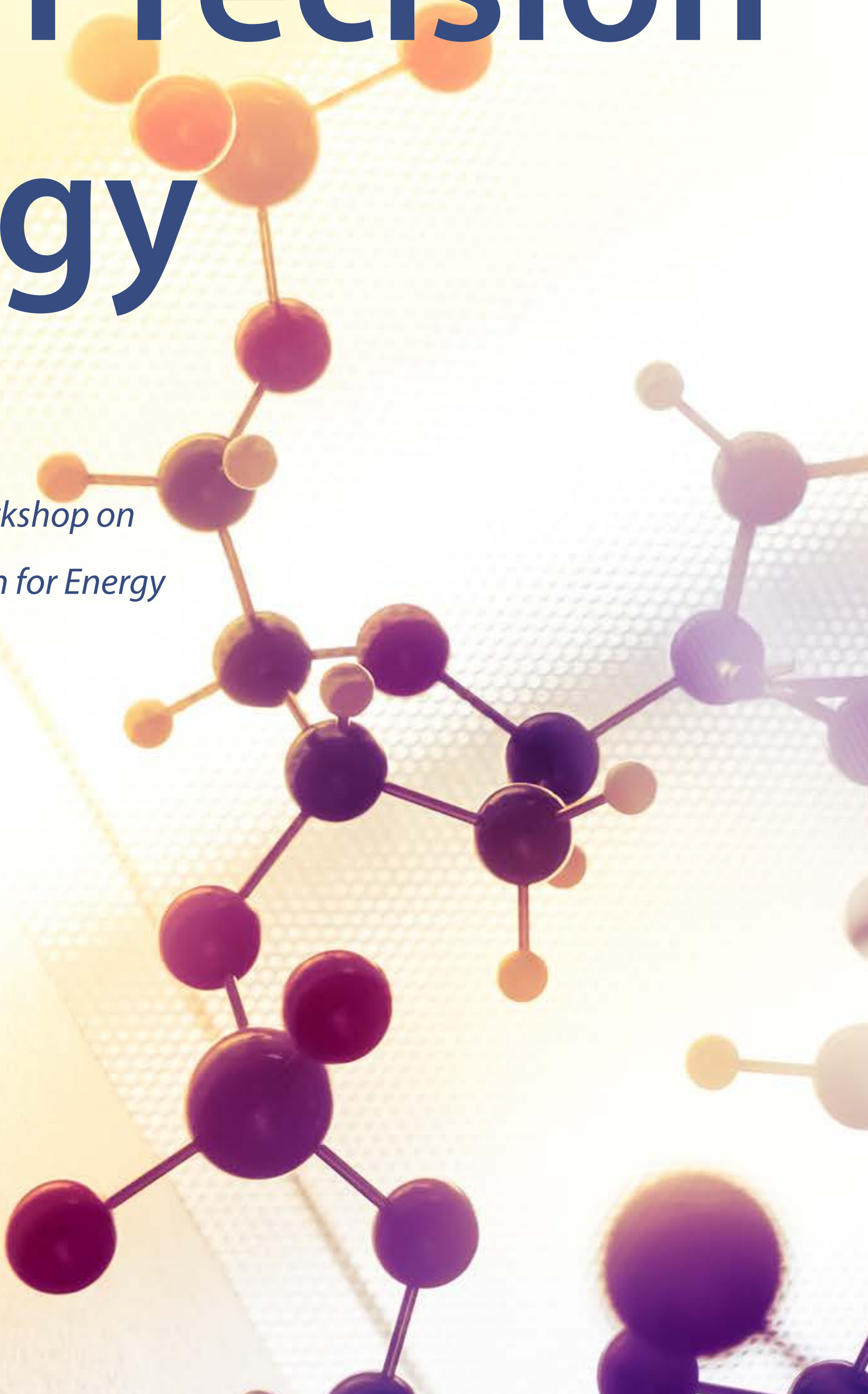
Atomic Precision for Energy

2016

Whitepaper based on Foresight Institute Workshop on Breakthrough Technologies: Atomic Precision for Energy Generation, Transmission and Use Reduction



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Foreword

We can't continue like this.

Our civilization needs energy like the human body needs food; it won't flourish when it's scarce. But fossil fuels, the not-so-secret stash of energy hidden inside our earth that have fueled our growth, are neither as abundant nor as gratuitous as we would like to believe.

We have seen the rise and fall of civilizations over the past millennia. Rarely ever were great civilizations conquered. Rather, excess, lack of foresight, and cultural blind spots led to their undoing. Our relationship with energy may be such a cultural blind spot. With a lack of global foresight and decisive action, we're steering towards the most painful "told you so" moments in human history.

Now, in traditional images, energy is smelly, messy, toxic, and loud. We're wasteful on all levels, starting at energy production, through storage and transport, all the way to consumption of energy. It is especially tragic that the crudeness with which we handle energy is not only wasteful, but also pollutes our planet. But the technology of the future doesn't have to be that way. As our command of the physical world increases, so does energy-related technology shift from crude to refined, from messy too precise all the way down to the atomic level. Precision is the antithesis to waste, pollution, and inefficiency.

It is peak time for a technological breakthrough for energy. For this reason, Foresight Institute brought together leading scientists, technologists, policy makers, and domain experts from all over the world.

Foreword

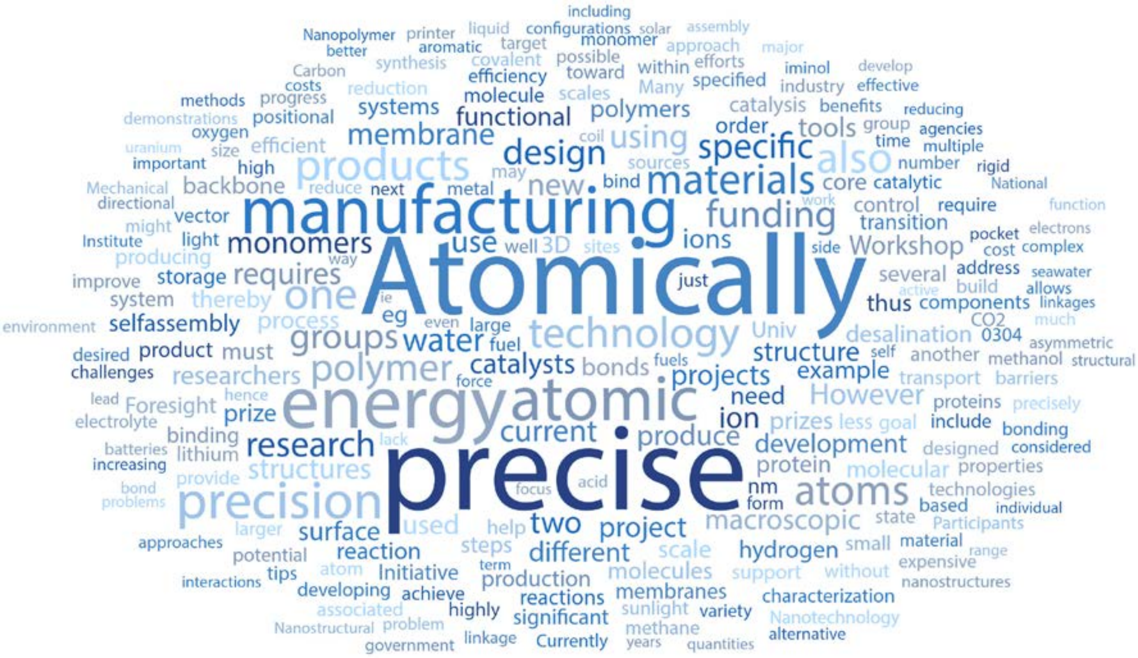

Figure 1: A visual rendering of the terms used in this report, scaled by their frequency.

What you are about to read are parts of the outcomes of this summit in May 2016. Other outcomes are less tangible: Ideas have been exchanged and debated. Collaborations and friendships have been formed. Discussions went on until deep into the night and continue to this day. Minds have been changed. (We have prepared a video with candid impressions for you in our video channel.)

The message that emerged is clear: There are paths toward a clean, abundant future. We are pointing to a few of them. As it is the nature of bold ideas, not all of them may make it to final implementation, and some will change from their initial conceptualization. That is okay. On the journey to technological breakthrough, we will see experimentation and serendipity. I invite you to read this report with a mindset of possibility.

03

Foreword

Beyond the details of the technical proposals, this report is a testament to human hope and ingenuity. Our way out of an energy crisis is not backwards, but forwards into a new technological golden age.

As you read the proposals, you can almost feel the scientists' zest for action. There is an entire world of atomic precision in energy waiting for us. But they can't embark on their journeys by themselves. It takes teams, labs, money, and public support.

We often think that being one person, there's not much we can do to tackle a challenge this massive. But here's an opportunity where you, the single reader, can have an impact. Get this report in front of the right people to make things happen. Spread the word that our most powerful lever to improve the state of the world is novel technology. Support Foresight Institute to extend the frequency and scale of our efforts.

What if your support turns out to be the key in our quest towards a golden age?

Julia Bossmann
President
August 2016

Technical Proposals

Sunlight-Driven CO2 Reduction

Tim Potter, based in part on notes by Richard Nesbitt

> *"By precisely controlling material properties, atomic precision can lead to high-efficiency synthesis of solar fuels."*

The advancing technology of atomic precision enables the environmentally friendly manufacture of high technology materials at costs comparable to agricultural products, owing to its integrated knowledge of chemistry and engineering [1]. Atomic precision unlocks for humanity a motif of natural creation: where sunlight interacts with CO2 in the air giving rise to hydrocarbons and alcohol [2].

Without atomic precision, partial successes have been obtained by combining perovskite-structured metal halide photovoltaics with an electrochemical cell using oxidized gold and iridium dioxide electrodes and using water as an electron source, to efficiently reduce carbon dioxide to carbon monoxide. This can be used with established chemical processes to produce methanol, hydrocarbon fuels, and other commodity chemicals [3]. However, catalysts and membranes designed and fabricated using atomically precise methods provide the potential to replace expensive electrode materials with abundant and inexpensive components, to eliminate side reactions due to dissolved impurities, and to obtain higher efficiencies.

Photocatalytic reduction of carbon dioxide (CO2) is a photo physio-chemical reaction in which the photoexcited charge carriers like electrons and holes travel to the surface of the semiconductor material and react with the adsorbed species such as CO2, thereby reducing it to carbon monoxide (CO) or hydrocarbons [4,5,]. For the effective photocatalytic reduction of CO2, the catalysts used must possess several characteristics such as a high surface area, optimal light absorption, efficient charge separation, long carrier lifetime, high carrier mobility and selectivity towards a single product [5,6]. They must achieve turnover frequencies equivalent to that of nanoscale light concentrators with enhanced light harvesting to augment charge carrier concentration to unprecedented levels. For this purpose, both broadband and selective narrow band light absorption must be investigated [7,8]. A nanoscale light concentrator works in conjunction with macroscopic light concentrators to concentrate and direct photons at each catalytic site thereby increasing the carrier concentration. Concomitantly it needs to serve as a proton gradient channel without disturbing its optical properties. A further essential factor is membranes which separate atmospheric air as well as deliver CO2 molecules/ electrons to the catalysis site to facilitate its function at night or in the absence of sunlight. It is critical that these membranes do not interfere destructively with the nanoscale light concentrators.

Figure 2: The largest photovoltaic plant to date in North America at Nellis Air Force Base. Attribution: Wikimedia Commons

The use of this technology indirectly reduces energy consumption by displacing energy-intensive industrial processes with eco-friendly, renewable sunlight-driven production of both base and exotic materials, thereby leading to clean and renewable production of liquid fuels. Efforts should be directed towards addressing the issues which restrain the full large-scale potential of this technology, such as synthesis of highly efficient catalysts and low-cost membranes. Key researchers pursuing this technological development must remain fully funded to improvise the key components of the technology. Advancements in photocatalytic reduction of CO2 can be realized by atomically precise methods for synthesis or fabrication of catalysts and membranes as it enables tailoring the catalyst and membrane properties at the atomic scale, which lends the materials unique properties [9].

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Light-based Desalination Using Solar-Driven Protein Ion Pumps

Allison Duettmann, Dr. Richard Nesbitt

> *"Target-specific protein-based microporous membrane desalination driven by solar energy offers economical, energy efficient alternatives."*

Growing population demands and the effects of global warming lead to the rapid overdraw and depletion of water reserves (groundwater, water recycling and conservation) and the occurrence of permanent droughts in many developing countries [1]. This impending crisis is the driver for current investment in desalinated sea-water for both human consumption and agriculture [2,3]. Desalination involves depletion of minerals from saline water to transform it into fresh water, which is suitable for domestic and industrial needs. However, desalination is expensive because of the extensive energy needed to process the water [4]. In addition, the costs associated with transporting energy sources and water also contribute to the overall cost of desalination projects. This problem is likely to worsen in the future: according to the US Intelligence Community Assessment of Global Water Security, by 2030, humanity's global water requirements will exceed current sustainable water supplies by 40% [5]. Thus it is imperative to draft projects focusing on water purification, distribution of water facilitated by local production, as well as water storage. These projects should also aim at attaining the objectives with minimal adverse effects on the environment and at achieving long-term sustainability by using renewable sources of energy (solar energy) while taking cost factors into consideration.

Traditionally, the desalination process is achieved by distillation wherein the water is boiled to form water vapor which is then collected and condensed to turn liquid, leaving behind salt and impurities [6]. However, as this process heavily relies on heat, it is not energy efficient: Although novel desalination systems incorporating membrane-based reverse osmosis consume less energy than does thermal distillation, these systems are still not energy efficient as they are also connected to an outside energy source [7]. Atomically precise manufacturing can play a vital role in addressing this technological problem [8]: Protein molecules which are manufactured with atomic precision can be used to create a membrane that can be coupled with light, thus creating a sunlight based desalination system. Instead of connecting this desalination system to an outside solar source, the system itself would be powered by sunlight directly.

