Directed Programmable Matter for Energy Applications

Insights, analysis and implications for society

CASE STUDY DOCUMENTATION

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Summary

The workshop on Energy and Directed/Programmable Matter (D/PM) examined the potential for precise materials and devices to significantly improve energy production, storage and use.

Contents:

Introduction

World energy demand will increase significantly in the next few decades. Meeting this demand sustainably and at affordable cost is a major challenge, especially for developing nations (Holmes et al. 2015). The Foresight workshop on Energy and Directed/Programmable Matter examined how high-precision materials and devices could help address this challenge.

Long-term, atomically precise materials offer transformative improvements throughout the economy, including the energy sector. However, the focus of this workshop was on the shorter-term goal of identifying ways in which currently developing precision technologies could improve the energy sector.

With this focus, the goals of the workshop were to

- identify the main, and possibly overlooked, areas in which atomically precise technologies could make a global difference for energy
- identify and start removing roadblocks to this advance
- advance research by those already working in the field
- help early career researchers enter the field
- establish collaborations among researchers with complementary expertise and interests

The workshop participants had diverse backgrounds and interests. They included a range of experience (from senior researchers to graduate students), institutions (universities, government and industry) and expertise. This diversity was important due to the interdisciplinary nature of designing and manufacturing precise materials, as well as identifying large-scale applications to the energy sector.

The workshop distinguished atomically precise materials and devices from the broader term “nanotechnology.” Atomic precision refers to materials in which most atoms are in precisely specified locations. Biology provides the most complex such materials, e.g., proteins constructed of sequences of amino acids as specified by DNA. Nanotechnology, on the other hand, often refers to materials with structures precisely defined on scales of up to, roughly, 100 nanometers, which is far larger than the atomic scale. This includes current microelectronics, with engineered features as small as a few nanometers. Thus both atomically precise materials and nanotechnology products are small and precise by conventional engineering standards. Atomic precision refers to the smaller end of this range, with subnanometer precision. Moreover, atomic precision involves placing every atom of the material precisely, thereby considerably extending current demonstrations of placing and manipulating a few atoms on a surface. This distinction is important as atomically precise materials have more potential than larger-scale nanodevices to significantly improve chemical reactions. Such potential applications include producing or using fuels with higher efficiency and few or no side reactions that produce waste products.

Building with atomic precision covers a wide range of products. The simpler end of this range consists of atomically-precise materials, with each atom in a designed location. More complex products include computationally active materials, as smaller scale versions of ``smart matter'' made from current micromachine (MEMS) technology.

Energy Technologies and Current Limitations

The energy sector of the economy faces a number of limitations. These constrain and motivate the choice of new technologies to improve energy production, storage and use.

Major challenges arise from the environmental impact of the energy industry, particularly the use of fossil fuels. Moreover, current technologies are ill equipped to meet rapidly growing global energy demand without further environmental degradation.

This challenge remains in spite of significant exploration and development of renewable energy sources. This is because such sources currently lack the necessary scale, cost, reliability, and distribution infrastructure. Moreover, renewable energy sources have their own difficulties. One such problem is their intermittency, e.g., due to cloudy days or calm weather reducing solar or wind power, respectively. Another problem is finding acceptable locations. Suitable areas are often far from major sources of demand, requiring additional infrastructure to move generated power to customers' locations.

Another challenge is that much of the energy produced is wasted. This waste arises throughout the energy industry, from production to consumption. For instance, energy production at commercial scales typically involves transferring energy in large steps between the source, e.g., a hot furnace, and sink, e.g., cool water. Such transfers are thermodynamically less efficient than releasing energy in small, controlled steps as done, on much smaller scales, in biology.

Another form of waste arises in the production and use of chemical fuels, e.g., gasoline. The chemical reactions also create unwanted byproducts, e.g., pollution from automobile exhaust.

Constraints on energy technology arise from both public policy and consumer demand.

For instance, policies developed for current energy infrastructure can limit the scale up of new technologies. Another example is consumers want affordable automobiles with rapid acceleration, long range, and rapid refueling. This limits the options for alternative fuels, especially while new technologies are still relatively expensive and lack widely distributed support for refueling and maintenance.

Precision Materials and Devices for Energy

Workshop participants discussed a variety of precision materials that could improve current energy technologies. These included

- solar cells
- catalysts to produce chemical fuels
- membranes for fuel cells
- supercapacitors
- flywheels

Other energy technologies are less suitable near-term targets for improvement through higher-precision materials. These include fossil fuel and geothermal power plants, and energy storage through movement of bulk materials, such as pumping water to elevated reservoirs or compressing large quantities of air.

