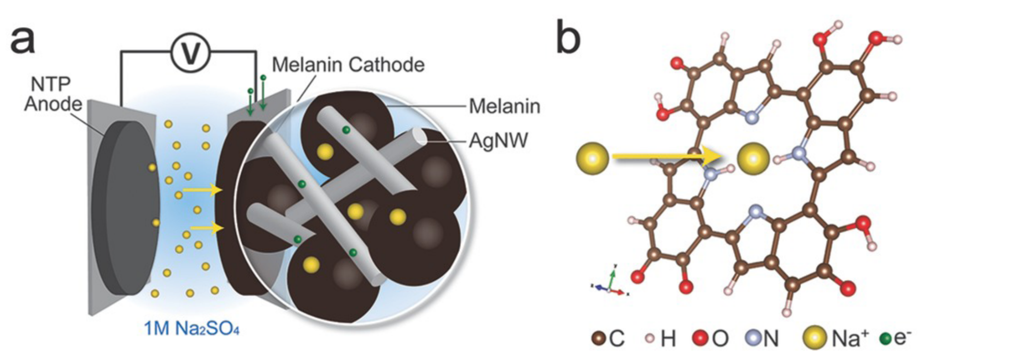

Figure 13 – Natural melanin pigment shows promise as a novel organic battery material *[25]*.

Synthetic biology can also be used to develop new structures, from two-dimensional stack layers, pore systems, and even three-dimensional structures, whereby small units (i.e., proteins, DNA, etc.) can self-assemble into hierarchical structures. Microbial cellulose produces hydrogels of defined porosity and high surface area that could be integrated into low cost batteries with reduced usage of expensive metals (e.g., platinum). Silks and other protein based materials offer the potential for programmable self-assembly and incorporation into 3D printing platforms. Finally, templated materials, for example by phage, could be used for battery components and to produce batteries with improved properties (e.g., structural rigidity).

The combination of new materials and new structures can be used to enable ion transport systems relevant to energy/power devices. For example, new engineered membrane systems with precisely tuned biological transporters and membrane pores could provide new synthetic cascading electron transport devices to store or convert energy and efficiently couple electron/ion transport. Similarly, new molecules with finely tuned chirality[1] features could drive advances in molecular spintronics (or spin-based electronics) for electrochemistry-driven energy/power applications.

Beyond simply replacing conventional materials with bio-derived alternatives, participants emphasized the opportunity to use the capabilities of synthetic biology to develop unique and unconventional approaches to solving energy storage problems. Initially, this could be the identification of new biological chemistries needed to meet design criteria. In the future, researchers could potentially develop Darwinian selection methods to obtain desired material properties. Systems could be developed with the capability to self-organize into functional materials or devices using programmed self-assembly across multiple length scales. **Researchers should work to imagine biological systems that don't just mimic existing chemical solutions but meet or exceed defined device performance metrics in unique ways.**

Microorganisms at the Biotic/Abiotic interface

Another important synthetic biology research area relevant to energy/power applications is microorganisms at the biotic/abiotic interface. Broadly speaking, the biotic/abiotic interface can be defined as the point of interaction between the biological component of a system (bacterial cell, living tissue, protein, etc.) and a non-biological surface, such as a medical device, mineral in the subsurface, or electrode. Although the biotic/abiotic interface has been recognized to play a significant role in many facets of society for a long time (e.g. medical devices, corrosion, and fouling of ships) it has only been within the last 20 years or so that it was recognized that living cells can exchange electrochemical information in the form of electrons at this interface. While naturally-occurring systems have evolved to interface with minerals, surprisingly many of these microorganisms—dubbed exoelectrogens—can also electrochemically interface with electrode materials. These discoveries have spurred investigations into how to exploit the charge transfer mechanisms at the biotic/abiotic interface for the development of microbial electrochemical technologies, such as microbial fuel cells [26].

An on-going body of research has revealed diverse mechanisms of electron flow between microorganisms and their environment [27]. Bacteria have evolved multiple electron transfer pathways in order to efficiently and rapidly adapt to energy requirements in environments where available potential energy at the biotic/abiotic interface changes rapidly depending on subsurface chemistry (Figure 14). Bacterial cells can directly perform heterogeneous electron transfer reactions with electrodes using redox active proteins. To date, these have been reported to be multi-heme c-type cytochromes that form electron transfer conduits between the oxidative metabolism of the cell and the extracellular environment. Further, some bacteria are able to form conductive biofilms that span gaps of 10's of microns with conductivities rivaling those of synthetic polymers [28]. These studies provide both design rules for charge transfer at the biotic/abiotic interface and 'parts' for synthetic biologists.

Microbial fuel cells (MFCs) use microbially-mediated oxidization of organic molecules to produce electricity. **Because they can generate power using dilute sources of chemical energy, microbial fuel cells hold great promise as persistent sources of power in remote locations, including at the bottom of the ocean.** Another emerging technology, microbial electrosynthesis cells, can use renewable energy to make covalent bonds, including the ability to synthesize fuels from CO2 [29]. Synthetic biology could be used to address these technologies, as well as enable further control of these processes at the biotic/abiotic interface for applications in energy and power platforms. For example, microorganisms with very wide metabolic ranges have been engineered to be exoelectrogens, which increases the variety and number of fuels that can be used in MFCs to produce electricity.

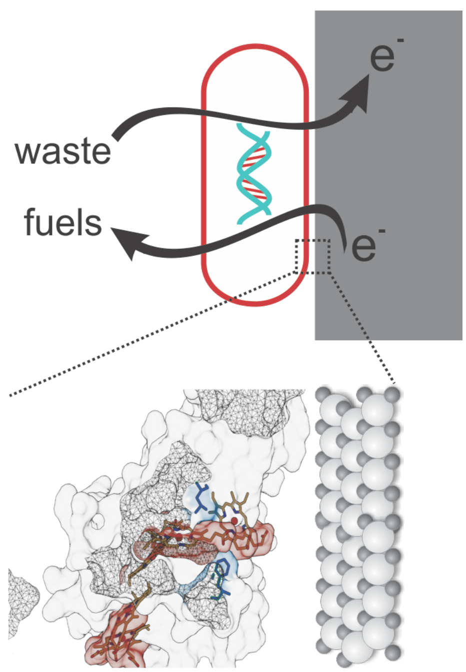

Figure 14 – The microorganisms at the biotic/abiotic interface can interconvert chemical and electrical energy (top), but pose significant characterization (bottom) and engineering challenges. (Credit: adapted from [30] and [31])

1 Mondal, et al., 2018 Small Methods, 2(4): 1700313. *https://doi.org/10.1002/smtd.201700313*

Synthetic Biology Research Challenges and Proposed Trajectory

To realize the potential for synthetic biology to enable advanced materials and structures for energy and power applications, there are several key conceptual and technical obstacles that will need to be overcome over the next 20 years.