Figure 3: Water desalination plant in Ras Al Khaimah, United Arab Emirates. *Attribution: Wikimedia Commons*

The concrete objective of the proposed project is to remove ions such as chloride and sodium from seawater, using target-specific proteins that directly use sunlight as ion pumps. This can be accomplished by embedding target-specific proteins in the pores of a mesoporous silicon nitride (Si3N4) membrane separating the saltwater from the deionized chamber[9]. The dimensions of the pores could range from 5-20 nm, small enough to ensure that the membrane is stable and large enough to assist in the transport. However, the one-way movement of salt water through the membrane into the deionized chamber alone is not sustainable for desalination in the long run since accumulated material would get stored at one side of the membrane leading to fouling and blocking of the membrane. To avoid the fouling a bi-directional process has to be ensured, which requires energy. To harness solar energy, the protein will be furnished with a covalently bonded photosensitive molecule (FMN), so that it can undergo a conformational change by absorbing light. If the photosensitive molecule encounters light, it will absorb a photon and go into higher energy state, thereby signaling the protein to rearrange. The protein will undergo a stroke transporting the previously bound salt ion through the membrane. When the photon is released again, the transportation finishes and the process repeats. In short, the transport consists of a switch between two actions: binding action (the protein binding an ion), the switch (absorption of a photon), and transport action (moving the ion through the membrane and releasing it on the other side). Initial efforts can be focused on targeting and transporting one specific ion, but could progress to targeting multiple ions, like sodium and chloride for desalinated and dechlorinated water. The resulting purification units could be widely distributed and enable decentralized storage of the purified water.

The development of these ion pump proteins requires molecular precision - a specific protein for each ion [10]. The design of the target-specific protein structures requires intensive research into different research fields, e.g. Directed Evolution (DE). Selection pressure of DE can also be used to resolve the challenge associated with protein binding efficiency, especially in cases when the transporter protein strokes even when there is no ion to bind and transport. If this happens too often it might diminish the efficiency of the system.

Critical factors to be considered for the viability of this technology encompass robust protein-design [11], inexpensive membrane design [12] and energy calculations. For efficient functioning of the mesoporous membrane, the design of the proteins must ensure that their binding to the membrane is not affected by the fluctuations in the pore size attributed to the motion of the membrane. In order to ensure that the proposed system is less expensive than the existing membrane systems, which rely on alternative energy sources, it must be tested if the energy saved by using light-based desalination constitutes a significant saving versus the existing generic membrane system, which could run using alternative energy sources, e.g. external solar-based energy provision. However, given that the light-based desalination can be used anywhere, thereby eliminating transport costs for energy sources and water this is likely to be the case.

This idea is the result of joint efforts by experts from various research fields in line with the Energy workshop’s goal, which is to foster interdisciplinary collaboration to seek novel and innovative solutions to various problems. Financial assistance in terms of funding or grants is essential to support research efforts and collaborations to advance such technological developments with minimum adverse effects on the environment.

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Nanostructural Self Assembly Project

Jim Lewis, Gauri Vilash

The Nanostructural Self-Assembly project is based on the intellectual property owned by Steve Fowkes and Tom Nufert, working at Nanopolymer Systems [1]. They utilized proprietary vector-directional polymers to achieve bottom-up manufacturing through nanostructural self-assembly. Nanopolymer Systems has a toolset of related monomers under development for making a variety of nanostructures, some of which exhibit atomic precision. This project proposes a tight coil as the R&D structure, but the toolset is capable of making a variety of nanostructures suitable for different purposes.

“There is no polymer folding problem with vector-directional polymers since the interactions are with the nearest neighbor”

Nanostructured self-assembly with this class of polymers (iminols) is based upon tetra functional monomers [2]. The monomers are aromatic rings with four functional groups attached. As with all polymers, the monomers are polymerised by the reaction of the "head" function of one monomer (a carboxylic acid group) with the "tail" function of the next monomer (an amine group), releasing a molecule of water and forming the initial aramid linkage and the "backbone" of the polymer. The "leg" function (an annular nitrogen atom) is attached near the tail and the "arm" function (an alcohol group) is attached near the head.

After the formation of the covalent backbone linkage, the leg forms a hydrogen bond with the backbone linkage behind it, while the arm forms a hydrogen bond with the backbone linkage in front of it. These hydrogen bonds stabilize the backbone linkage and they "freeze" each linkage in the polymer into a specific conformation, thus giving the polymer a nanostructured backbone. There is thus no polymer folding problem with vector-directional polymers since the interactions are with the nearest neighbor.

This combination of strong covalent bonds from head-tail interactions and weak hydrogen bonds from arm and leg interactions with the backbone linkages allows temporary disruption of the linkage nanostructure by mechanical forces sufficient to break hydrogen bonds, but not sufficient to break covalent bonds, thus allowing the nanostructures to temporarily bend, fold or stretch and then reform as the energy from the broken hydrogen bonds is dissipated.

A variety of monomers are available, and backbone linkages can form between different pairings of head monomers and tail monomers [3]. Although the prototypical monomer can be visualized to have one head, one arm, one leg and one tail, the most useful monomers have two heads and two arms, or two legs and two tails, because heads do not react with heads, nor tails with tails, nor arms with heads, legs with tails, or arms with legs [4]. Depending on the ring positions of the two heads and two tails, the polymer backbone is either straight or bent at a 60° angle (which can be ±60°). Rarely, some monomers can accomplish a 120° bend. When an extremely simple monomer sequence is chosen with a constant vector, circular rings and helical spirals (nano coils) are formed. Depending on the size of the monomers (number of aromatic rings), and the vector combination, nano coils of varying diameters can be formed. If the backbone alternates between negative and positive vectors, it will result in a zig-zag or sinusoidal polymer.

"For any given pair of monomers, only one nanostructure will self-assemble."

The four functional groups used in these “vector-directional" iminol polymers include two groups (carboxylates and amines) that are common to industrial polymers (Kevlar and Nomex) and two others (hydroxy and annular nitrogen atoms) that are common to biological systems (proteins and DNA). So in a significant sense, these vector-directional polymers are biomimetic, even though their functional amino and acid groups are entirely aromatic instead of aliphatic.

At the current stage of development, most monomers are single ring aromatics, but there is a two-ring aromatic. But the defining characteristic is a nanostructured backbone of units with both size and direction, hence the term vector-directional polymer. When one combines only two monomers or monomers of non-opposite sign (either positive or negative) vector-directional polymers form a backbone with constant curvature, which invariably forms coils with the same pitch (axial distance per coil), but with varying diameter of the coil. A salient characteristic of these systems is the lack of structural heterogeneity. For any given pair of monomers, only one nanostructure will self-assemble, assuming that there is no tangling or kinking that gets in the way of the coiling (π-stacking) process.

One way to describe these self-assembled nanostructures is to say that at a length scale of several nm they are "as rigid as cooked spaghetti", but at the atomic level, they are "as rigid as a vibrating wire sculpture". They can flex from coil to coil but there is very little stretching from monomer to monomer. They can thus flex axially to a substantial degree, but not radially. These rigidities are similar to carbon nanotubes, which are axially more flexible but radially rigid.

Every aromatic ring has the potential for an extra arm and an extra leg so some monomers have six functional groups, for example sulfonic acid as an extra arm and a fluorine atom as an extra leg.

A library of monomers is available, permitting a variety of structures from different pairings. The monomers in the current core library are joined by iminol linkages (N=C) in tautomeric equilibrium with aramid linkages (amide bonds joining aromatic residues, with the amide carbon double bonded to the oxygen).

The polymer described in this manuscript is iminol polymer NSC-0304, which exhibits a core geometry of six oxygen atoms spaced at 0.28 nm so that the oxygen lone pair electrons are precisely oriented into the core of the coil formed by the polymer. The two monomers used for this polymer are 2, 3-diaminopyrazine and 2, 3-dihydroxyterephthalic acid.

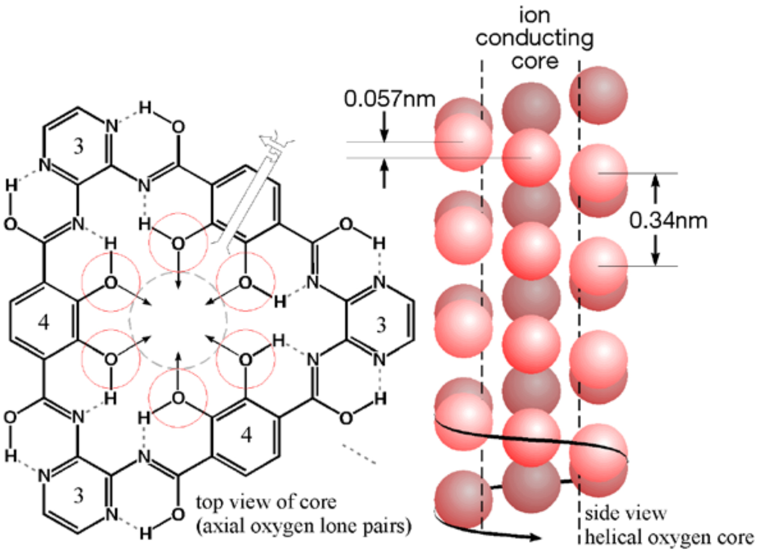

Figure 4: Iminol polymer NSC-0304 has a core geometry with six oxygen atoms spaced at 0.28 nm center-to-center distance, and with axially directed lone pair orbitals. This geometry suggests possible metal-binding and small-ion conductivity applications. Assuming uniform ring strain and even distortion, the oxygen atoms and radially directed oxygen sp2 orbitals should be staggered in a conformation lining the core, with 0.057 nm spacing. This could allow a proton or lithium ion stepping-ladder for cation conductivity. Lithium-ion or proton movement (technological issues C and D, respectively, page 14 below) would be pseudo-helical, paralleling the polymer backbone, "hopping" the less than 0.05-nm gaps between oxygen orbital centers. Attribution: Steve Fowkes and Tom Nufert, Nanopolymer Systems.

Due to the hydrogen bonding and donor-acceptor pairs flanking the iminol linkages, the polymer formed from these monomers follows a helical conformation, with a pitch of 0.057 nm between each of the six adjacent equivalent oxygen atoms in one turn of the helix. The pitch of one turn of the helix is thus 0.34 nm. Each monomer also has two more functional groups in addition to the two used for the iminol linkages. The polymer structure is further stabilized by the π-π electron interactions between vertically aligned aromatic rings.

The objective of Nanopolymer System's platform is to address several technological issues pertaining to catalysis, uranium mining from seawater, a replacement for the liquid electrolyte in lithium-ion batteries and application in fuel cells.

A. Organizing several different metal ions or atoms in atomically precise positions with respect to each other to increase catalytic efficiency. Following the simulation results from density functional theory [5], researchers were able to produce catalysts with an "atomically homogeneous" metal distribution. Several metals produced as gelled oxy-hydroxides "reveal a synergistic interplay between tungsten, iron, and cobalt in producing a favourable local coordination environment and electronic structure that enhance the energetics for OER (the oxygen evolution reaction)." Would an atomically precise positioning of several metals improve the results over an "atomically homogeneous" metal distribution? Would metal-to-metal bonding in the 0304 structure provide enhanced catalytic activity compared to mere "local" proximity of metals or oxides found in a gel? Is there a tiny percentage of specific proximities in a "homogeneous gel" that are responsible for the high catalytic activity? And can those specific proximities be reliably replicated by atomic-precision methods?

B. Efficient harvest from seawater of uranium (or other valuable minerals, such as thorium, gold, radium, platinum, palladium) or removal of uranium (or mercury or other toxic material) from industrial effluent or ground water. This work [6] does not approach atomic precision but does demonstrate that a specific process to combine disparate nanostructures into hydrogels produces a novel structure that is a potential adsorbent for uranium from seawater for use as a nuclear fuel. Would methods of combining these components to form atomically defined mesoscopic structures yield even better results? Also raised "in committee" was the idea that in situ release of bound heavy metals by mechanical means (tidal action) might be dramatically more efficient than chemical extraction [7].

C. The current liquid electrolyte in lithium-ion batteries requires lithium ions to follow a long, tortuous path between electrodes (through the electrolyte and separator membrane). A concept of using hydrogen-bonded supramolecular solid electrolyte to act as an ion-migration path will facilitate fabrication of high-performance electrolytes [8]. Would lithium ions flow through properly designed atomically precise channels embedded in a membrane give a superior performance? Would the shortening of "ion hopping" to subatomic scales via atomic precision positioning of counterions reduce ion movement resistance losses [9]?

D. Hydrogen storage. It would also be worthwhile to investigate whether hydride ions or protons in a properly designed atomically precise channels provide greatly increased hydrogen storage for fuel cells, compared to, for examples, metal organic frameworks (MOF's), in which the hydrogen would be less accessible, or to polysulfonyl perfluorocarbon proton-exchange membranes (Nafion, DuPont).

However, current nanotechnologies do not provide nanostructures that self-assemble in sub-micron domains or greater quantities into atomically precise structures that can be designed to be specific for target guest ions. In other words, the freedom of rotation in standard polymers allows negatively charged functional groups to move in response to electrical repulsion forces resulting in separations that necessitate cation hopping. These are some of the challenges which should be considered.

How could atomically precise manufacturing help?

- The toolkits for nanostructural self-assembly being developed by Nanopolymer Systems provide ways to design and manufacture polymers that will adapt atomically precise secondary structures on large scales. Polymers can be designed to be either coils or sinusoidal, and coils can have varying diameters and be lined with different functional groups to accommodate various guest atoms or ions.
- These toolkits are also adaptable to build block copolymers so that different functions could be implemented in different portions of the nanostructure.
- The few other atomically precise structures that could be considered are rigid, such as metal organic frameworks. These vector-directed polymers contain weak bonds

(hydrogen bonds, lithium bonds) that can be reversibly broken and re-assemble as the energy from disruptive forces is dissipated.

- Ion channels designed with atomically precise structures can also be expected to resist fouling since they will not admit guests that should not be present. Such channels might, for example, protect lithium batteries from harmful side reactions by contaminants that could be excluded or trapped within the coil pores.
- Furthermore, the vector-directional polymers developed by Nanopolymer Systems are exceptionally stable, being thermally stable over 200 °C.

With respect to catalysis (A above), several different combinations of monomers could be designed to form a pocket, specific to individual transition metal ions or atoms. These could be arranged as stacks in block copolymers or as bundled coils embedded in a membrane so that several atomically precise configurations of several different atoms could be compared for catalytic activity, with each other and with the randomized distribution reported in reference 5.