Solar energy is a significant potential energy source, since the earth receives far more solar energy than current global energy demands. Photovoltaic materials convert light directly into electrical energy. Laboratory demonstrations show precision materials can improve solar energy. For instance, nanostructured materials can directly convert sunlight into mechanical work (Okawa et al. 2009). As another example, nanowires can improve efficiency of solar cells and reduce their cost (Kempa et al. 2013).

In addition to producing energy for immediate use, solar energy can produce chemical fuels for later use, thereby overcoming the intermittency of available sunlight. Reactions producing such fuels often have large activation energies. Supplying this energy in bulk, e.g., with high temperature or pressure, not only wastes energy, but also activates other, undesirable reactions, reducing yield and producing waste products.

An alternative, as amply demonstrated in biological systems, is the use of catalysts that selectively lower activation barriers to just the desired reactions. This allows the reaction to proceed rapidly under mild conditions, and produce the desired product with high yield.
This approach to energy production improves efficiency by proceeding in small steps, thereby getting closer to the thermodynamic limit.
An example in nature is light-harvesting by plants, which involves a complex sequence of reactions. Engineered nanoscale cavities can perform similar functions (Noriega et al. 2015). For instance, nanoparticle surfaces can enhance photocatalytic fuel-forming reactions. An example is using solar energy to produce hydrogen from water (Muhich et al. 2013, Manthiram et al. 2014).

More complex catalysts could create fuels from carbon dioxide, analogous to the processes in plants, but with reactions designed, for example, to produce hydrocarbon fuels. These are more convenient fuels than hydrogen in that extensive infrastructure already exists for their use. Produced from sunlight by catalysts, this fuel production would be sustainable and avoid the waste products from current technologies. An example is producing methanol from carbon dioxide (Lim et al. 2014).

After producing fuels, a key challenge is using them effectively to generate energy. Simple burning is a common approach to using chemical fuels, but has limited efficiency and produces numerous undesirable products. Fuel cells are an alternative approach. These rely on membranes that selectively allow only certain molecules to pass through, while forcing charges to travel through external circuits, thereby producing electrical energy. Improved selectivity and reliability of membranes is a significant opportunity where higher precision materials could make highly effective fuel cells for a variety of chemical fuels.

The waste associated with the energy industry could be significantly reduced with the use of precise materials and devices that more specifically control energy harvesting, storage, local distribution and use.

Energy technology involves tradeoffs among competing goals, such as efficiency, safety, sustainability and cost. Before precise materials are commercially available to handle the full task of energy production, small amounts of such materials can also be useful. For instance, a small amount of precise material added to conventional fuels can help simultaneously achieve multiple, apparently conflicting goals for energy production. In particular, a small quantity of specifically designed molecules can improve fuel safety without compromising efficiency (Wei et al. 2015). Another instance is modifying the microscopic structure of batteries to improve energy storage (Liu et al 2015).

These examples illustrate the potential energy applications of precise materials. These benefits increase as the material precision improves toward the atomic scale.

Challenges for Creating Precise Materials

Significantly improving the energy industry with precise materials and devices requires addressing two major challenges: developing enabling technologies and improving communication among diverse groups to coordinate and fund interdisciplinary work.

Challenge: manufacturing technologies

Researchers are exploring a variety of approaches to high-precision materials. Chemical synthesis is one approach, which relies on self-assembly to produce atomically precise materials. Self-assembly faces significant challenges in designing reaction sequences to achieve high yield of highly complex materials, e.g., involving large molecules and supramolecular assemblies.

Another bottom-up approach directly manipulates atoms on surfaces, e.g., with scanning tunneling microscopes (STM) and atomic force microscopes (AFM). These allow direct manipulating of atoms, avoiding the stochastic limitations of self-assembly, but are severely limited in the number of atoms they can arrange in a reasonable amount of time.

Biotechnology is a third bottom-up approach. Proteins form many useful catalysts.

Unfortunately, proteins with novel functions are difficult to design, and energy applications are not limited to physiological conditions. An alternate engineering approach is designing macromolecular structures whose bonding prevents folding. This simplifies the design of macromolecules with desired properties (Schafmeister et al. 2008), e.g., for efficient energy harvesting.

The top-down approach to precise materials and devices, used by the semiconductor industry, can produce large quantities of products. However, this approach is limited to precision of a few nanometers and does not produce atomically precise products. Moreover, fabrication factories for this technology are very expensive.