At a high level, the first step will be to develop interdisciplinary collaborations between the synthetic biology and energy research communities. Currently, each community lacks awareness of the needs, interests, and capabilities of the other, especially quantitative metrics of performance. This leads to miscommunications and missed opportunities. This was quite apparent even in the language used by the participants at the workshop. For example, common terms like catalysis, co-factor, and robustness meant completely different things to the physical and life science researchers in the workshop. **With different vocabularies and limited interaction between the two communities, new mechanisms will be needed to help build interdisciplinary connections and foster collaboration.** As these collaborations become more prevalent and the number or researchers working in this area grows, the community will develop its own language for communicating at this interface.

The workshop participants framed the important technical challenges for the three research areas within the context of development of:

- Computational frameworks, as well as theory to model and predict biological design of materials
- Analytical tools to characterize interfaces and charge transfer in biological and bio-derived systems
- Bioprocess engineering strategies to enable manufacturing of bio-derived energy materials at appropriate scales
- Strategies to decouple cellular and engineering objectives
- Processes for decentralized, on-demand synthesis
- Biological systems that can scavenge energy from the environment for long-term deployment

All of these topics are linked by the common need for establishing active collaborations across disciplines through interdisciplinary projects and conferences.

The specific synthetic biology research challenges and proposed trajectory are organized along four themes: (1) bio-inspired catalysts, (2) bio-derived energy storage materials, (3) bioprocess engineering frameworks for making new biomaterials/polymers, and the (4) biotic/abiotic interface. Each of these is described in detail in the following sections.

Bio-Inspired Catalysts

While the application of synthetic biology was agreed to have tremendous potential, participants acknowledged certain obstacles to progress. First, further investigation of the fundamental mechanisms of biological catalysts is needed to translate their unique functions into principles that can be used to create new design rules for materials scientists. To obtain this information, new characterization techniques are needed to better understand the catalyst active site and identify the relevant mechanisms that control activity, selectivity, and stability. Once a greater understanding of biological catalysts is obtained, research can move in three directions simultaneously: 1) materials scientists can develop design concepts based on biological systems and use these concepts to synthesize high performance catalysts; 2) synthetic biologists can modify cellular machinery to enhance the performance of existing biological catalysts by reducing enzyme footprint or modifying the active site, and 3) materials scientists and synthetic biologists can work together to create multifunctional catalysts from biological and materials parts.

Whether enzymes are the inspiration for better catalysts or engineered to facilitate reactions directly, a number of research challenges in this space remain. To effectively implement any design rules learned from studying biological systems, materials scientists will need to develop new synthesis approaches to better control and design active sites. A possible alternative will be the adaptation of synthetic biology tools to create synthetic catalytic materials or structures that cannot be accessed with traditional synthesis or nanotechnology methods. This would require close collaboration between chemists and biologists to develop an entirely new biological toolkit for materials synthesis.

The modification of existing biological catalysts will also require significant work. With a richer structure-function understanding, we can first determine the smallest size of a biological catalyst that still performs a desired reaction, thus facilitating the engineering of lower footprint catalysis. Moving forward, the use of synthetic biology tools to engineer new catalytic systems with cellular machinery will open the door to the discovery of new active site chemistry or binding environments. High throughput screening may be one avenue to pursue in order to leverage evolutionary or library based modification of specific biological catalytic sites.

"Moving forward, the use of synthetic biology tools to engineer new catalytic systems with cellular machinery will open the door to the discovery of new active site chemistry or binding environments."

A synthetic biology approach can also be used to develop new hybrid catalysts that take advantage of the beneficial characteristics of bio- and chemical catalysts while avoiding their disadvantages. For example, protein structures designed to bind a reactant of interest with high affinity could be used to enhance selectivity in heterogeneous and homogenous reactions. Alternatively, new materials could be used to stabilize and enhance enzymes with smaller footprints. Hybrid catalysts also promise to create new cascade and multistep reactions, enabling chemistries that are not possible through the use of a single type of catalyst. Incorporating both biological and material diversity into high throughput design-build-test approaches is one possible route to the development of these new technologies.

Participants discussed the parallel growth of new computational frameworks to aid in the advancement of understanding and design of bio-inspired and biological catalysts. Such frameworks could help researchers to identify optimal catalytic properties and develop a better connection between enzyme structure and activity or selectivity. However, these advances would require faster and more detailed characterization techniques in order to provide the data needed to drive these computational models accurately.

To address these challenges, the panelists propose the following research trajectory:

Short-term Research Trajectory (5-10 years):

- Develop biologically-inspired design of catalytic active sites
- Create new characterization tools, including in-situ techniques, to identify active site intermediate binding geometries

Long-term Research Trajectory (10 -20 years):

- Develop a new biology-based toolkit to create materials and structures for catalyst synthesis
- Harness cellular machinery to reduce enzyme footprints and introduce modifications to active sites for improved performance
- Establish multi-scale computation methods to understand and predict structure-property relationships that can drive rational design

Bio-derived Energy Storage Materials

The importance of a common language and mutual understanding between biologists and material scientists is especially important for developing bio-derived energy storage materials. This is essential in order for researchers to clearly articulate and understand performance specifications and key parameters for materials and devices.

Once clear communication has been established, researchers can begin to use synthetic biology to synthesize useful energy storage materials as discussed in the Current Research and Future Opportunities section. When discussing the use of bio-derived materials for energy storage applications, the main challenges are large scale synthesis of bio-derived materials, characterization methods, and the compatibility of biochemistry with reactive energy storage environments.

Most importantly, new techniques and theories are needed to aid the development of these new materials. New testing platforms will be needed to characterize materials across multiple length scales, and the potential capabilities of synthetic biology require new theoretical frameworks to help link accessible biological molecular structures with materials properties. Ideally, these new frameworks will help provide modeling tools to understand and predict materials properties and architectures. Computational approaches will also be useful as researchers study how to program and control the production and assembly of biological materials. Further, new biocatalytic approaches to materials themselves are needed.

Short-term Research Trajectory (5-10 years):

- Establish better communication between the synthetic biology and energy communities to build an understanding of device/materials properties and metrics
- Identify new biological chemistry needed to meet design criteria and expand our chemical/biochemical reaction capabilities
- Develop engineered translation systems for manufacturing novel sequence defined polymers

Long-term Research Trajectory (10-20 years):

- Develop unconventional materials and methods using a uniquely synthetic biology approach
- Develop multiscale computation and characterization methods to further understanding of structure-function relationships and drive rational design
- Program self-assembly of energy storage materials/devices using guided production and organization

Bioprocess Engineering Frameworks for Making New Biomaterials/Polymers

Unlike the biomedical applications of synthetic biology, extending the field to energy/power challenges requires a much greater consideration of scale. The scaling issue underpins a great need and opportunity to create new bioprocess engineering systems that can meet the demand for high volume materials needed in energy and power applications.