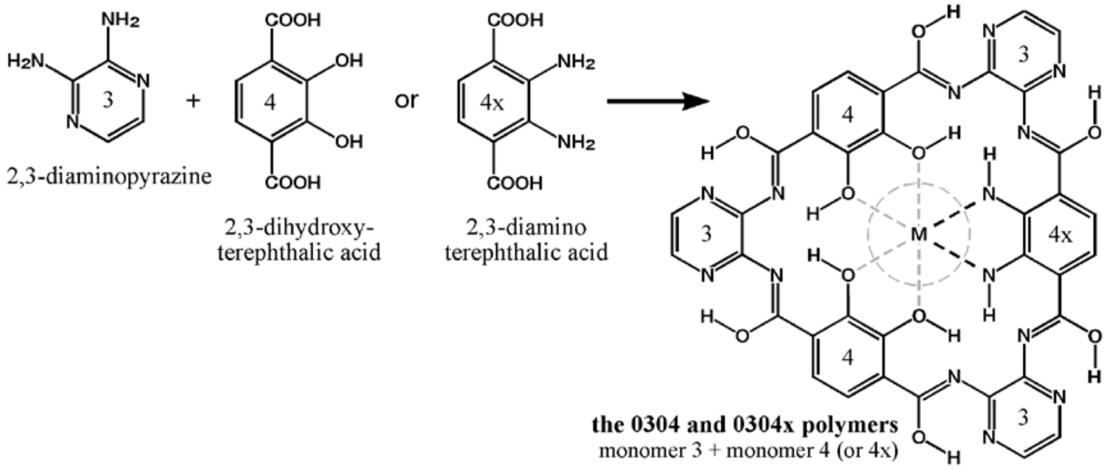

Figure 5: With nitrogen atoms instead of oxygen atoms (substituting monomer 04x for monomer 04), the core would be "pre-charged" with protons. Attribution: Steve Fowkes and Tom Nufert, Nanopolymer Systems.

For uranium harvest from seawater or removal from industrial effluent, the size of the uranium ion requires a sinusoidal polymer that can accommodate binding pockets for large atoms. The combination of primary covalent and secondary hydrogen bonds achieves the S-structured semi-rigid backbone. With mechanical stretching, the secondary bonding that would otherwise encourage the S-shaped backbone is readily disrupted without affecting the covalent primary bonding, which breaks up the multi-dentate large-ion binding sites. Then, when the stretching force is released, the polymer is free to re-form its secondary bonds and begin binding with another set of large ions, thus eliminating the need for chemical extraction of the metal ions from the polymer.


Figure 6: One possible application: energy storage, i.e. better batteries. *Attribution: Wikimedia Commons*

Energy needs pertaining to hydrogen-bonded supramolecular solid electrolyte and hydrogen storage in fuel cells can be considered with respect to iminol polymer NSC-0304. Such a helical polymer provides a core into which can be stacked a column of Li ions or protons. This polymer represents a class of polymers in which both the diameter of the inner core and the functional groups lining this surface can be varied. So each monomer pair produces a different nano coil with a different pore size and surface. Some examples:

The 0304 polymer core is lined with phenolic oxygen atoms.

The 0609 polymer core is lined with iminol hydroxy groups.

The 0514 polymer core is lined with sulfonyl groups.

The 0314 polymer core is so tight that nothing but protons can pass through it.

The 0304 polymer core is about 0.35 nm.

The 0504, 0904, 0706 pores are larger than 1.5 nm.

The best guess based on knowledge of the size of the pore and atomic dimensions of the atoms and their ions is that polymer 0304 might be too small to fit a sodium ion. It will surely fit lithium ions and protons. However, it might be hard to fit larger ions like potassium, calcium and the first d-block row of transition metals (3d electrons, period 4). These are the current practical challenges for implementing this project.

Atom size decreases with ionization. A vanadium+7 ion is likely to be small enough to fit within the 0304 core, but the high charge may affect the flow of such ions to a prohibitive degree. The binding of secondary atoms to the vanadium ion (like trioxide, tetraoxide) might be too tenacious to alter, or leave the vanadium ion which is reactive towards the oxygen lone pair electrons of the 0304 core. Speculatively, the halides and oxides of first-row transition metals with linear structures might get filtered through the 0304 polymers. It seems likely that first-row transition metal ions would have a good chance of sticking and becoming trapped within the core at a level of binding that would be stable enough for functional use (for example, as electrochemical catalysts).

The energy needs pertaining to a liquid electrolyte in lithium-ion batteries presents perhaps the simplest application of nanostructured self-assembly, which is replacing the liquid electrolyte in the batteries with ionic channels to conduct cations between the electrodes [8]. An alternative to the pore approach of the 0304 polymer is to use external sulfonyl groups in immediate proximity to each other, thus in immediate proximity to each other, thus eliminating the losses from "ion hopping" in standard batteries. Because they are negatively charged (and strongly acidic), sulfonyl group are well suited to conduct cations. NSC's vector-directional polymer design places sulfonyls immediately adjacent to each other (0.35 nm center-to-center separations, < 0.1 nm surface-to-surface separations), which is predicted to reduce "hopping" to its theoretical minimum. Hopping of cations from one randomly distributed sulfonyl group to another in conventional liquid electrolytes decreases energy density and shortens battery lifespan. Further, sulfonyl groups are unlikely to bind lithium ions irreversibly. Such may also be said of the 0304 nanocoils but for different reasons: The only lithium bonding sites—the oxygen atoms—(1) are aromatic and hence partially positively charged and (2) their negatively charged orbitals are staggered in a helical configuration, which limits lithium cation interaction to one oxygen atom at a time, or to two at a time with bad binding geometries. The NSC-0314 polymer core, which is so tight that nothing but protons can pass through it, would similarly present an improved electrolyte for acid gel batteries and possibly proton-exchange membranes. They may also prove suitable for reversible storage of hydrogen for fuel cells.

In spite of the several attractive features of this project there are some challenges which require attention:

- The design of the membranes into which the nanostructured polymers need to be embedded
- The lack of automated design of polymer components and constituents for specific guests (the initial configurations of components for specific target guests have been designed by hand)
- The lack of detailed atomically precise characterization of specific self-assembled nanostructures
- The need for collaborators for certain functional tests, such as plasmonics
- A demonstration project such as assembling a proton transport channel in a membrane and demonstrating a change in pH through the membrane

However, these challenges can be addressed by designing software that will produce vector-directed polymers to channel specific target guests, by acquiring financial assistance or funding for demonstration projects and by collaborating with researchers for atomically precise structural characterization and functional assays.

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Atomically Precise Asymmetric Catalysis

Tim Potter, Acknowledgement: Gauri Vilash

"Screening and designing of atomically precise stereo selective centers for efficient catalysis."

The current state of catalysis is inefficient and ineffective compared to foreseeable technology [1].Rather than relying on existing synthesis strategies, atomic precision allows the creation of catalysts that function based on their precise structures.

For many industrial catalysts, only a small fraction of the surface contributes to most of the catalytic activity [2]. The advantage of bottom-up atomically precise synthesis is that it is possible to have all sites actively involved in catalysis. The drawback of having inactive sites is that they are just as expensive to fabricate and yet their unwanted reactants must be cleaned up after catalysis. Atomic precision increases the reaction density, the reaction speed, and uses significantly less energy, producing a chemically pure product, and also permits possibilities of developing new catalysts which are presently uncontrollable. Reaction rates can be improved by one to two orders of magnitude and in some cases even to nine orders of magnitude [2].

Many catalytic reactions are highly reactive and are stabilized in nature with atomically precise asymmetric pockets within enzymes. Though we are beginning to understand the desired atomically precise structure for a given catalyst, designing proteins that fold into an atomically precise desired configuration that is highly effective is still elusive [3]. The shape and subsequently the catalytic properties of a protein are easily altered with its environment, limiting its applications.

Computer simulations can predict the transition state between a reactant and a reaction product for a given reaction [4,5]. It is thought that proteins tightly bind this transition state and do not bind the reactant or the product. With the transition state map generated by simulations, a corresponding map of atoms known as the active site can be made which will tightly bind the transition state.

An atomically precise rigid scaffolding can then be designed and synthesized using organic stereochemistry to support the precise atomic arrangement of the active site [6,7]. The stereo centers of the scaffolding can be varied, the scaffolding can be functionalized with the same R groups that proteins use, and inorganics can also be used as functional groups in the structure [8].

Organic Stereochemistry allows synthesis of scaffolding which is relatively simple to design. The algorithm required to place atoms precisely in a rigid 3D structure is known, while the algorithms needed to precisely fold a highly functional designer protein are not yet complete. Though rigid scaffolds can be synthesized easily compared to the protein folding structures, novel computational tools must be used to facilitate the design of complex asymmetric structures.

The structure-property relationship that directs highly reactive reactants in nature is generally an atomically precise asymmetric pocket and this same motif is also the basis of the structure-property relationship of the proposed method. Stereocenters, R groups, and inorganics form an atomically precise asymmetric pocket with a surface that binds to, or stabilizes, the transition state. This atomically specific structure can perform catalysis in one step and also precludes the need for membranes because the asymmetric pocket functions as a membrane by accepting only the desired reactant. Because of the bottom-up synthesis it is possible for all sites to be active. Inactive sites are just as expensive to fabricate, yet must be cleaned up after catalysis.

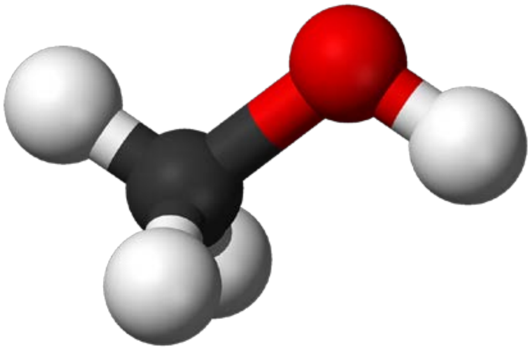

Figure 7: Methanol molecule, the result of the conversion of methane to methanol. Attribution: *Wikimedia Commons*

One application of this technology is the conversion of methane to methanol. Methanol is useful as an energy carrier because it is easier to store than methane.

Methane is a tetrahedral molecule with four equivalent C–H covalent bonds. This equivalency presents a challenge to react with any one of the four bonds. After breaking the first C-H bond in reaction, the molecule is highly reactive and unstable.

An asymmetric pocket allows the first C-H bond to be broken in an environment where it is stabilized. The pocket stabilizes the reaction through the transition state by binding the transition state and allowing the reaction to carry out in a controlled manner until the desired product methanol is obtained. The pocket prevents methanol from reacting with the next methane molecule during its catalysis.

Developing this technology to maturity requires developing a periodic table of chemistry and building a tool-kit of self-assembling monomers. Furthermore, software is required to predict transition states and which monomers and which functional groups are needed to build the atomically precise active sites. Software is also required to build the macromolecular structures.

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The Atomically Precise 3D Printer

A case for research and development in the manufacturing of an atomically precise 3D printer using functional tips.

Lori Luttrell, Acknowledgement: Rei-Wen Wang

"Atomically precise 3D printing reduces cost and energy-use by providing precise control of properties."

Despite Moore's Law, manufacturing is reaching a limit to how rapidly we can continue to make smaller and more efficient devices including computers and cellular phones. More than being a law, Moore's Law is an observation that for the foreseeable future, manufacturers could double the number of transistors on a microprocessor chip every two years [1]. We're already approaching the limit to manufacturing computer chips out of silicon. This ability will not continue indefinitely, and we need to look to other ways to produce better quality materials providing longer sustainability of products that today are often low quality and discarded rapidly [2]. It's time to invest in research in atomically precise manufacturing. If we don't do it, someone else will.

The atomically precise 3D printer is one of those promising technologies [3]. By manufacturing materials to atomic precision, fabrication of ultra-small devices and materials with better performance is possible. For instance, an atomically precise 3D printer could be used to fabricate mechanical transistors at nanoscale to operate at high frequency with low energy consumption. For one proposal, see reference [4].

We propose to make a 3D printer using functional tips. IBM started research in this area using a combination of the MEM's (Micro Electro Mechanical Systems) and the AFM (Atomic Force Microscope) to produce nanometer scale, but not yet atomically precise features on surfaces using tips. The project involved atomic force probes in a 1000+ tip scanner to write memory[5]. Its intended application was in high-density memory, but was found to be economically unviable upon the development of flash memory. The multi-tip array then became obsolete and the project was essentially abandoned.

Also, research and development into an atomically precise 3D printer hadn't caught on because it was considered too small a scale and extremely specific. Many in industry and commercialization thought overall development in atomically precise manufacturing was too risky to fund because it that appeared to be a costly undertaking without guaranteed results. The focus at the time was on bulk purpose machines that generate revenue quickly with a broad range of customers [6]. APM is fairly unexplored territory and if the Millipede project hadn't been canceled development in a 3D printer might be further along.

Figure 8: A fabrication lab featuring multiple 3D printers: A space for experimentation with atomically precise 3D printing? *Attribution: Wikimedia Commons*

In the future, atomically precise manufacturing could be used to make ultra-high efficiency computers and small devices and systems with emergent performance characteristics. With it will come an increased efficiency in catalysts and a 1000x decrease in energy use than present-day CMOS style. It will be a more adequate energy conversion with cost decreases across the board. Importantly, there will be far less waste as devices manufactured using atomically precise technology will last longer and have far greater quality and efficiency.

"We want to expand the millipede project to a megapede, a 1 million STM tip array."

There are several ways to fabricate atomically precise 3D printers – print materials by an electrospun nano jet, build up materials with a catalytic tip, use focused ion and electron microscopies, two-photon lithography etc. [7, 8]. Currently, if you wanted to make a dime out of atomically precise 3D printing with one STM tip patterning element, it would take 10 years. One tip is too slow; we need 10^6 tips. The potential path forward is to use a multi-tip array and make atomically precise templates using tips or catalysts. We want to expand the millipede project to a megapede, a 1 million STM tip array. However, tips have been a problem in scan probes. An idea would be to make carbon nanotube scaffolds.

Using a multi-tip array is one way to scale up and improve the process of manufacturing a product one atom at a time. The tip-based method emits electrons or ions positive or negative, that interact with the surface. Presently, we can write 50 atoms/sec. So we need to scale up to 50 x 10^6 atoms per sec. Each tip needs to have maneuverability so that the tips won't be in the same spot relative to one another. Each cone needs to be able to move on its own and needs to have springs on the side and can't have two tips next to each other. A system should be compact laterally so tips can move up or down.

To achieve this, we need a lot of computing power, scanners, vibration isolation and the ability to control the power from getting too hot. There is the idea of doing some of these experiments in liquid. A desirable team required to work on this project would include scientists with different backgrounds in a multidisciplinary approach including a NEMS/ FAB group, and organic chemists to make building blocks [9].