None of these approaches is yet capable of manufacturing the commercial quantities of atomically precise materials required to provide the improved energy capabilities discussed at the workshop. Thus an important direction for further development is improving the accuracy of tools for atomic-scale manipulation, fabrication and characterization of the resulting materials.

Challenge: design tools

Design is a major hurdle for creating useful atomically precise materials and devices. Thus, in addition to developing manufacturing technologies, it is important to create design tools to help determine what arrangements of atoms will provide required capabilities. This is primarily a software development issue. Unfortunately, agencies that fund material development provide little funding for design tools necessary to take full advantage of new material manufacturing capabilities.

To rationally design materials, simulation tools are vitally important as a guide to the most promising directions to devote fabrication efforts. Software issues and access to processing power were identified by all the disciplines present at the workshop as the biggest roadblock slowing the achievement of atomic precision.

In particular, there is a substantial gap between what is needed to model a pharmaceutical — a relatively small unit — and what is needed to model the much larger size and complexity of atomically precise materials envisioned at the workshop.

Some existing design tools evaluate material properties at micron scales and larger. These include continuum models based on numerical solution of partial differential equations. Other software programs aid the bottom up approaches by modeling small groups of atoms, at sizes of about a nanometer.

Between these two size regimes is a large gap that presently lacks adequate modeling software. The field of atomically precise construction needs software to design nanoscale structures. The field also requires software to model those structures interacting with complex environments. One critical need is for a multi-scale physics package that allows designing a structure on the atomic scale, and then continue the calculations for that material as the structure grows — up to the micron size regime — all the while maintaining the data for the atomic scale interactions.

An example is developing computer simulations for molecular design of catalysts that will convert carbon dioxide through several intermediates into hydrocarbons. This involves trying many variations via simulations to find a few good potential catalysts for subsequent synthesis and testing. This requires significant computation capability to search through large design space of possible catalysts.

Molecular dynamics codes running on graphics processing units (GPUs) provide an increasingly effective approach to examine atomic-scale behaviors. However these do not address quantum effects in bond formation, which are important for evaluating catalysts. Quantum simulations are substantially slower, making it difficult to simulate behavior with a large enough number of atoms and for long enough time to connect with relevant macroscale behavior, e.g., large-scale production of fuels from sunlight.

Thus there is an important unmet need for better algorithms and computational hardware to guide the design of more precise materials, including those with the potential to significantly address global energy problems.

Challenge: communication among diverse research groups and funders

Creating high-precision materials and devices requires contributions from diverse fields, including the physics of materials, synthetic chemistry of large molecules, electrical and mechanical engineering to incorporate new materials into complete products, and production engineering to scale up from laboratory demonstrations to large-scale commercial products. This also requires software engineering of design tools that account for the different dominant physical effects at different length scales.

This diversity makes it difficult to assemble teams with the necessary expertise, and requires a significant time commitment from members of those teams to become familiar with the capabilities and language of the other fields.

This communication challenge also applies to funding agencies, which generally focus on only a few aspects of the full design problem. Thus there is an important need for more communication of funding opportunities from agencies such as DOE and DARPA to encourage interdisciplinary exploratory projects on designing and manufacturing precise materials for a variety of applications, including energy.

Next Steps

Encouraging researchers and funding agencies to address the roadblocks to creating and applying precision materials to energy are the next steps identified at the workshop.

To help this process, researchers should identify short and intermediate term goals, easily explainable to funders, which are useful in their own right and also as steps toward the long-term goal of atomic precision for applications including energy.

One useful technique to aid this goal setting is backcasting. This exercise imagines the problem solved some number of years in the future and then identifies prior steps that led to that solution. This procedure can identify which among many fundable short-term goals also help realize longer-term goals. This is important since there are often many scientifically appealing projects with roughly equal short-term merit. Only a few of these may also significantly advance longer-term goals. In addition, projects for enabling technologies, such as software development, are often viewed as beyond the scope of agencies charged with developing materials. Communicating how such technologies are important steps toward significant applications may help gain support for these enabling technologies in spite of their lack of immediate application to new materials.

In summary, atomically precise materials have the potential to move energy production toward sustainable sources and eliminate unwanted byproducts. Many research groups have demonstrated fabrication of precise materials or devices, and their potential advantages for energy production and storage. A major challenge is scaling up these demonstrations to commercial use. While the focus of this workshop was on energy applications, improving capability to design and manufacture precise materials could also significantly improve other significant areas, such as medicine and environmental remediation.

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