The issue of scale arose frequently throughout the workshop and across all small group discussions. Bioprocessing frameworks discussed include understanding the appropriate titers, rates, and yields of relevant processes.

A key challenge to achieving large scale is to balance the synthetically engineered objectives with the interference this causes to the microorganism's endogenous metabolic processes and functions. New insight from biology have led to better circuit design and more success in scaling up various bioprocesses. This must continue to be developed. However, an alternative solution is to decouple the endogenous objectives of a cell from its engineered objectives by using cell-free systems (Figure 15). Cell-free systems have particular advantages. First, the open nature of the reaction allows the user to directly influence biochemical systems of interest. As a result, new components can be added or synthesized, and maintained at precise concentrations. Second, cell-free systems bypass viability constraints

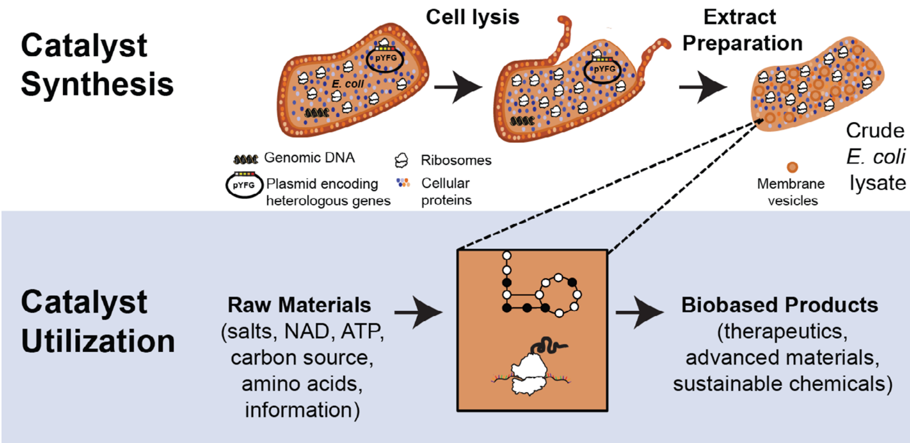

Figure 15 – Cell-free synthetic biology is emerging as a transformative approach aimed to understand, harness, and expand the capabilities of natural biological systems. (Credit: Michael Jewett, Northwestern University)

making possible the production of proteins at titers that would otherwise be toxic in living cells. Third, processes that take days or weeks to design, prepare, and execute *in vivo* can be done more rapidly in a cell-free system, leading to high-throughput production campaigns on a whole-proteome scale with the ability to automate.

Aside from cell-free systems, other possible manufacturing strategies discussed included hybrid biological/chemical synthesis, and microbial consortia.

In producing energetic materials in living cells, the core challenge is the ability to convert a need for a particular polymeric or nanostructure to the control of multiple genes. The production of a monomeric precursor involves the introduction of recombinant genes from diverse organisms and the optimization of carbon flux through metabolism, from sugar to the precursor metabolites. To create desired structures that do not exist in nature, multiple enzymes from different organisms/pathways will need to be combined so that the chemically-modified metabolite can be converted into the final chemical required. This will require the systematic analysis of the specificity and compatibility of large enzyme libraries and the computational algorithms in order to accurately combine these enzymes and to retro-synthetically create a final chemical from the metabolite. Further, the pathways by which microbes build intricate non-carbon (metal, silicate, etc.) pathways are poorly understood. The ability to design particular nanostructures will require the ability to manipulate metal transporters and protein and lipid-based mechanisms for the crystallization and layering of composite structures. Finally, to fully exploit the potential of biology, mechanisms for self-assembly have to be developed. This consideration extends to the molecular level, where protein-protein interactions, as well as DNA/RNA techniques could be used to create structures at the nanometer scale. Assembling structures from the micron to meter scale requires the control of cells over long distances and during growth processes. This will require more precise control over cell-cell communication and the division of labor amongst differentiated cells. Tight control of complex materials synthesis and conformations will require that processes be staged to occur at different times. For instance, a stepwise process could include: 1) the initial production of primary building blocks of a polymer, 2) its polymerization into a precise primary structure, 3) the control over 3D assembly, and 4) the final post-processing of the product. If costs can be lowered and reaction longevity extended, cell-free systems may offer an interesting opportunity here. This will require new modes of energy regeneration in these systems.

Short-term Research Trajectory (5-10 years):

- Establish test-beds and metrics for design to ensure that properties of bio-based materials meet specifications
- Institute training programs to educate a workforce that is proficient in a common vocabulary between physical and life scientists
- Develop new theory to model and predict properties of unique materials accessible by engineering biology
- Build fundamental understanding of biological systems and ion transport mechanisms
- Develop computational frameworks to advance biological design (both of active sites for catalysts, and polymeric materials)
- Develop new approaches that decouple the production of chemicals/materials from the need to maintain living cells, for example, for toxic products
- Develop technologies for the rapid design of biological materials to the production of sufficient quantities for prototyping in devices
- Establish new hybrid chemical/biological syntheses strategies

Long-term Research Trajectory (10-20 years):

- Develop a framework for the synthesis of sequence defined polymer structures
- Tailor design and synthesis of materials using predictive modeling of biopolymer architectures
- Construct on-site distributed biomanufacturing capabilities that can derive energy from diverse waste sources, for example garbage at a forward-operating base
- Develop bioprocess strategies and flexible manufacturing facilities for the rapid scale-up of biomaterials production
- Integrate large-scale chemical and biological processing
- Integrate design platforms that simplify the design of a material to physical specifications, for example rate and scale metrics, to the creation of genetic systems to implement and scale production
- Design integration of scale between the atomic, micro- and macro- domains

Biotic/Abiotic Interface

While the use of living microorganisms as living catalysts that facilitate charge transfer and storage holds tremendous potential for distributed energy and renewable energy, there are many obstacles to maturing such technology to be competitive with conventional batteries and fuel cell devices. The chief advantage to using a living system vs. a bio-inspired or bio-derived catalyst is the ability of the living system to self-regenerate. However, similarly to non-living biocatalysts, living systems require a greater depth of understanding of the mechanistic principles that can create new design rules for incorporating them into energy related devices or materials. As is the case for non-living biocatalysts, this may require development of new characterization techniques, including the development of high throughput electrochemical screening techniques that couple both charge transfer and cellular energy transfer to the abiotic surface. By increasing our depth of understanding on this push and pull between cellular growth and energy demand and the ability of a cell to act as a charge transfer mediator or storage device, the research can move in three directions much the same as noted above for bio-inspired catalysts.