It's time to put into place some longer-term goals and develop ways to communicate ideas regarding APM to political decision-makers, investors and the general public. We have to develop some standard capabilities and make some regulatory changes to allow testing and deployment. The importance of communicating and educating the public can't be overstated. In order to make an atomically precise 3D printer and continue manufacturing products, conserve resources and reduce waste, we must look to APM and invest in research and development.

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Prize Proposals

Prizes can motivate the development of new technology by rewarding significant accomplishments on the path toward that technology. Prizes also build public interest. For a general discussion about the concept of prizes for technological progress, please see *Prizes for significant steps toward atomically precise manufacturing* under *Approaches* in *Technical Background Information*.

The prizes mentioned below should include seed funds for small groups, including students, to access facilities that can characterize the materials, opening the prize to a wider range of participants than just researchers who already have access to those tools.

"Molecular motors could use positional control to achieve the required multistep synthesis."

The workshop used these prize ideas in a backcasting exercise: participants considered a hypothetical future scenario in which their team had won one of these prizes. Teams discussed how they had won. More generally, the backcasting technique can help researchers apply their creativity to identify keys steps toward atomically precise manufacturing and explain their importance, by assuming the step is completed and describing how that happened. Conversely, when evaluating projects with appealing short-term benefits, backcasting can be used to explore possible negative outcomes, such as that the project failed to advance your long-term goal, and to imagine what went wrong. This future-oriented perspective can help a group focus on efforts with near-term payoffs that also contribute to long-term goals.

Positional control prize

Demonstrating a major step toward atomically precise manufacturing using positional control. This idea involves a set of catalyzed reactions that start from the same molecule and produce different products depending on the order in which they operate on intermediate molecules. If reactions occur randomly, e.g., with chemicals diffusing in solution, the result will be a mix of different products. The prize could require demonstrating positional control to force the steps to occur in a specific order, thereby producing just one of the possible products. One feasible approach to this task is using molecular motors to move a molecule along a track between surface-bound catalysts, each of which performs one step of transforming the initial molecule to the desired target. Prize criteria could include:

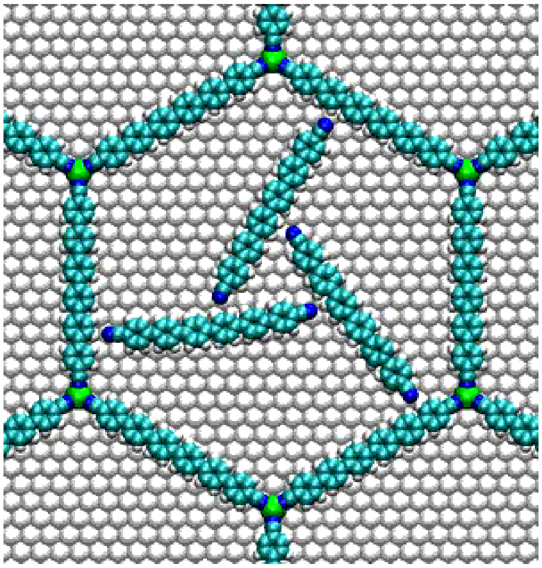

Figure 9: A possible starting point: Rotation and dynamics of a supramolecular motor caged in a hexagonal lattice (outer diameter = 6.7 nm) on a silver surface at ~ 250 K. See "Nanoscopic observation of molecular rotation" at https://en.wikipedia.org/wiki/Synthetic_molecular_motor and publications cited therein. *Attribution: By Palma, C.-A.; Kühne, D.; Klappenberger, F.; Barth, J.V. (Technische Universität München) [Public domain], via Wikimedia Commons.*

Animated version: https://commons.wikimedia.org/wiki/File:MD_rotor_250K_1ns.gif

- The number of steps
- The purity of the product
- Time allowed
- Complexity of the product
- Positional precision for each step, e.g., whether just placing intermediates near each catalyst is sufficient to produce the reaction, or whether intermediates must also be correctly oriented or pushed into active sites on the catalyst.

Increasingly challenging criteria provide a way to define a series of prizes, each of which requires a significant advance over prior steps.

Desalination prize

A $1 million prize for desalination with the goal to purify 1 liter of water using atomically precise filters that require less than half the energy used by current desalination methods, e.g., reverse osmosis.

Methane to Methanol conversion prize

A prize for converting methane to methanol requiring the use of atomically precise catalysts to speed up specific reactions. This prize would proceed through a series of steps with seed funding for multiple groups and an ultimate $1 billion prize. (While this prize magnitude may seem very large, it is appropriate in the context of the value of solving this global problem.) Specifically, the goal is atomically precise catalysts with two orders of magnitude better performance than current methods to produce methanol. This demonstration would have large economic value by allowing capture of methane in natural gas instead of burning it. Currently, there is no economical way to convert the methane to fuel because oxidizing reactions tend to run to completion (i.e., burn the methane) rather than selectively stop at a convenient liquid fuel (methanol). Success for this prize would pave the way for creating precise catalysts for many other reactions.

Flexible Positional Chemistry prize

A prize for flexible positional chemistry. This would require multiple nanorobotic manipulators with molecular recognition binding sites at their ends. These manipulators must then push molecules toward each other to force an exothermic reaction, and use that energy to reset the manipulators.

Atomically Precise 3D Printing prize

A prize for atomically precise 3D printing, using multiple tips, achieving a rate of more than a trillion atoms per second. Success for this prize would enable printing 10 billion mechanical switches a second on a surface. Such molecular switches, based on rotating single carbon-carbon bonds, would use less than 10-19 joules per operation and readily operate at 1012 Hz, thereby using less power and providing faster switching than current electronics.

Technical background information

Atomically Precise Manufacturing

“Advance atomically precise manufacturing and improve the energy sector."

Atomically precise manufacturing means producing products with atoms in precisely specified locations and with specified bonds to their neighbors. Current technology can make such products, but only at very small sizes with relatively few atoms. The manufacturing discussed at the workshop extends to macroscopic products.

An analogy for thinking about the benefits of increasing precision is that in the 19th century, the micron length scale was not relevant to the manufacturing economy. Developing engineering at that scale in the 20th century led to major new industries that eclipsed the value produced previously. Similarly, we can expect commercial availability of precise engineering at the atomic scale to create significant new industries and benefits. Countries and companies that lead this development could capture much of this new value. A major focus of this workshop was on evaluating this possibility for the energy sector.

Macroscopic atomic precision will not only improve today’s materials, but also allow producing programmable materials composed of active microscopic machines that can sense, compute and exert forces on their neighbors to alter their spacing. Such materials could change properties such as shape, strength and optical response under computer control. In particular, such changes in response to external forces could make the material very flexible, unlike the brittleness expected from large-scale atomically-precise crystals.

"Costs of atomically precise products should be front-loaded: cost more to design, less to build."

A key issue for commercial use is production cost. While costly in the R&D phase, per-unit production costs should eventually be comparable to agriculture, which currently produces many molecular machines via exponential growth using cheap materials and sunlight. That is, products could eventually cost about $1 per kilogram. Thus the economics of atomically precise manufacturing is similar to that of digital goods: i.e., expensive to design and test new products, but cheap to produce copies.

> *"Atomically precise catalysts could produce the products we want and avoid undesirable side products."*

Atomic precision contrasts with the broader term “nanotechnology” which refers to materials with structures defined on scales below 100 nanometers, which is far larger than the atomic scale.

This includes current microelectronics, with features as small as a few nanometers. This distinction is important because atomically precise materials can have significantly higher performance than materials that are precise only at nanometer or larger scales. For instance, the strength of atomically precise materials can reach theoretical values of materials without defects. This could improve strength-to-weight ratios of structural materials by a least an order of magnitude.

Another example is catalysis, which depends on the atomic structure of surfaces. Atomically precise surfaces could produce just the desired product, e.g., a fuel, without other parts of the surface catalyzing unwanted reactions that produce waste products. This variation arises in current materials due to their heterogeneity at the atomic scale. When used as catalysts for chemical reactions, a few of the atomic arrangements in the material catalyze the reaction far more effectively than the majority of the arrangements. This minority of the most effective sites can dominate the activity of the entire material. If we could find those most effective arrangements and make materials with just those (i.e., manufactured with atomic precision), we would have far more effective catalysts, rapidly producing just the products we want and avoiding undesirable side products that later need to be removed by costly purification steps.

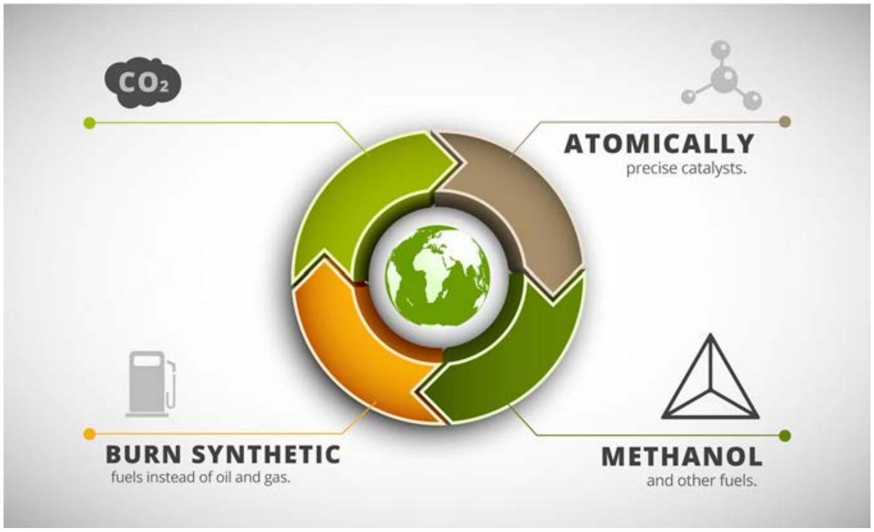

Figure 10: *Attribution: Foresight Institute; Artist: Gina Miller*

Opportunities for Energy

Atomically precise manufacturing could have significant benefits throughout the world economy. This workshop focused on the energy sector and found opportunities to improve both the supply and demand sides of the energy sector.

Regarding supply, atomic precision could make the energy supply more efficient and sustainable. This includes improved production, storage and delivery of energy. Precise manufacturing could also reduce waste products and pollution associated with energy production.

For example, atomic precision could create much better catalysts for energy production. One such application is harvesting sunlight to produce chemical fuels while reducing pollution from unwanted reactions and reducing the need to extract such fuels from the earth. Another application of better catalysts is to capture methane and CO2 by catalytic conversion from natural gas or the atmosphere to fuels.

One example is manufacturing structural materials having close to the theoretical strength of the materials. This would allow using lighter materials, which in turn require less energy to transport. Another example is producing atomically precise membranes, which could separate chemicals in solutions with much less energy than required with current membranes. Applied to water desalination, this would reduce the energy needed to supply fresh water in arid regions. Also, atomically precise manufacturing will enable the production of highly efficient computers, thereby significantly reducing the electricity requirements of today’s large data centers.

> *"Atomically precise manufacturing would reduce the energy required to manufacture, transport and consume products"*

Challenges

Atomically precise manufacturing requires

- Capability: bond atoms and molecules in macroscopic quantities at low cost
- Design: determine arrangements of atoms giving useful products

- Characterization: evaluate whether a design was manufactured correctly and, if so, whether it has desired properties

Addressing these requirements requires sustained funding for basic research, engineering and tool development. This, in turn, requires decision makers recognize the opportunity. Significant barriers stand in the way of achieving this opportunity.

“Currently, there is no consensus on what are the limits of macroscopic atomic precision.”

Lack of scientific consensus

Currently, there is no consensus on how to achieve macroscopic atomic precision. The benefits claimed for atomically precise manufacturing can appear too good to be true, leading some authorities to relegate this technology to the realm of science fiction. Others suppose progress will require many decades and hence think it premature to devote scarce research funds to such development. Moreover, until there are high-profile funded projects, the lack of funding itself is a barrier, giving the appearance that other funding sources have evaluated and rejected this research.

One objection is that current demonstrations of manipulating individual atoms on a surface cannot scale up: building materials by moving one atom at a time will take prohibitively long to produce macroscopic quantities of atomically precise products. This neglects two possibilities: (1) using modular self-assembly or positional assembly of multi-atom molecules to build larger structures, and (2) using massively parallel manipulators and, in particular, the exponential growth process seen in cell division whereby a single cell divides to produce an organism with tens of trillions of cells in a relatively small number of doublings.

“'Atomic precision' means specifying number, position, and bonding for each atom."

Another objection is that, even if such products could be produced, they would not be stable because thermal fluctuations necessarily require macroscopic materials to have defects. However, covalent bond energies are sufficiently larger than thermal energies at ambient temperatures to prevent such rearrangements of covalently bound materials. That is, it is a mistake to assume that atomic precision is analogous to precisely placing unbound atoms next to each other on a surface at cryogenic temperatures and then expecting the structure to remain in place when warmed up.

Contributing to the lack of consensus is a confusion of terminology between "atomically precise" and "atomic scale". Many scientists use the term atomically precise to apply to atomic-scale structures, such as atomic layer deposition and nanoelectronics (with 10nm features), and hence incorrectly assume these examples represent the best we can expect to achieve with atomic precision. Instead, examples of atomically precise nanomachines are bacteriophages and flagellar motors, which are structures with atoms precisely positioned with respect to each other. Adding to this confusion, some researchers also use "atomic precision" to include less stringent requirements, such as just a specified number of atoms rather than also specified position and bonding for each atom.

"Two methods for atomic precision are self-assembly and positional control."

Manufacturing

Atomic precision is already implemented today at the molecular scale, e.g., producing specific molecules through chemistry in solutions or moving atoms on a surface with probe microscopes. However, the full potential of atomically precise manufacturing requires producing macroscopic products.

Two methods for atomic precision are self-assembly and positional control. Both face challenges in producing macroscopic, atomically precise products.

"Self-assembly creates structures from components whose interactions allow them to bind together only in specific, well-defined configurations."

Self-Assembly

Self-assembly creates structures from components whose interactions allow them to bind together only in specific, well-defined configurations. In this case, randomly moving those components around each other can eventually have them meet in the proper configurations and bind together. At a small scale, molecular diffusion from thermal fluctuations provides this random motion.

Self-assembly is the basis of chemistry in solutions and can produce atomically precise molecular structures. Template surfaces, defined at somewhat larger scales, can aid this process. Self-assembly can produce large quantities of product by operating in parallel.