A major hurdle to realizing the potential of living organisms to act as precision charge transfer mediators or charge storage devices is the complexity of the system itself. With only a few well-defined model systems to work with, including Geobacter and Shewanella, researchers lack the ability to predict protein function or macrostructure from genomic sequencing. Moreover, electron transfer conduits in these bacteria require metal cofactors and are known to be tied to complex regulatory and maturation systems that are not well-understood. For these reasons, it will be difficult for synthetic biologists to transfer them to other organisms that may be better suited for applications in power and energy. It also creates challenges for predictive protein engineering because many aspects of protein function will need to be considered, including membrane localization, cofactor, and maturation. Additionally, metabolic modeling will be necessary to predict the cellular energy requirements for growth vs. protein turnover in order to precisely control the number of electrons that cells keep for their own metabolism and homeostasis versus relaying to the power system.

Our understanding of bacterial extracellular electron transfer has exponentially increased over the last two decades owing to the blossoming of the interdisciplinary field of microbial electrochemistry, or sometimes referred to as electromicrobiology. Interdisciplinary teams of microbiologists, electrochemists, physicists, and engineers have worked together to answer fundamental questions on the nature of long-distance biological charge transfer, yet the details of such processes remain elusive. New instrumentation is needed to monitor electron and ion transport under physiologically-relevant conditions. Any new technique should also be amenable to the high-throughput biological engineering that is the hallmark of synthetic biology.

A synthetic biology approach can be used to precisely control the production of electron transfer mediators in living systems that fit the needs of energy storage devices. For example, if the design requirements are known, electron transfer conduits can be transferred to bacteria that survive under conditions of high alkalinity or acidity. Synthetic biology can also be used to model and tune cellular metabolism for carbon and energy storage much the same way that it has been used for metabolic energy to create biofuels and pharmaceuticals.

Participants discussed the need to expand the community of researchers involved in developing the biotic/abiotic interface to incorporate new tools for screening and predictive modeling. This may include development of a new lexicon for communicating across the large number of disciplines that contribute to this space. Ultimately, protein engineering should be considered to design precise modifications of charge carrying proteins to improve catalysis.

Short-term Research Trajectory (~5-10 years):

- Bring new tools from electrical engineering, photosynthesis, to bear on characterization
- Develop higher throughput experiments and models to predict ion/electron fluxes
- Use biotic/abiotic interface to stimulate behavior
- Develop education, training, and a more interdisciplinary community

Long-term Research Trajectory (10-20 years):

- Investigate fundamental processes and components in target organisms
- Bring Protein Engineering into this space
- Design systems that exist at the organic/inorganic interface

Conclusions

Synthetic biology represents the movement of life sciences from a descriptive science to an emerging creative technology and a new approach to meet grand challenges. As such, it has made immediate contributions to biomedicine and has started to make inroads into the energy and power space, primarily through biofuels. However, further extension of the synthetic biology toolkit could enable new solutions to meet global energy needs.

This workshop brought together a truly multidisciplinary group of scientists, including synthetic biologists, chemists, materials scientists, and engineers to discuss the possibilities at this intersectional space. The consensus was that there is significant potential to advance the application of synthetic biology for energy and power, especially in the areas of storage and ion transport. To achieve this potential, basic research must occur to: (i) foster collaboration and develop common language between the synthetic biology and energy communities, (ii) advance new integrated theory to model and predict catalyst, material, and interfacial properties, (iii) enable high-throughput experimentation tools and analytics that accelerate design-build-test loops, (iv) facilitate manufacture of new types of materials, and (v) develop strategies to address biomanufacturing at scale, as well as strategies suitable for decentralized, on-demand syntheses, including cell-free systems.

The development of sustainable and efficient energy platforms is a grand challenge of our time, one that requires creativity and an interdisciplinary approach including chemistry, engineering, and materials science. Simply improving upon current technologies with known methods will not be enough to address future energy needs. Rather, new concepts, design tools, and technologies will be needed to develop novel approaches to capture, convert, and store energy. Thus the intersection of the synthetic biology and energy/power research domains, with the proper pathways and resources, can enable powerful solutions to address the ever-changing landscape of energy needs and support a sustainable energy future.

Appendix I – Workshop Attendees

Panelists

Caroline Ajo-Franklin

Lawrence Berkeley National Lab, Staff Scientist
cajo-franklin@lbl.gov

Dr. Ajo-Franklin's research group uses biophysics and synthetic biology to engineer and explore the nanoscale interface between living microbes and fabricated materials. They are particularly interested in the basic mechanisms underlying charge transfer and assembly of materials at this living/non-living interface. Ultimately, their research has applications in autonomous sensing, bio-solar energy generation, and hierarchical assembly of nanostructures. She received her PhD in chemistry from Stanford University.

Fred Burpo

United States Military Academy, West Point, Department Head
john.burpo@usma.edu

Colonel Burpo is the Department Head for West Point's Department of Chemistry and Life Science which offers majors in chemistry, chemical engineering, and life science. Prior to that he served as the Deputy Department Head, an Academy Professor, and the Life Science Program Director in the department. He teaches courses in biochemistry, bioengineering, biotechnology, biology, biomechanics, and general chemistry. He also leads the Multi-Functional Materials Laboratory as part of West Point's Center for Molecular Science. The lab develops 3-dimensional nanomaterials to provide lightweight energy storage and sensor solutions for Soldiers. Colonel Burpo has field Army experience in light infantry, armor, and Stryker units with operational deployments to Rwanda, Bosnia, and Iraq.

Moh El-Naggar

USC, Professor of Physics, Biological Sciences, & Chemistry
mnaggar@usc.edu

Mohamed Y. El-Naggar is the Robert D. Beyer Early Career Chair in Natural Sciences, and Associate Professor of Physics, Biological Sciences, and Chemistry at the University of Southern California. El-Naggar and his interdisciplinary group investigate biological electron transfer and energy conversion (universal features of life as we know it) with special emphasis on the interface between biotic and abiotic systems. Their work, which has important implications for fundamental cell physiology and astrobiology, may also lead to the development of new hybrid materials and renewable energy technologies that combine the exquisite biochemical control of nature with the synthetic building blocks of nanotechnology.

Sarah Glaven

Naval Research Lab, Research Biologist
sarah.glaven@nrl.navy.mil

Dr. Sarah Glaven is a Research Biologist at the Naval Research Laboratory (NRL) in Washington, DC. She joined the NRL in 2009 to study microbial electrochemistry under Dr. Lenny Tender, a pioneer in the field of microbial fuel cells. Using a combination of electrochemistry, genomics, transcriptomics, and proteomics Dr. Glaven has contributed to our fundamental understanding of long distance electron transfer in microbial biofilms. Her current research focuses on how synthetic biology can be used to engineer the interaction between bacteria and electrodes to improve energy from microbial fuel cells, improve biocatalysis during electrosynthesis, and direct cellular behavior using electricity as an input or report on cellular behavior using an electrical output. Dr. Glaven currently serves as the President of International Society for Microbial Electrochemistry and Technology (ISMET).

Jeffrey Gralnick

University of Minnesota, Associate Professor
gralnick@umn.edu

Jeffrey Gralnick has extensively studied the physiology of Shewanella, gram-negative bacteria found worldwide in aquatic environments. By understanding the molecular mechanism of this species to respire a diversity of compounds - including insoluble minerals - he hopes to engineer strains that can generate power in microbial fuel cells or react against certain toxic metals in the environment. Working with Prof. Daniel Bond, Gralnick made a key discovery about how bacteria can convert organic compounds into electricity. They observed that riboflavin (commonly known as vitamin B-2) was responsible for much of the energy produced by the bacteria growing on electrodes. Riboflavin produced by the bacteria carried electrons from the living cells to the electrodes, and rates of electricity production increased by 370 percent as riboflavin accumulated. This finding has major implications for the development of scaled-up microbial fuel cells. Gralnick is developing strains, tools and techniques for increasing the robustness of using Shewanella for metabolic engineering and downstream applications in both Bioenergy (microbial fuel cells), Bioremediation and Biocatalysis.

Justin Jahnke

US Army Research Laboratory, Chemical Engineer
justin.p.jahnke.civ.@mail.mil

Justin Jahnke is a research chemical engineer at the US Army Research Laboratory with interests in bio electrochemistry, bio-abio interfaces and biology-based materials.

Michael Jewett

Northwestern University, Associate Professor
m-jewett@northwestern.edu

Michael Jewett is the Charles Deering McCormick Professor of Teaching Excellence, an Associate Professor of Chemical and Biological Engineering, and co-director of the Center for Synthetic Biology at Northwestern University. He is also an Institute Fellow at the Northwestern Argonne Institute for Science & Engineering. Dr. Jewett's lab seeks to re-conceptualize the way we engineer complex biological systems for compelling applications in medicine, materials, and energy by transforming biochemical engineering with synthetic biology. Dr. Jewett is the recipient of the NIH Pathway to Independence Award in 2009, David and Lucile Packard Fellowship in 2011, the DARPA Young Faculty Award in 2011, the Camille-Dreyfus Teacher-Scholar Award in 2015, the ACS Biochemical Technologies Division Young Investigator Award in 2017, among others. He received his PhD in 2005 at Stanford University and completed postdoctoral studies at the Center for Microbial Biotechnology in Denmark and the Harvard Medical School.

David Kaplan
Tufts, Professor
david.kaplan@tufts.edu
David Kaplan holds an Endowed Chair, the Stern Family Professor of Engineering, at Tufts University. He is Professor & Chair of the Department of Biomedical Engineering and also holds faculty appointments in the School of Medicine, the School of Dental Medicine, Department of Chemistry and the Department of Chemical and Biological Engineering. His research focus is on biopolymer engineering to understand structure-function relationships, with emphasis on studies related to self-assembly, biomaterials engineering and functional tissue engineering/regenerative medicine. He has published over 600 peer reviewed papers and edited eight books. He directs the NIH P41 Tissue Engineering Resource Center (TERC) that involves Tufts University and Columbia University. He serves on the editorial boards of numerous journals and is Associate Editor for the ACS journal Biomacromolecules. He has received a number of awards for teaching, was Elected Fellow American Institute of Medical and Biological Engineering and received the Columbus Discovery Medal and Society for Biomaterials Clemson Award for contributions to the literature.

Chong Liu
UCLA, Assistant Professor
chongliu@chem.ucla.edu
Prof. Liu earned his BS in chemistry from Fudan University, China, in 2008, and a PhD in chemistry from the University of California, Berkeley in 2013 under the supervision of Prof. Peidong Yang. His thesis focused on artificial photosynthesis that uses solar energy to synthesize selective chemicals. He continued his career at Harvard University, working with Prof. Daniel Nocera as a Lee Kuan Yew postdoctoral fellow. At Harvard, he developed inorganic/bio hybrid systems of solar-driven CO2 and N2 fixation with the efficiencies higher than natural counterparts. Prof. Liu joined UCLA Chemistry & Biochemistry in 2017.

Corey Love
NRL, Alternative Energy Section, Materials Engineer
corey.love@nrl.navy.mil
Dr. Corey Love is a materials research engineer in the Alternative Energy Section of the Chemistry Division at the U.S. Naval Research Laboratory (NRL) in Washington, DC. His research focuses on safe implementation of lithium-ion batteries through fundamental materials research and development as well as fault and damage detection diagnostics. Corey received his BS in Materials Science and Engineering from Virginia Tech in 2003 and PhD in Materials Science and Engineering from the University of California-San Diego in 2008. Dr. Corey completed a postdoctoral fellowship through the American Society for Engineering Education at NRL. In 2009 Corey became the Chemistry Division's first Jerome Karle Research Fellow and began his career as a staff researcher. In 2010 Corey received the Chemistry Division's Young Investigator Award to pursue independent research in lithium-ion battery safety and the development of battery state-of-health monitoring diagnostics. Dr. Love has numerous publications in the areas of corrosion, mechanics of materials and electrochemical energy storage. His work "Impedance Diagnostic for Battery Health Monitoring" was named an NRL Top 20 Accomplishment of 2011. He serves on technical review panels and working groups in support of various federal and state agencies.

Cynthia Lundgren
Army Research Lab, Electrochemistry Division, Power and Energy Division, Chief of Electrochemistry Branch
cynthia.a.lundgren2.civ@mail.mil
Dr. Lundgren, chief of ARL's electrochemistry branch, is working to create fuel cells that are lighter and more efficient to reduce the weight a soldier carries by a third to a half. Her group is investigating new types of energy devices that allow for ubiquitous energy, for example making fuel out of water. Dr. Lundgren received a PhD in chemistry from the University of North Carolina at Chapel Hill.

Sarah Milsom
Touchlight Genetics, DNA Nanotechnology Lead
sarah.milsom@touchlight.com
Sarah Milsom has a background in biomedical engineering, and received a Bachelor of Arts and Engineering with Honors in Biomedical Engineering and Arts, from Auckland University. At Touchlight, she is establishing and running projects in non-therapeutic, industrial and nanotechnology applications of doggybone DNA. Her previous roles were in Life Sciences management consulting and medical device design and manufacture.