Biological organisms use self-assembly to produce atomically precise molecular-scale materials with a wide range of functions, e.g., harvesting energy from sunlight for chemical synthesis. Growth through cell division rapidly produces macroscopic quantities through an exponential process of repeated doublings.

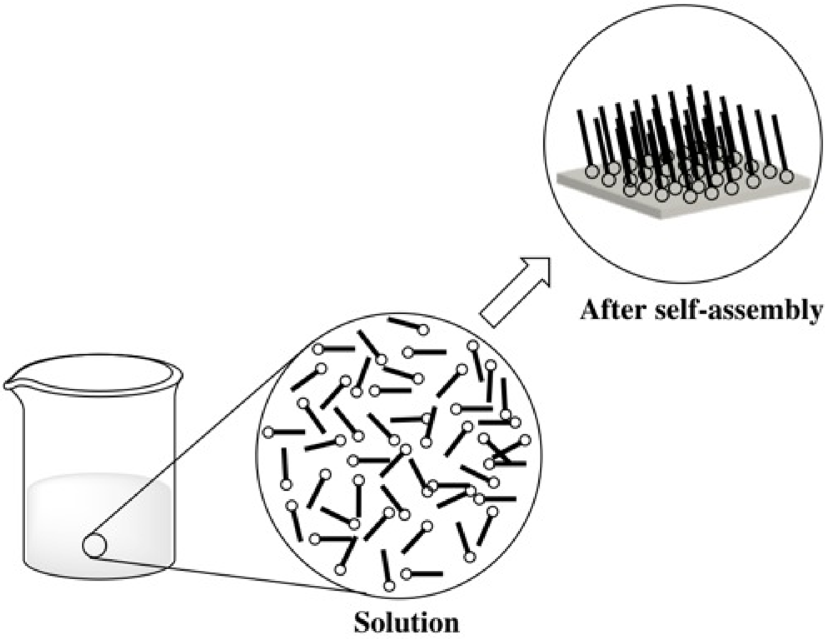

Figure 11: An example of self-assembly of nanoparticles in a solution: A disordered system forms an organized structure which can be due to specific interactions among the particles. However, the organized structure is only atomically precise in the interaction of the nanoparticles with the surface. Atomically precise manufacturing will use atomically precise molecular building blocks assembled with atomic precision in position, orientation, and bonding. *Attribution: By Fasantos (Own work) [CC BY-SA 3.0 (http://creativecommons.org/licenses/by-sa/3.0)], via Wikimedia Commons*

However, at larger scales, bindings of components are generally not specific, resulting in a mixture of different structures rather than a single atomically precise product. Moreover, diffusion is very slow at large scales, thereby requiring complex additional transport and mixing of materials to maintain self-assembly. Thus self-assembly alone does not today produce macroscopic quantities of complex atomically precise materials.

Positional control

Positional control uses external manipulators or other positional constraints that force components to meet each other at only precisely specified locations and orientations. In this case, even if components could bind in a variety of configurations, they are only allowed to meet and bind into one of those configurations.

> *“Positional control forces components to meet each other at precisely specified locations and orientations.”*

Factories use positional control to produce a wide variety of macroscopic products that are not atomically precise. These factories use automation to mass-produce products cheaply. On a much smaller scale, ribosomes construct proteins by positioning and joining precise

"Self-assembly provides atomic precision at small scales; positional control produces complex macroscopic objects or atomic precision for only a few atoms."

sequences of amino acids as specified by DNA. Another example is manipulating and reacting atoms on surfaces with scanning tunneling microscopes (STM) and atomic force microscopes (AFM). This technology directly manipulates atoms, avoiding the stochastic limitations of self-assembly. However, this approach is severely limited in the number of atoms it can arrange in a reasonable amount of time, and thus cannot build macroscopic products with atomic precision.

Thus, currently, self-assembly provides atomic precision, but only at small scales, while positional control produces complex macroscopic objects, without atomic precision, or atomic precision for only a few atoms. Atomically precise manufacturing of macroscopic products requires overcoming these limitations.

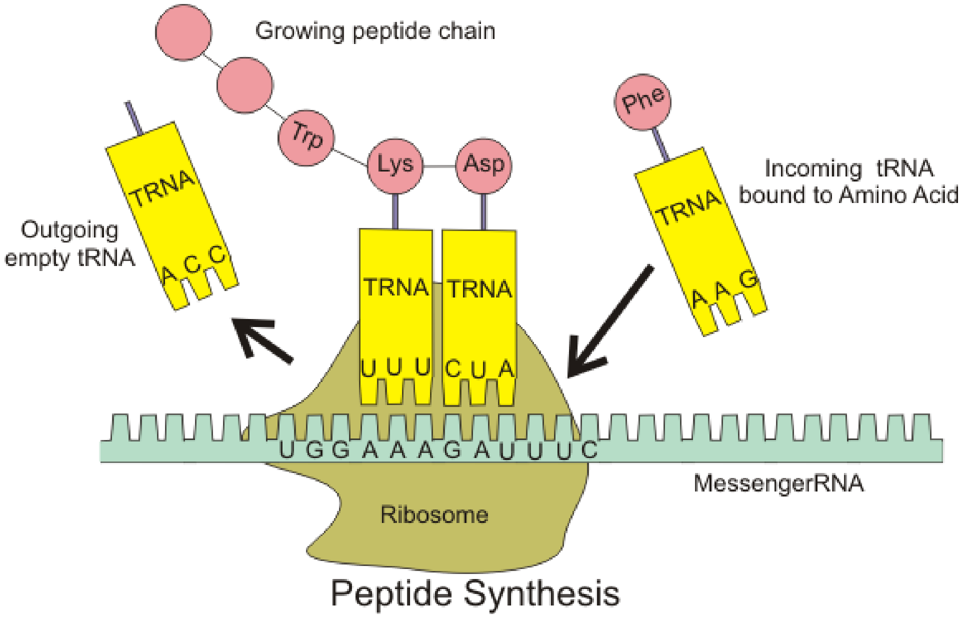

Figure 12: The ribosome is a cellular organelle synthesized by the atomically precise self-assembly of dozens of RNA and protein molecules. This complex biological molecular machine system precisely orients tRNA molecules, each charged with a specific amino acid, in the order specified by interaction with the mRNA, such that another part of the ribosome can add a specific amino acid to the growing peptide chain. *Attribution: Wikimedia Commons*

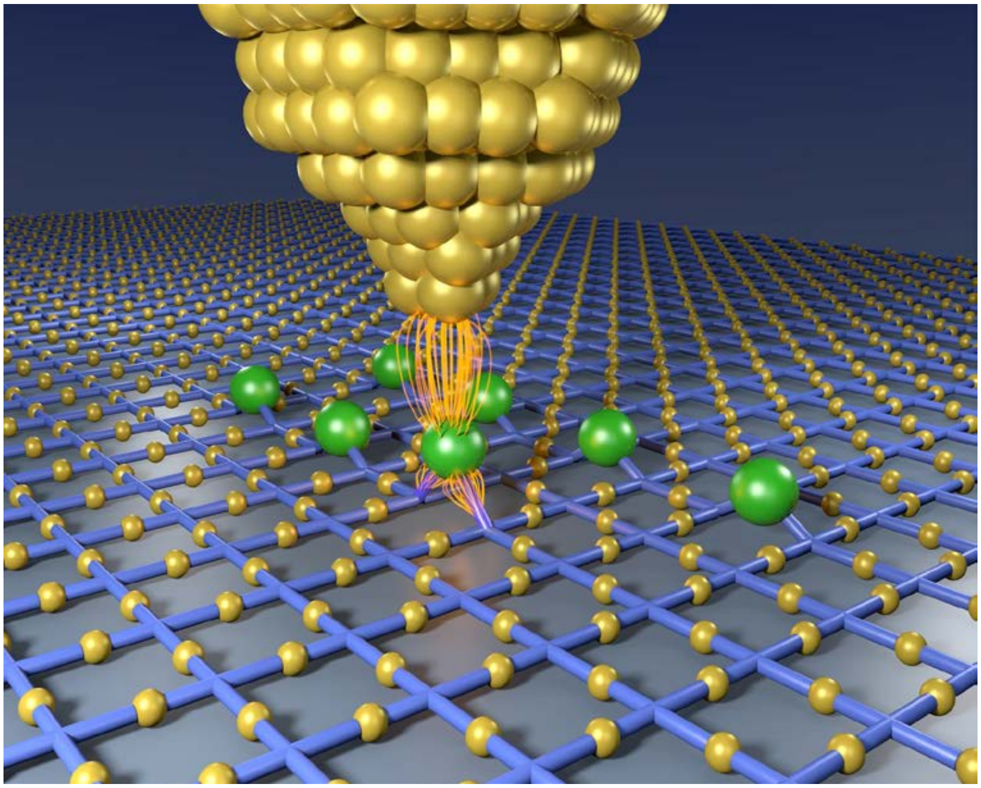

Figure 13: The world's smallest magnetic data storage. Press release from the Deutsches Elektronen-Synchrotron, A Research Centre of the Helmholtz Association. Atomically precise assembly of an atomic-scale antiferromagnet with the tip of a scanning tunneling microscope. Iron atoms are placed onto a copper nitride surface and bound by two nitrogen atoms (blue rods) into a regular array separated by one copper atom (yellow). *Attribution: Sebastian Loth, CFEL Hamburg, Germany, used with permission.*

Design

"Funding for design tools is needed to better determine which arrangements of atoms are useful to provide required capabilities."

Exploiting a new manufacturing technology requires not only the technology itself, but also knowledge of how to design products that fully exploit that technology. In some cases, design is relatively simple, e.g., producing defect-free structural material to achieve its theoretical strength. Other cases, however, can require significant effort to determine which placements of atoms provide the most benefit. Novel catalysts are an important example for energy applications, e.g., to determine atom configurations that efficiently catalyze fuel production without undesired side reactions.

Thus we need design tools that determine which arrangements of atoms provide required capabilities. This is primarily a software development task, i.e., producing a programming environment that helps design molecular machines, analogous to existing computer-aided design (CAD) software. These tools must evaluate many large-scale molecular machines, particularly for molecules that we currently have little experience with, i.e., complex, non-biological molecules. The tools must also handle design at multiple scales, from individual molecules to macroscopic products. The scales differ in the dominant physical effects and require correspondingly different computational approaches that smoothly integrate across scales.

Currently, individual research groups develop such tools for their own use. Progress would be faster with funding to improve the robustness, usability and compatibility of such tools. This would allow multiple research groups to use and contribute to a common set of tools. For example, an important design problem is that of binding sites for catalysts. Simulations of various groups of atoms around the target molecule could evaluate how well a design promotes a desired reaction. Directed evolution techniques could then find better designs, e.g., by making mutations and evaluating the results. Each mutation is an independent evaluation and hence readily evaluated in parallel.

Characterization

An important enabler of manufacturing is the ability to characterize products, thereby identifying any mismatch between the design specification and the actual product. For atomically precise products, this characterization requires tools that can determine the structure with atomic precision.

Current microscopy allows identifying the structure of some molecules and atomic positions on surfaces. Atomically precise manufacturing requires improved characterization tools that can handle complex, macroscopic products. Such tools could be expensive, thereby requiring funding to support access to these tools.

"Other challenges apart from adequate characterization for macroscopic products are inadequate funding and excessive administrative burdens"

Funding and administration

Currently, neither government nor private funders provide significant support for developing atomically precise manufacturing. For instance, Silicon Valley is eager to fund $100K startups to develop apps, but is less willing to fund the much larger costs of chemistry startups. Within large technology companies, investment in atomically precise manufacturing may lead to reduced profits from their current technology, adding financial risk to the already high technical risk of such projects.

The high administrative burdens associated with government grants and university governance wastes enormous amounts of researcher time. This is particularly challenging for starting new research in atomically precise manufacturing where significant results may take many years to achieve. In the meantime, the cost of administrative support can consume much of the already limited funding, thereby discouraging such research.

Approaches

Overcoming the barriers to atomically precise manufacturing requires funding. The workshop discussed several approaches to reach large-scale macroscopic atomically precise manufacturing. These involve identifying near-term demonstrations of steps toward this goal. Such demonstrations serve to focus attention on the manufacturing process in addition to specific products and reduce the risk for program managers considering funding the projects. The design and analysis of demonstrations will identify technical barriers to scaling up atomic precision, show which new advances funding agencies could support to address these barriers, and provide platforms for scaling to larger-scale production.

"To develop macroscopic APM: demonstrate initial steps, award prizes, educate thought leaders, APM initiative to extend the NNI."

Obtaining funding requires educating thought leaders within the scientific community, political decision makers, and those presenting science to the general public. Workshop participants explored approaches to this education process. As one example, groups developed short presentations for the next presidential science advisor. These presentations highlighted opportunities for investing in atomic precision through a new national technical initiative for atomically precise manufacturing. Other sessions explored the design of potential prizes and developed new R&D projects suggested by interdisciplinary discussions at the workshop.

Initiative for atomically precise manufacturing

For two decades, the National Nanotechnology Initiative (NNI) has provided funds for developing nanotechnology, focusing broadly on the control of matter at dimensions between approximately 1 and 100 nm. This initiative successfully advances capabilities at this scale. However, this work using current technologies is rapidly approaching its limits, e.g., as photolithography struggles to continue shrinking devices to below a few nanometers.

The NNI has not addressed the possibility of atomically precise manufacturing. With our improved tools for manipulating and imaging individual atoms, now is the time for creating a new initiative for R&D on pathways exploiting atomic precision, leading to both near-term payoffs and, in the longer-term, low-cost atomically precise manufacturing of macroscopic products. Defining this initiative requires distinguishing problems requiring atomic precision from other problems for which atomic precision is not necessary (even if involving nanomaterials). Educating researchers and program fund managers on this distinction is crucial to focus this initiative on the new opportunities of atomic precision.

While consensus on this opportunity is built on the federal level, an earlier alternative is an initiative funded at the state level. This could be similar to California's early funding of stem cell research or New York's funding of semiconductor technologies.

A diverse set of research groups and approaches may contribute to this initiative, including projects created by students. Enabling the broadest possible participation by these groups requires access to characterization tools whose cost is beyond the reach of small groups. Thus an initiative for atomic precision should support access to characterization tools hosted by larger institutions, e.g., national labs. Enabling broad participation will also motivate and educate students in this new area.

Prizes for significant steps toward atomically precise manufacturing

Prizes can motivate the development of new technology by rewarding significant accomplishments on the path toward that technology. Prizes also build public interest. Examples of such incentive or inducement prizes include the X Prizes and Foresight Institute's Feynman Grand Prize.

Designing incentive prizes for new technologies is challenging. The experience with the X Prizes suggests criteria such as:

- steps achievable in a few years,
- clear, specific goals,
- goals that could create a new industry rather than one-off demonstrations,
- a series of increasingly difficult goals building capability for successive prizes on the way to general-purpose high-throughput atomically precise manufacturing.

The prize incentive structure should match the interests and funding constraints of participants likely able to achieve the goal. Examples include winner-take-all prizes, prizes for multiple winners, or a sequence of increasingly ambitious prizes with increasing levels of prize money for groups who succeed with earlier steps.

Several prizes were proposed at the workshop, which are outlined in Prize Proposals.

Funding for research projects

Figure 14: Much basic research is government-funded. *Attribution: Wikimedia Commons*

In the past few decades, government agencies have been major funders of basic research. Unfortunately, the traditional proposal process focuses on relatively near-term projects with low risk. These criteria are difficult to satisfy for long-term projects that may lead to atomically precise manufacturing.

One alternative is private funding by high net worth individuals with interest in helping address major social problems, and funding development of technologies they see could address those problems. New online sources, such as Benefunder, help to match funders with researchers.

“One alternative to fund long-term, high-risk projects: private funding by high net worth individuals.”

New government initiatives can help researchers, particularly at small companies, identify and apply for funding within the government. An example is the Defense Innovation Unit Experimental (DIUx) program. Such programs can identify complementary strategic directions between commercial researchers and government agencies, rather than using funding to alter a company’s direction to meet different requirements of the funding agency.

Accessing these new sources of funding, as well as traditional sources, requires researchers to explain their projects in terms accessible to people outside their fields, including the general public. In particular, descriptions should explain:

Figure 15: A major obstacle towards atomically precise manufacturing is inadequate funding. Source: Wikimedia Commons

- What big problem does the research address?
- Why can’t other approaches address the problem?
- How does the proposed research address that problem?
- What are barriers to achieving the solution?
- How will the requested funding overcome the barriers?

Research projects and collaborations

During the workshop, participants explored several collaborative research projects applying atomically precise materials to the energy sector. After defining the project goal and approach, the discussion addressed the following questions:

- What aspect of energy does the project address?
- Why can’t current technology achieve the project goal?
- How could atomically precise manufacturing achieve the goal?
- What’s preventing development and deployment of this project? Particularly, identifying key roadblocks, such as building or characterizing individual devices in a lab, and scaling up from lab demonstrations to commercial use at reasonable cost.

- What's needed to achieve the project? This includes research skills, tools, funding and addressing regulatory constraints.

Technical Proposals (see above) describes these projects.

Next Steps

Education

Gaining support for atomically precise manufacturing requires educating decision-makers and their advisors on the scope of this opportunity, and how that differs from broader nanotechnology. These people include program managers at funding agencies, senior scientists (e.g., from the National Academies, national laboratories, universities and industry), policy advisors and professional societies such as AAAS, IEEE, APS and ACS. This education should also proactively engage regulatory agencies so they start considering the wide range of new products atomically precise manufacturing will produce.


Figure 16: Air pollution in Beijing. *Attribution: Wikimedia Commons*

Explaining the benefits of precise manufacturing in terms relevant to daily life is important to develop interest among the general public. These benefits include reducing pollution, lowering costs and creating new industries.

Foresight could play a major role in this process with workshops bringing together researchers and program managers at funding agencies. Such workshops could help researchers refine proposals for atomically precise manufacturing, facilitate collaborations, and build support in professional societies. Foresight could help spread the ideas by hosting a website for atomic precision resources, including summaries of these workshops. Foresight's background in policy implications of atomically precise manufacturing could help educate regulators and the legal community more generally, similar to ongoing workshops discussing regulatory issues related to the increasing use of robots, such as the WeRobot workshops (http://robots.law.miami.edu/2016/).

Research Strategy

Achieving atomically precise manufacturing requires developing a roadmap toward this goal. This roadmap could include a sequence of atomically precise demonstrations with increasing numbers of atoms. Ideally, these intermediate steps toward macroscopic atomic precision will themselves be commercially viable products to encourage their development by industry. The roadmap should also include tool development, to aid design and characterization of atomically precise products.

"Achieving atomically precise manufacturing requires developing a roadmap."

Collaborators with significant resources and commercialization experience could come from industries facing increasing difficulty with conventional manufacturing. These companies might fund development of atomically precise manufacturing for their products once they understand the opportunity. One example is the semiconductor industry, where current lithographic techniques are increasingly expensive and less effective as component sizes decrease below 10 nm. Another example is the energy industry, which faces increasing concern with environmental consequences of burning hydrocarbon fuels.

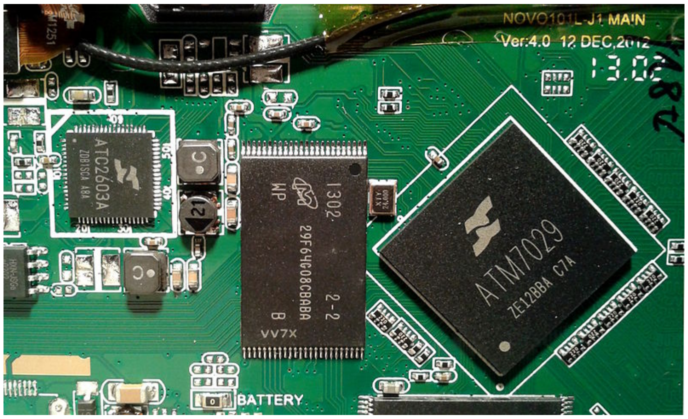

Figure 17: The semiconductor industry could be a major beneficiary of atomically precise manufacturing. *Attribution: Wikimedia Commons*

Standardization is important to quantify progress toward atomically precise manufacturing. We need metrics for partially precise materials, e.g., a fraction of atoms in a material that are correctly placed. Metrics could define precision according to a sequence of increasingly challenging criteria, such as having a specified number of atoms, then a specified position of each atom, and finally specified bonding of each atom with its neighbors. Widely understood metrics will not only demonstrate progress, but also help researchers and funding agencies focus on atomic precision.

Conclusion

"Atomically precise manufacturing would reduce the energy required to manufacture, transport and consume products"

Atomically precise manufacturing could significantly improve performance, efficiency and sustainability throughout the economy. This workshop focused on applications to energy production, transportation and use. Technical challenges and lack of scientific consensus are the major barriers to developing this manufacturing capability. These conclusions extend and solidify the preliminary evaluation of these applications at the 2014 Foresight Energy workshop.

Educating policy makers, demonstrating progress toward atomic precision, and identifying alternative funding for interdisciplinary projects could help create a major initiative to develop atomically precise manufacturing and realize its many benefits.

Participants

This list contains the names of all invited participants in alphabetical order.

Johan	Andreasson	Stanford Univ
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Cody	Geary	Caltech
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Tom	Nufert	Nanopolymer Systems
Gayle	Pergamit	Covalent / AguaVia
Cary	Pint	Vanderbilt Univ
Michael	Ross	UC Berkeley
Christian	Schafmeister	Temple University
Justin	Siegel	UC Davis
Michelle	Simmons	Univ of New South Wales
Volker	Schweikhard	Rice Univ
Dario	Stacchiola	Brookhaven Nat'l Lab
Isabell	Thomann	Rice Univ
Victoria	Vesna	UCLA
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Wei-Ren	Wang	Rice Univ
Stanley	Whittingham	NorthEast Cntr for Chem Energy Storage

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This workshop, documentation, and resulting projects wouldn't have been possible without our supporters.

Tad	**Hogg**	**Inst for Molec Manufacturing**
Gauri	**Vilash**	**Foothill College Nanotechnology**
Lori	**Luttrell**	**Molecular Biology**
Richard	**Nesbit**	**Bio Q Pharma**
Traci	**Parker**	**Launch Media Enterprises**
Tim	**Porter**	**NASA, ASL**
Wei-Ren	**Wang**	**Rice Univ**
Chris	**Sapyta**	**Menlo School**
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Roby	**Behrens**	**Lucid Productions**
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We’re united by a passion for future technologies and the drive to improve the state of the world.

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FORESIGHT
INSTITUTE

Appendix

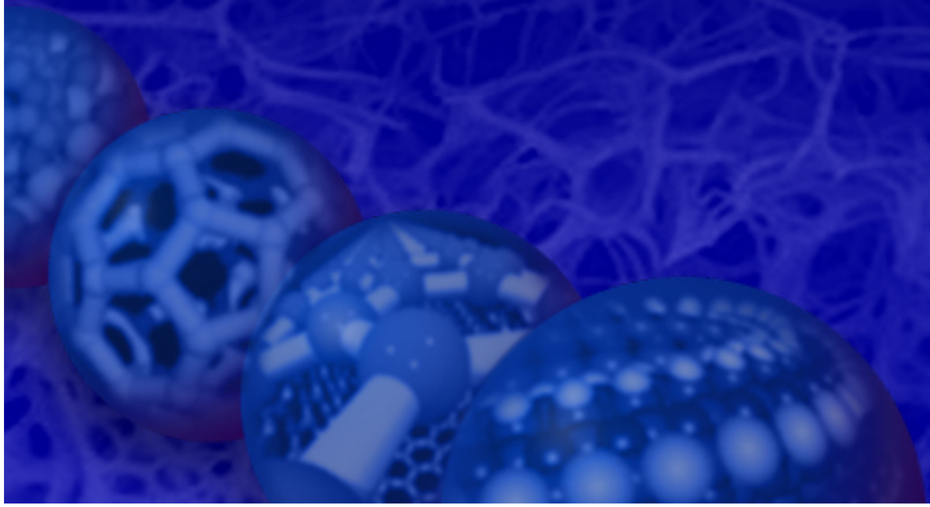
U.S. Department of Energy

Progress in Atomically Precise Manufacturing at the Advanced Manufacturing Office

David R. Forrest, Sc.D., PE, FASM

U.S. DEPARTMENT OF
ENERGY

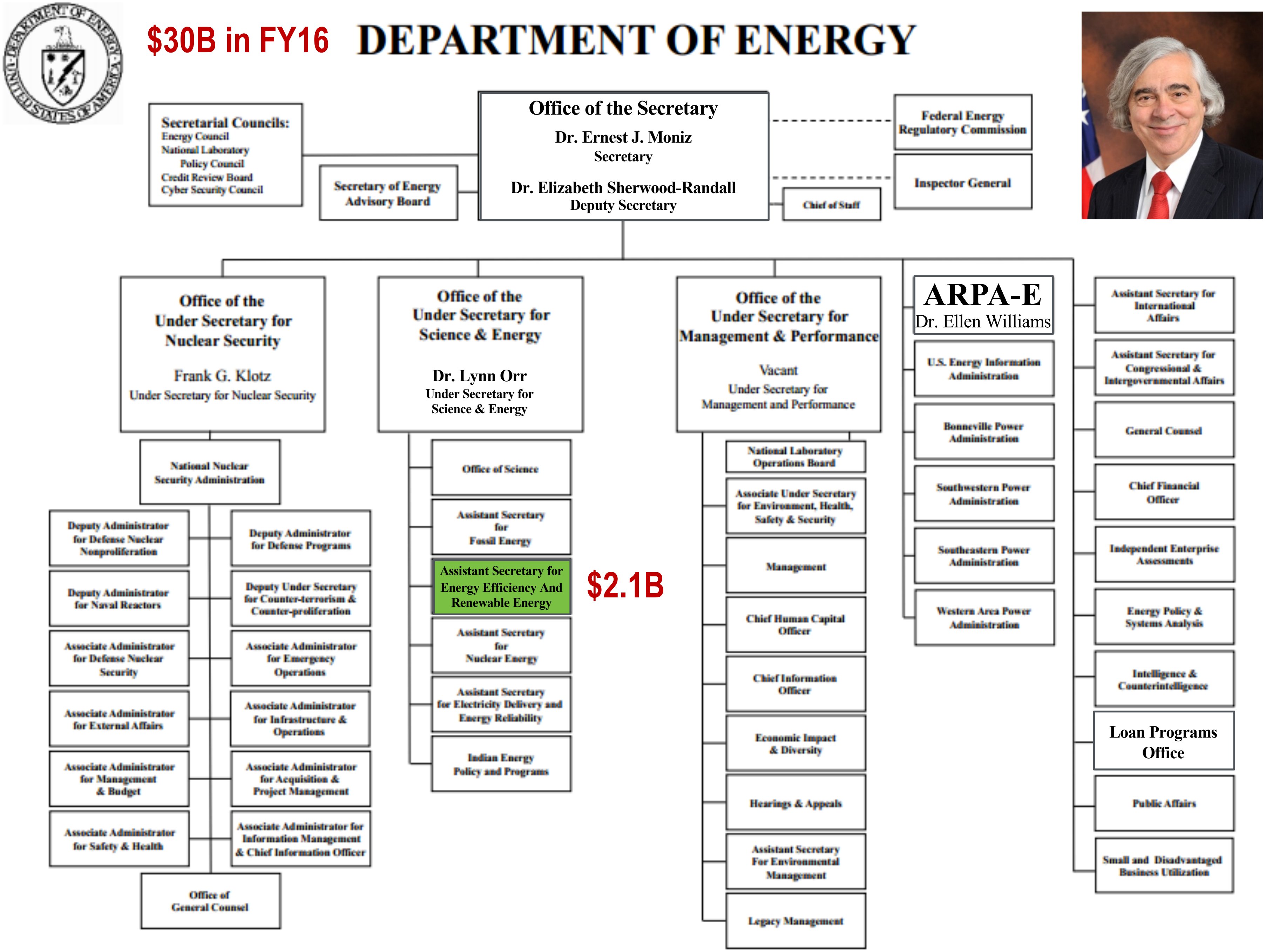
Progress in Atomically Precise Manufacturing at the Advanced Manufacturing Office



Outline

- About the Advanced Manufacturing Office
- Why are we interested?
- Specific programmatic efforts
- 2105 Berkeley Workshop on Integrated Nanosystems for Atomically Precise Manufacturing
- Some thoughts about ongoing challenges: changing the culture and mindset

DOE Organization Chart



$30B in FY16

DEPARTMENT OF ENERGY

Office of the Secretary
Dr. Ernest J. Moniz
Secretary
Dr. Elizabeth Sherwood-Randall
Deputy Secretary

Secretarial Councils:
- Energy Council
- National Laboratory Policy Council
- Credit Review Board
- Cyber Security Council