Banahalli Ratna
*NRL, Center for Bio/Molecular Science and Engineering, Direc*tor
banahalli.ratna@nrl.navy.mil
Dr. Banahalli R. Ratna is the Director for the Center for Bio/Molecular Science and Engineering (CBMSE) at the Naval Research Laboratory. In this capacity, she provides executive direction and technical leadership in the development of objectives and policies necessary to conduct basic and applied research in areas of bio/molecular science and engineering to meet DON/DoD operational needs. Under her supervision, basic science research projects are pursued that investigate biological and biomimetic processes at the molecular level and learn from biology to design and develop novel systems. The results of the basic science are translated to develop applied technology projects such as alternate energy sources and sensors for broad spectrum pathogen identification and chem/bio agents. She acts as a subject knowledge expert on bio/molecular science and engineering and provides advice to the NRL management. She was selected to the Senior Executive Service (SES) in March 2009.

Joaquin Rodriguez-Lopez
University of Illinois at Urbana-Champaign, Assistant Professor
joaquinr@illinois.edu
Dr. Rodríguez-López is an Assistant Professor of Chemistry at the University of Illinois at Urbana-Champaign. Joaquin's group combines interests in electroanalytical chemistry and energy materials by developing chemically-sensitive methods for studying ionic and redox reactivity in nano-structures, redox polymers, highly-localized surface features, and ultra-thin electrodes for energy storage and conversion. In the energy storage space his group created a size-ex-

clusion flow battery that combines inexpensive membranes with redox-active polymers. Awards include: Society of Electroanalytical Chemistry Royce W. Murray Young Investigator Award (2017), Scialog Fellowship (2017), Toyota-Electrochemical Society Young Investigator Fellowship (2017), Sloan Research Fellowship (2016).

Nicholas Roehner
Raytheon BBN, Scientist
nicholas.roehner@raytheon.com
Dr. Roehner is a postdoc in the CIDAR lab at Boston University and the MIT-Broad Foundry at the Broad Institute of MIT and Harvard. Currently, he is a researcher on projects under the 1000 Molecules component of the DARPA Living Foundries program, including software for designing genetic libraries (Double Dutch) and a database for storing and tracking changes to combinatorial genetic designs (Knox). He earned a PhD in bioengineering from the University of Utah (2014), working with Prof. Chris J. Myers on computational methods for genetic design automation. Additionally, he served as an editor of the Synthetic Biology Open Language (SBOL) and contributed to the development of the SBOL 2.0 data standard.

Oscar Ruiz
Air Force Research Laboratory, Senior Biological Scientist
oscar.ruiz@us.af.mil
Dr. Ruiz is the lead scientist directing the Fuel Biodeterioration Research Program at the Fuels and Energy Branch of the Air Force Research Laboratory (AFRL). Dr. Ruiz serves as expert in the fields of fuel microbiology, biotechnology, biofuels, and conventional fuels for the Aerospace Systems Directorate of AFRL. He received a PhD in Biomolecular Sciences from the University of Central Florida.

Claudia Schmidt-Dannert
University of Minnesota, Professor
schmi232@umn.edu
Dr. Schmidt-Dannert is Distinguished McKnight Professor in the Department of Biochemistry, Molecular Biology and Biophysics, at the University of Minnesota. She studied Biology and Biochemistry at the Carolo Wilhelmina University Braunschweig (Germany), where she received her PhD in Biochemistry in 1994. She held a Group Leader position in Molecular Biotechnology at the University of Stuttgart (Germany) and joined the faculty at the University of Minnesota in 2000. Her current research focuses on developing and studying systems to carry out multi-step enzymatic synthesis in vitro and in microbial systems for the synthesis of valuable compounds.

Yang Shao-Horn
MIT, W.M. Keck Professor of Energy
shaohorn@mit.edu
Professor Shao-Horn is the W.M. Keck Professor of Energy at the Massachusetts Institute of Technology (MIT), as well as, a Professor of Mechanical Engineering, and Materials Science and Engineering. Professor Shao-Horn earned her BS degree from Beijing University of Technology and her PhD degree from Michigan Technological University, both in Metallurgical and Materials Engineering. She joined the MIT faculty in 2002.

Wolfgang Sigmund
University of Florida, Professor
sigmund@ufl.edu
Dr. Sigmund is professor of Materials Science at the University of Florida since 1999. He studied chemistry at the University of Heidelberg, and got his doctorate at the University of Mainz from the Max-Planck Institute of polymer research under Prof. G. Wegner. He served as visiting professor at the University of Florida, Universidade de Pernambuco in Brazil, and RIKEN in Japan, and worked at the Powder Metallurgical Laboratory within the Max-Planck Institute of Metals Research as deputy director for the associated University of Stuttgart institute of nonmetallic inorganic materials. He also held a guest professorship at Hanyang University in South Korea from 2009-2013. He has published more than 200 articles and patents. His current work focuses on fabrication and processing of ceramic nanomaterials using electrospinning and surface science.

James Sumner
Army Research Laboratory, Chief, Biotechnology Branch
james.j.sumner4.civ@mail.mil
James Sumner received a BS in chemistry (summa cum laude) from High Point University and a PhD in chemistry from Clemson University. He joined the Army Research Laboratory (ARL) in Adelphi, MD in 2002 after working as an American Society of Engineering Education (ASEE) Postdoctoral Fellow at ARL. Dr. Sumner has over 15 years experience as an analytical chemist. His current work focuses on biophotonic and bioelectronics research as applied to biological and chemical sensor development including studies of DNA hybridization by electrochemical and spectroscopic methods as well as research and development in bioelectrochemical systems. He has also been conducting collaborative research in the field of novel biotechnology applications in the areas of power and energy and waste remediation. Dr. Sumner has produced 25 open literature publications and book chapters, which have been favorably cited over 600 times, as well as 2 patent disclosures.

Jin Suntivich
Cornell, Assistant Professor
jsuntivich@cornell.edu
Dr. Suntivich is an assistant professor in Materials Science and Engineering at Cornell University. His group works on electrocatalysis for energy conversions, in situ characterizations, and chemical applications of photonics. He holds an ScD in Materials Science and Engineering from MIT.

Yinjie Tang
Washington University in St Louis, Associate Professor
yinjie.tang@wustl.edu
Yinjie Tang at Washington University has expertise in environmental microbiology, kinetic modeling, and metabolic flux analysis. He received his PhD in Chemical Engineering at the University of Washington (with Dr. Barbara Krieger-Brockett). During his postdoctoral period (2004-2008), he worked on genomics projects at Lawrence Berkeley National Laboratory (with Dr. Jay Keasling). He moved to Washington University in 2008, where his research focuses on characterizing and engineering nonmodel microorganisms for bio-manufacturing.

Leonard Tender
Naval Research Lab, Microbial Electrochemist
tender@nrl.navy.mil
Leonard M. Tender earned a BS in chemistry from MIT where he was fortunate to be mentored by Mark Wrighton, and a PhD from UNC Chapel Hill where he was again fortunate to be mentored by Royce Murray. He has been at the Naval Research Laboratory since 1999 where he is a research chemist and branch head.

Christopher Voigt
MIT, Professor
cavoigt@gmail.com
Prof. Voigt obtained his Bachelor's degree in Chemical Engineering at the University of Michigan, Ann Arbor and a PhD in Biochemistry and Biophysics at the California Institute of Technology. He continued his postdoctoral research in Bioengineering at the University of California, Berkeley. His academic career commenced as an Assistant and Associate Professor at the Department of Pharmaceutical Chemistry at the University of California-San Francisco. Dr. Voigt joined the Department of Biological Engineering at MIT as Associate Professor in 2011.

Hailiang Wang
Yale, Assistant Professor
hailiang.wang@yale.edu
Dr. Wang has a PhD in Chemistry from Stanford University. He leads a research lab and is on the faculty at Yale. His research employs chemistry, materials science, nanotechnology and surface science to tackle the challenges in electrochemical energy storage and conversion.

Ian Wheeldon
UC Riverside, Chemical and Environmental Engineering
iwheeldon@engr.ucr.edu
Prior to arriving at UCR, Dr. Wheeldon was a post-doctoral fellow at Brigham Women's Hospital, Harvard Medical School and the Wyss Institute for Biologically Inspired Engineering at Harvard University. As a postdoc, he developed new methods of high throughput biomaterials synthesis and screening. His doctoral research focused on the development of multi-functional enzymatic hydrogels for biofuel cells. This work built on his previous studies at the University of Buenos Aires, where he was a visiting scholar studying the electrochemistry of biological molecules. Dr. Wheeldon received his Master's degree in Applied Science from the Royal Military College of Canada, under the supervision of Dr. Brant Peppley, where he worked on fuel reforming and hydrogen purification technologies for high and low temperature fuel cells.

Workshop Co-Chairs

Michael Jewett, *Northwestern University*
Yang Shao-Horn, *MIT*
Christopher Voigt, *MIT*

Observers

Linda Chrisey, *Office of Naval Research*
Mike Finnin, *Institute for Defense Analyses*
J Aura Gimm, *US Army Research Office*
Laura Kienker, *Office of Naval Research*
Taeyjuana Lyons, *OUSD(R&E), Basic Research Office*
Esha Mathew, *OUSD(R&E), Basic Research Office*
Caitlyn McGuire, *OUSD(R&E), Basic Research Office*
Bindu Nair, *OUSD(R&E), Basic Research Office*
Petra Oyston, *UK DSTL*
Ben Petro, *OUSD(R&E)*
Dave Rampulla, *NIH/NIBIB*
Robert Reeve, *UK DSTL*
Alex Schlichting, *MITRE*
Tiffany Tsang, *MITRE*
Marc von Keitz, *ARPA-E, DOE*
Tsuetanda Zhelva, *US Army Lab*

VT-ARC Staff

Kate Klemic, *Program Manager*
Dorothy Brady, *Rapporteur*
Lynne Ostrer, *Rapporteur*
Lindsay Naves Anderson, *Rapporteur*

Appendix II – Workshop Agenda

Day 1 – Tuesday, March 6th, 2018

Time	Title	Speaker
7:45–8:15	**Registration**	
8:15–8:20	Welcome and Introductions	Dr. Christopher Voigt, *MIT*
8:20–8:30	ASDR&E Welcome	Dr. Ben Petro, *Human Performance, Training, & BioSystems Directorate*
8:30–8:45	Military Perspective on Energy and Power	Dr. Robert Reeve, *Defense Science and Technology Laboratory, UK*
8:45–9:05	Synthetic Biology Capabilities	Dr. Michael Jewett, *Northwestern U*
9:05–9:25	Energy Storage and Power Delivery Challenges	Dr. Yang Shao-Horn, *MIT*
9:45–11:30	Breakout Session I: Challenges and Opportunities	
11:45–12:30	Outbriefing from Breakout Session I	
12:30–1:30	**Lunch**	
1:30–3:30	Breakout Session II: Technical Capabilities and Challenges	
3:45–4:30	Report Out from Breakout II	
4:30–5:00	Summary of Day	Dr. Christopher Voigt, *MIT*
5:00	**Meeting Adjourned for the Day**	

Day 2 – Wednesday, March 7th, 2018

Time	Title	Speaker
7:45–8:15	**Registration**	
8:15–8:30	Day 1 Recap	Drs. Michael Jewett and Yang Shao-Horn
8:30–9:30	**'White Space' Discussion I** Discussion of topics which did not fit into the framework of day 1, but need to be discussed.	Drs. Michael Jewett and Yang Shao-Horn
9:30–10:30	**'White Space' Discussion II** Discussion of particularly far-out (or long-term), high-risk, high-impact ideas.	Drs. Michael Jewett and Yang Shao-Horn
10:45–11:45	Discussion of Key Ideas/Components for Report	Drs. Michael Jewett and Yang Shao-Horn
11:45–12:00	Closing Remarks	
12:00	**Departure**	

Appendix III – Bibliography

[1] Lazard, "Levelized Cost of Energy Analysis 10.0," 2016. [Online]. Available: https://www.lazard.com/perspective/levelized-cost-of-energy-analysis-100/.

[2] G. Church, M. Elowitz, C. Smolke, C. Voigt and R. Weiss, "Realizing the potential of synthetic biology," *Nature Reviews Molecular Cell Biology*, vol. 15, pp. 289-294, 2014.

[3] B. Des Soye, J. Patel, F. Isaacs and M. Jewett, "Repurposing the translation apparatus for synthetic biology," *Current Opinions in Chemical Biology*, vol. 28, pp. 83-90, 2015.

[4] C. Liu, M. Jewett, J. Chin and C. Voigt, "Toward an orthogonal central dogma," *Nature Chemical Biology*, vol. 14, pp. 103-106, 2018.

[5] BloombergNEF, "Wind and solar boost cost-competitiveness versus fossil fuels," BloombergNEF, 5 October 2015. [Online]. Available: https://about.bnef.com/blog/wind-solar-boost-cost-competitiveness-versus-fossil-fuels/.

[6] I. R. E. Agency, "Renewable energy technologies: cost analysis series," 2012. [Online]. Available: https://www.irena.org/documentdownloads/publications/re_technologies_cost_analysis-hydropower.pdf.