- Secretary of Energy Advisory Board
- Federal Energy Regulatory Commission
- Inspector General
- Chief of Staff

Office of the Under Secretary for Nuclear Security
Frank G. Klotz
Under Secretary for Nuclear Security

- National Nuclear Security Administration
  - Deputy Administrator for Defense Nuclear Nonproliferation
  - Deputy Administrator for Naval Reactors
  - Associate Administrator for Defense Nuclear Security
  - Associate Administrator for External Affairs
  - Associate Administrator for Management & Budget
  - Associate Administrator for Safety & Health
  - Deputy Administrator for Defense Programs
  - Deputy Under Secretary for Counter-terrorism & Counter-proliferation
  - Associate Administrator for Emergency Operations
  - Associate Administrator for Infrastructure & Operations
  - Associate Administrator for Acquisition & Project Management
  - Associate Administrator for Information Management & Chief Information Officer
  - Office of General Counsel

Office of the Under Secretary for Science & Energy
Dr. Lynn Orr
Under Secretary for Science & Energy

- Office of Science
- Assistant Secretary for Fossil Energy
- Assistant Secretary for Energy Efficiency And Renewable Energy
- Assistant Secretary for Nuclear Energy
- Assistant Secretary for Electricity Delivery and Energy Reliability
- Indian Energy Policy and Programs

$2.1B

Office of the Under Secretary for Management & Performance
Vacant
Under Secretary for Management and Performance

- National Laboratory Operations Board
- Associate Under Secretary for Environment, Health, Safety & Security
- Management
- Chief Human Capital Officer
- Chief Information Officer
- Economic Impact & Diversity
- Hearings & Appeals
- Assistant Secretary For Environmental Management
- Legacy Management

ARPA-E
Dr. Ellen Williams

- U.S. Energy Information Administration
- Bonneville Power Administration
- Southwestern Power Administration
- Southeastern Power Administration
- Western Area Power Administration

- Assistant Secretary for International Affairs
- Assistant Secretary for Congressional & Intergovernmental Affairs
- General Counsel
- Chief Financial Officer
- Independent Enterprise Assessments
- Energy Policy & Systems Analysis
- Intelligence & Counterintelligence
- Loan Programs Office
- Public Affairs
- Small and Disadvantaged Business Utilization

EERE Organization Chart

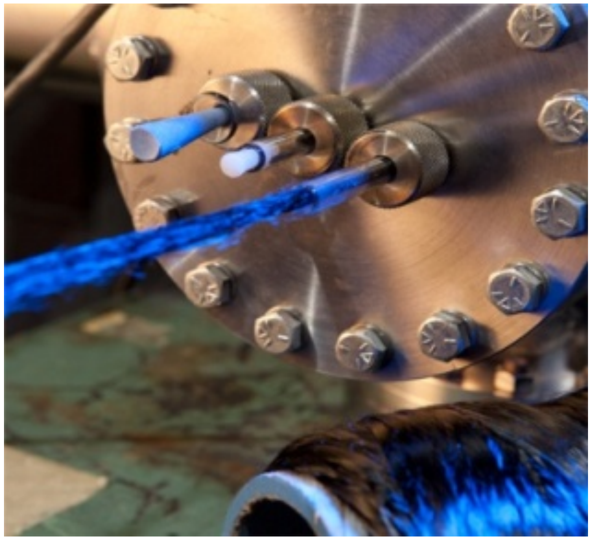
Assistant Secretary
David T. Danielson

Principal Deputy Assistant Secretary
Michael S. Carr

$2.1B

- **Energy Efficiency** Kathleen B. Hogan
  - **Building Technologies** Roland J. Risser
  - **Federal Energy Management** Timothy D. Unruh
  - **Advanced Manufacturing** Mark A. Johnson ($229M)
  - **Vehicle Technologies** Christy Cooper
  - **Weatherization & Intergovernmental** Anna M. Garcia
  - **Sustainability Performance** Jennifer C. MacDonald
- **Renewable Energy** Douglas W. Hollett
  - **Biomass Program** Valerie Sarisky-Reed (*Acting*)
  - **Fuel Cell Technologies** Sunita Satyapal
  - **Geothermal Technology** Douglas W. Hollett
  - **Solar Energy Technology** Minh Sy Le *(Acting)*
  - **Wind & Hydropower Technology** Jose R. Zayas
- **Business Operations** Merle L. Sykes
  - **Business Services** Derek Passarelli (*Acting*)
  - **Budget** A. Avon Meacham
  - **Information & Business Management** Douglas E. Kaempf
  - **Project Management & Evaluation** Scott E. Hine
  - **Golden Field Office** Carol J. Battershell
- **Strategic Programs** JoAnn Milliken (*Acting*)
  - **International Program** Robert L. Sandoli
  - **Analysis & Evaluation** (*Vacant*)
  - **Communications & Outreach** Karla Olsen
  - **Innovation & Deployment** JoAnn Milliken
  - **Legislative, Regulatory & Urban Affairs** Kerry C. Duggan

Advanced Manufacturing Office (AMO): Purpose



Carbon Fiber from Microwave Assisted Plasma (MAP)

Laser Processing for Additive Manufacturing

AMO's Purpose is to Increase U.S. Manufacturing Competitiveness through:

- ✓ **Manufacturing Efficiency - Broadly Applicable Technologies and Practices**
  - examples: Industrial motors, Combined heat and power (CHP), Industrial efficiency best practices.
- ✓ **Efficiency - Energy Intense Processes**
  - examples: Aluminum, Chemicals, Steel
- ✓ **Cross-cutting Innovations - Clean Energy Manufacturing Technologies**
  - examples: Wide-Bandgap semiconductors, Power electronics, Additive manufacturing, Advanced composites, Roll-to-roll processes, Digital manufacturing

Advanced Manufacturing Office (AMO): Structure

R&D Projects ($84M)

- Manufacturing Efficiency – Broadly Applicable
- Efficiency – for Energy Intense Processes
- Cross-cutting – for Clean Energy Manufacturing Technologies

R&D Facilities ($92.5M)

- Manufacturing Efficiency – Broadly Applicable
- Cross-cutting – for Clean Energy Manufacturing Technologies

Technical Assistance ($23.5M)

- Manufacturing Efficiency – Broadly Applicable

Programming in APM

Atomically Precise Manufacturing

the production of materials, structures, devices, and finished goods in a manner such that every atom is at its specified location relative to the other atoms, and in which there are no defects, missing atoms, extra atoms, or incorrect (impurity) atoms.

Integrated Nanosystems

Interconnected mechanical and electromechanical nanoscale devices and nanoscale structural components that operate together to perform a particular task under programmable control

Programming in APM: Strategic Goals

- Develop a suite of manufacturing technologies capable of building a broad range of atomically precise finished products (macroscopic)
- Transition to commercial practice:
  Will transform the U.S. manufacturing base to APM-centric production

Programming in APM: Why?

Materials, devices, and systems → properties and performance near their theoretical limits. Materials 10 X stronger, resulting in:

- Annual energy savings of greater than 50 quads/year
- Direct, clean production of finished goods from safe, inexpensive compounds
- Cars and aircraft weighing 90% less
- Single molecule switching for fast, low energy computers
- Quantum computers for complex problem solving (encryption/decryption)
- Low temperature catalysts for clean energy production of inexpensive fertilizers and fuels
- High efficiency membranes → Clean air and water

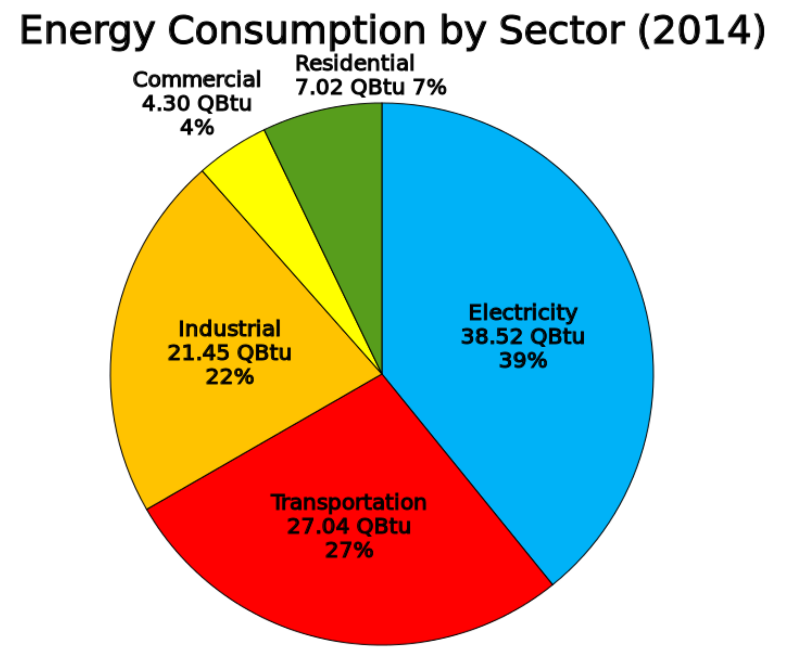
Programming in APM: Why?

To significantly improve the human condition

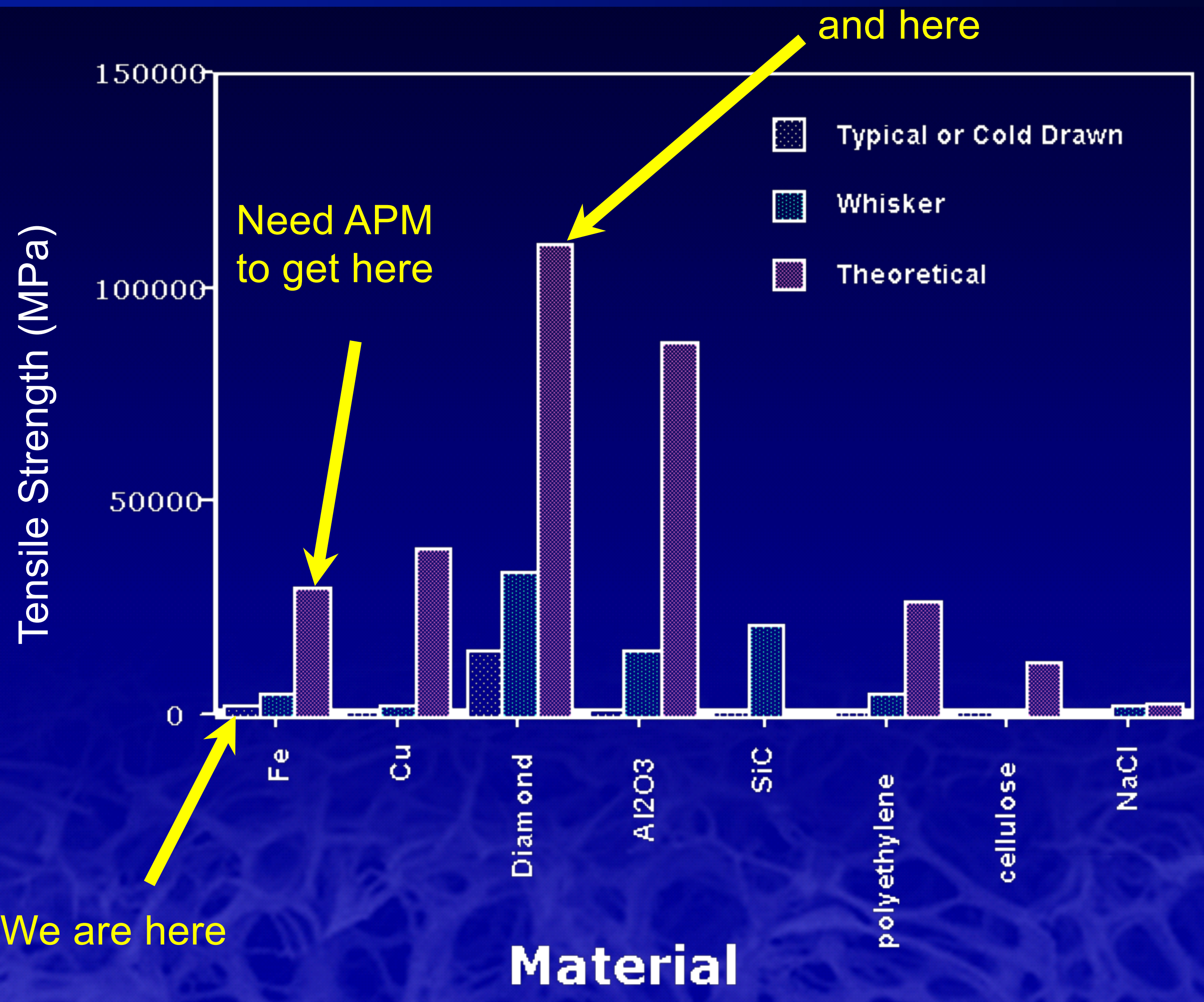
- Health
- Hunger
- Poverty
- Security

Mission-Centric Motivation
Reduction in Energy Consumption

- Lightweighting
  (90% weight reductions)
- Transportation:
  27 Quads down to 3 Quads
- Industrial processes
  (90% reduction in amount
  of material produced);
  21 Quads down to 2
- Less electricity needed for production
- Penalty for bandwidth gap: 50 Quads annually