[7] B. a. M. N. Nykvist, "Rapidly falling costs of battery packs for electric vehicles," *Nature Climate Change*, vol. 5, no. 4, pp. 329-332, 2015.

[8] B. K. H. T. J. Dunn, "Electrical Energy Storage for the Grid: A Battery of Choices," *Science*, vol. 334, no. 6058, pp. 928-935, 2001.

[9] S. W. Lee, B. M. Gallant, H. R. Byon and P. T. Hammond, "Nanostructured carbon-based electrodes: bridging the gap between thin-film lithium-ion batteries and electrochemical capacitors," *Energy & Environmental Science*, vol. 4, no. 6, pp. 1972-1985, 2011.

[10] W. T. Hong, M. Risch, K. A. Stoerzinger, A. Grimaud, J. Suntivich and Y. Shao-Horn, "Toward the rational design of non-precious transition metal oxides for oxygen electrocatalysis," *Energy & Environmental Science* , vol. 8, no. 5, pp. 1404-1427, 2015.

[11] J. Hwang, R. R. Rao, L. Giordano, Y. Katayama, Y. Yu and Y. Shao-Horn, "Perovskites in catalysis and electrocatalysis," *Science*, vol. 358, no. 6364, pp. 751-756, 2017.

[12] J. H. Montoya, L. C. Seitz, P. Chakthranont, A. Vojvodic, T. F. Jaramillo and J. K. Nørskov, "Materials for solar fuels and chemicals," *Nature Materials*, vol. 16, no. 1, pp. 70-81, 2017.

[13] E. V. Kondratenko, G. Mul, J. Baltrusaitis, G. O. Larrazabal and J. Perez-Ramirez, "Status and perspectives of CO2 conversion into fuels and chemicals by catalytic, photocatalytic and electrocatalytic processes," *Energy & Environmental Science*, vol. 6, no. 11, pp. 3112-3135, 2013.

[14] Y. Tanabe and Y. Nishibayashi, "Developing more sustainable processes for ammonia synthesis," *Coordination Chemistry Reviews*, vol. 257, no. 17-18, pp. 2551-2564, 2013.

[15] D. A. Kuznetsov, B. Han, Y. Yu, R. R. Rao, J. Hwang, Y. Román-Leshkov and Y. Shao-Horn, "Tuning Redox Transitions via Inductive Effect in Metal Oxides and Complexes, and Implications in Oxygen Electrocatalysis," *Joule*, vol. 2, no. 2, pp. 225-244, 2018.

[16] F. Abild-Pedersen, J. Greeley, F. Studt, J. Rossmeisl, T. R. Munter, P. G. Moses, E. Skulason, T. Bligaard and J. K. Norskov, "Scaling properties of adsorption energies for hydrogen-containing molecules on transition-metal surfaces," *Phys Rev Lett*, vol. 99, no. 1, p. 016105, 2007.

[17] D. Larcher and J. M. Tarascon, "Towards greener and more sustainable batteries for electrical energy storage," *Nature Chemistry*, vol. 7, no. 1, pp. 19-29, 2014.

[18] Y. Li and H. Dai, "Recent advances in zinc-air batteries," *Chem Soc Rev*, vol. 43, no. 15, pp. 5257-75, 2014.

[19] K. Lin, Q. Chen, M. R. Gerhardt, L. Tong, S. B. Kim, L. Eisenach, A. W. Valle, D. Hardee, R. G. Gordon, M. J. Aziz and M. P. Marshak, "Alkaline quinone flow battery," *Science*, vol. 349, no. 6255, pp. 1529-32, 2015.

[20] J. C. Bachman, S. Muy, A. Grimaud, H.-H. Chang, N. Pour, S. F. Lux, O. Paschos, F. Maglia, S. Lupart, P. Lamp, L. Giordano and Y. Shao-Horn, "Inorganic Solid-State Electrolytes for Lithium Batteries: Mechanisms and Properties Governing Ion Conduction," *Chemical Reviews*, vol. 116, no. 1, pp. 140-162, 2016.

[21] NHGRI, "DNA Sequencing Costs: Data," NIH, 2017. [Online]. Available: https://www.genome.gov/sequencing-costsdata/.

[22] ATCC, "Biological systems design and development," ATCC, 2018. [Online]. Available: https://www.atcc.org/Products/Synthetic_Biology_Solutions.aspx.

[23] V. Artero, "Bioinspired catalytic materials for energy-relevant conversions," *Nature Energy*, vol. 2, p. 17131, 2017.

[24] R. Lewis, M. Garcia-Borràs, M. J. Chalkley, A. R. Buller, K. N. Houk, S. B. J. Kan and F. H. Arnold, "Catalytic iron-carbene intermediate revealed in a cytochrome c carbene transferase," *PNAS*, vol. 115, no. 28, pp. 7308-7313, 2018.

[25] Y. J. Kim, A. Khetan, W. Wu, S. Chun. and V. Viswanathan, "Evidence of Porphyrin-Like Structures in Natural Melanin Pigments Using Electrochemical Fingerprinting," *Advanced Materials*, vol. 28, no. 16, pp. 3173-3180, 2016.

[26] L. Tender, C. Reimers, H. Stecher, D. Holmes, D. R. Bond, D. Lowy, K. F. S. Pilobello and D. Lovely, "Harnessing microbially generated power on the seafloor," *Nature Biotechnology*, vol. 20, pp. 821-825, 2002.

[27] L. Shi, H. Dong, G. Reguera, H. Beyenal, A. Lu, J. Liu, H. Yu and J. Fredrickson, "Extracellular electron transfer mechanisms between microorganisms and minerals," *Nature Review Microbiology*, vol. 4, no. 10, pp. 651-62, 2016.

[28] D. R. Lovley, "Electrically conductive pili: Biological function and potential applications in electronics," *Current Opinion in Electrochemistry*, vol. 4, no. 1, pp. 190-198, 2017.

[29] K. Rabaey and R. Rozendal, "Microbial electrosynthesis — revisiting the electrical route for microbial production," *Nature Reviews*, vol. 8, pp. 706-716, 2010.

[30] T. Fukushima, S. Gupta, B. Rad, J. Cornejo, C. Petzold, L. J. Chan, R. A. Mizrahi, C. Y. Ralston and C. Ajo-Franklin, "The Molecular Basis for Binding of an Electron Transfer Protein to a Metal Oxide Surface," *Journal of the American Chemical Society*, vol. 139, no. 36, pp. 12647-12654, 2017.

[31] M. TerAvest and C. Ajo-Franklin, "Transforming exoelectrogens for biotechnology using synthetic biology," *Biotechnology and Bioengineering*, vol. 113, no. 4, pp. 687-697, 2015.