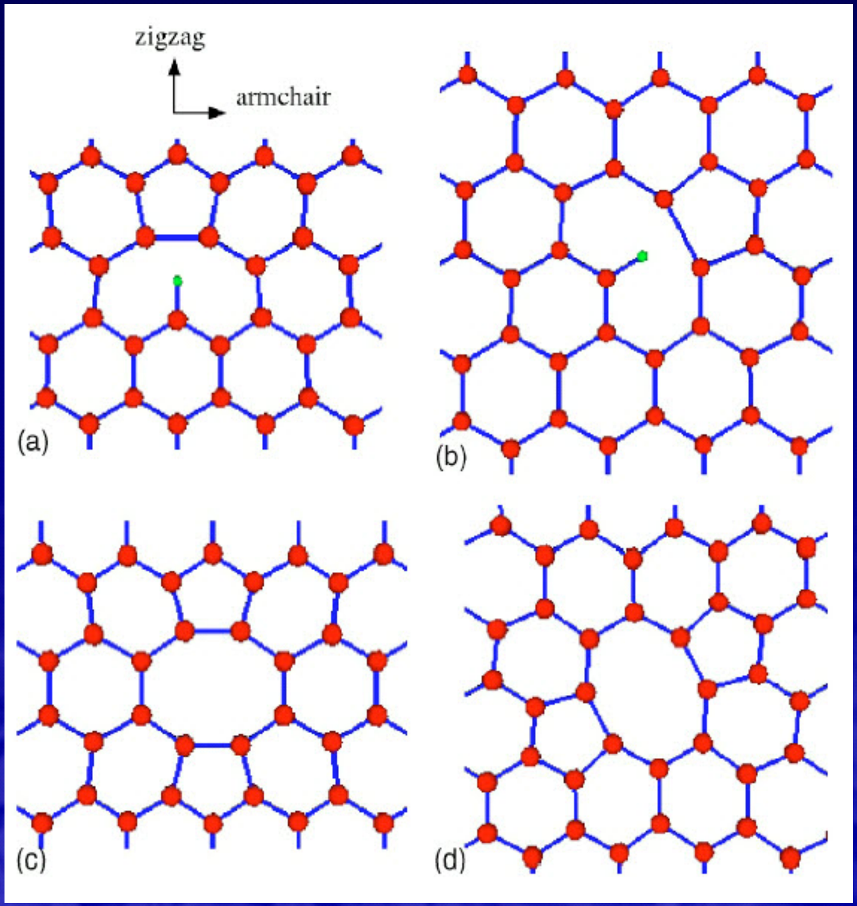


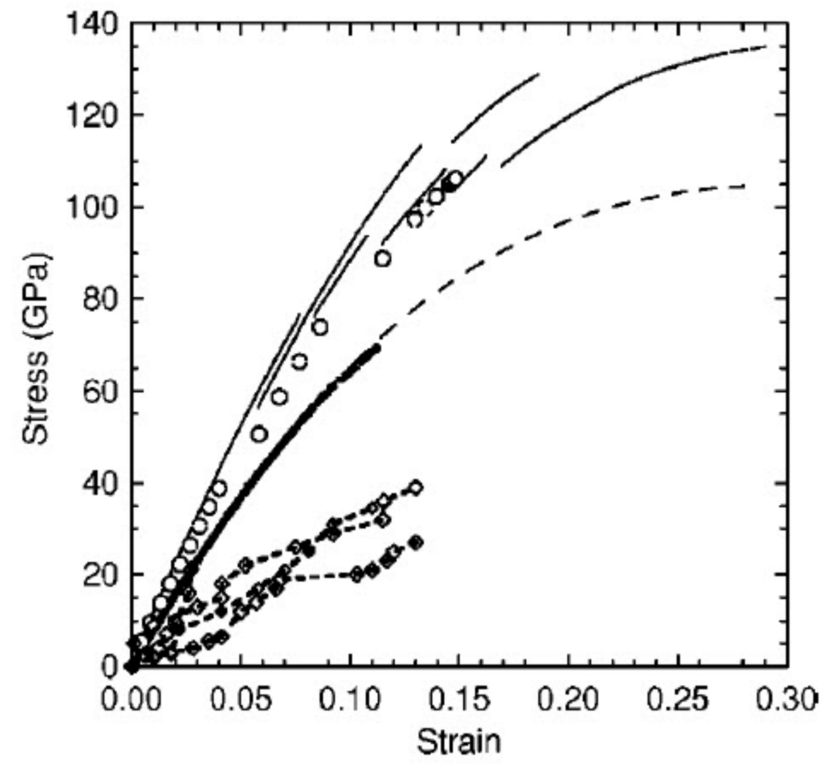
Strength Bandwidth



Example: Nanotube Lattice Defects

- Defects reduce strength of C nanotubes

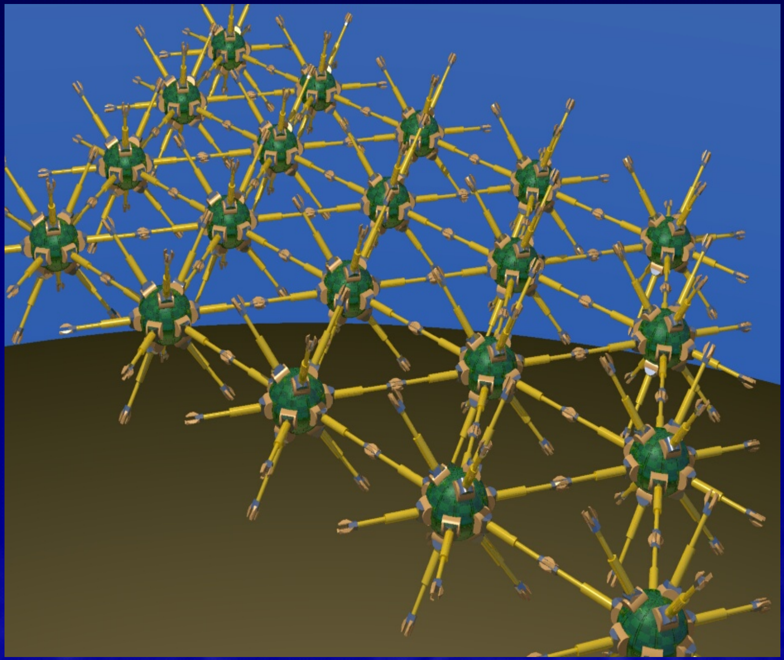




PHYSICAL REVIEW B **71**, 115403 (2005)

Lets you build materials like this

Rich integration of computers, sensors, and actuators → programmable materials



- Telescoping arms and nanoscale actuators could compensate for high (10%) elastic strains needed to achieve 10X strength
- Telescoping arms could accommodate large deformations and internal systems could reversibly store/dissipate energy

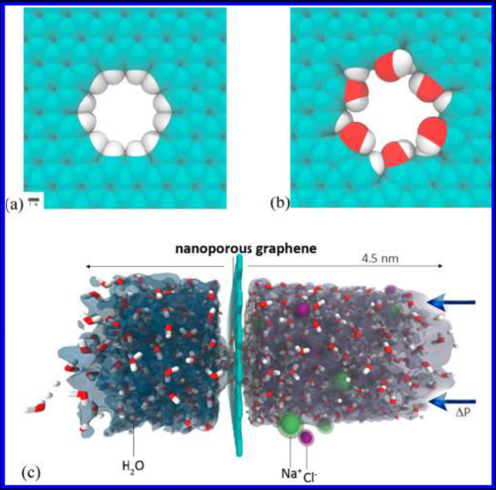
Strategy

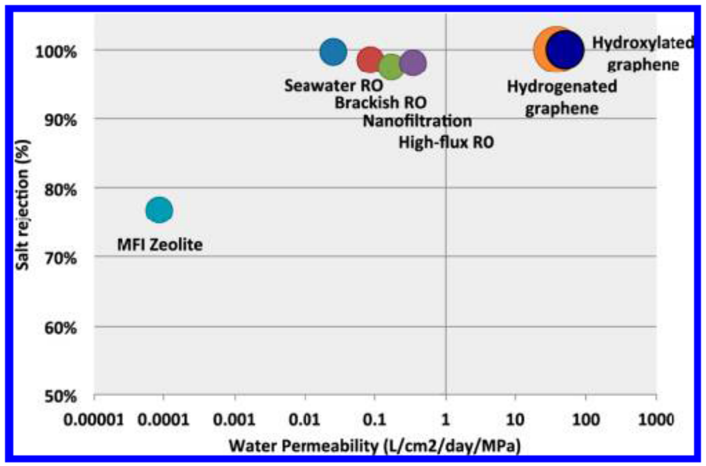
- Identify and provide funding for near term applications (SBIR, R&D Funding Opportunities)
- Develop and fund a long term program to advance the technologies for an integrated nanosystems approach
  - 2015 Workshop
  - 2016 Roadmap Framework
  - 2017^{+} Sustained roadmapping and (I hope) substantial funding program
- Engage National Laboratories leadership
- Engage NNI community (NNCO, face time at NSET)
- Engage Funding Agencies, OSTP
- Engage senior members of scientific community

We identified key near term applications

Membranes for separations,
e.g. desalination

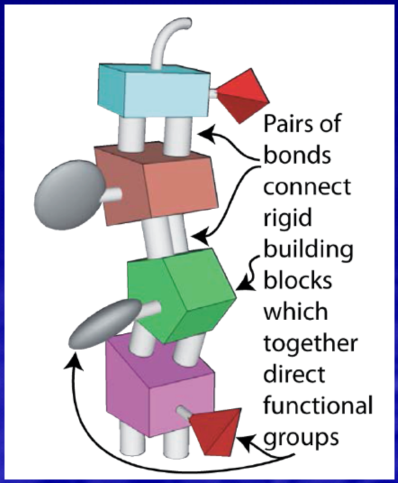
(MIT, Lockheed, Covalent)



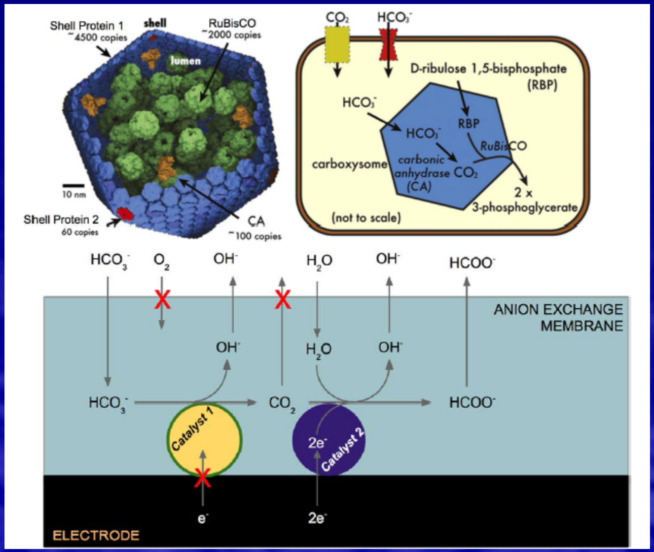


Catalysis,
e.g. $CO_2 \rightarrow CH_4$

(Schafmeister, Temple U.)



Pairs of bonds connect rigid building blocks which together direct functional groups

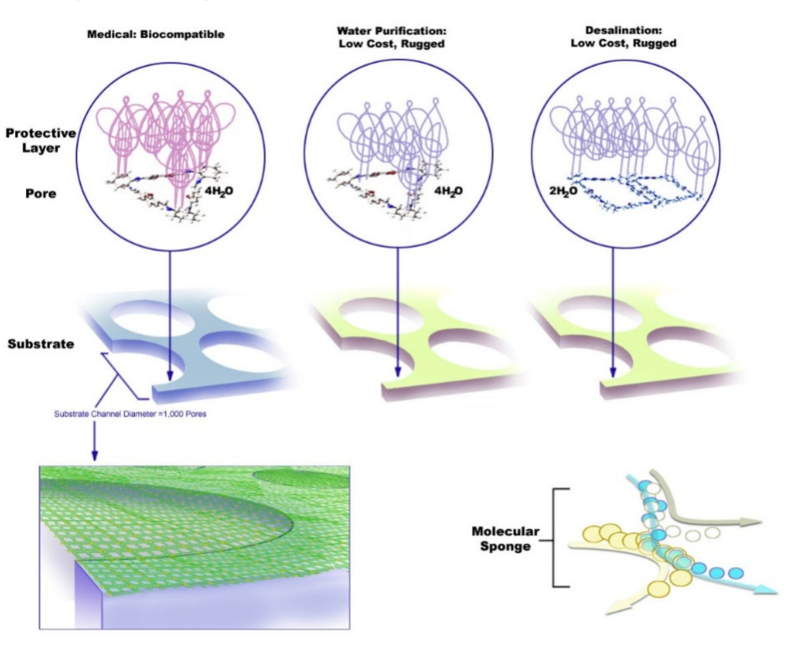


Funding to Support Near Term Applications

- SBIR FOA-0001164: Membranes $150k + $1M Phase II
- SBIR FOA-0001366: High selectivity [atomically precise] membranes, $1.5M
- SBIR FOA-0001417: Atomically Precise Structures and Devices for Catalysis $750k

Phase II SBIR: Covalent ($1M)

- Atomically flat membrane, one molecule thick
- Cross-linked, covalently-bound, ordered array
- Phase I: developed proof of concept for scalable manufacturing technique with Langmuir trough
- Atomically precise (molecular) pores were developed previously; to be integrated into membrane in Phase II
- 66% less energy than Reverse Osmosis, 50% less CAPEX and OPEX costs



Current Phase I's: High Precision or atomically precise membranes ($150k each)

Global Research & Development, Inc.	Water filtration membranes with built in continuous de-fouling
Techverse, Inc.	Novel Zeolite/polymer composite membrane
Mainstream Engineering Corporation	Membranes for highly selective separation and concentration of gasses
TDA Research, Inc.	Molecularly Precise Nanoporous Desalination Membranes
Luna Innovations Incorporated	CO2 Separation Membrane for Incipient Flue Gas
GRoWater Inc.	Development of Scalable Manufacturing Process for High-Selectivity Single-Layer Nanoporous Graphene Membranes
Novoreach Technologies LLC	Novel Nanoporous Inorganic Membranes for Energy Efficient Pervaporation Separation
Physical Sciences Inc.	2D Metal Organic Framework based Reverse Osmosis Membrane
HiFunda LLC	High Selectivity Gas Separation Membrane Assemblies
Compact Membrane Systems, Inc.	High Oxygen/Nitrogen Selectivity Membrane

Current Phase I's:
Atomically Precise Catalysts ($150k each)

Mainstream Engineering Corporation	Design and Synthesis of Bio-inspired Macromolecules Containing Atomically Precise Catalytic Active Sites
Sironix Renewables	Hierarchical Zeolite Catalysts for Renewable Surfactants Platform
Proton Energy Systems	Nitrogenase Inspired Peptide-Functionalized Catalysts for Efficient, Emission-Free Ammonia Production
TDA Research Inc.	Atomically Precise Catalysts for the Conversion of Glycerol to High Value Chemical Intermediates
BioHybrid Solutions	Rational Tailoring of Enzymes Stability and Performance via Polymer-Based Protein Engineering

Strategy

- Identify and provide funding for near term applications (SBIR, R&D Funding Opportunities)
- Develop and fund a long term program to advance the technologies for an integrated nanosystems approach
  - **2015 Workshop**
  - 2016 Roadmap Framework
  - 2017^{+} Sustained roadmapping and (I hope) substantial funding program
- Engage National Laboratories leadership
- Engage NNI community (NNCO, face time at NSET)
- Engage Funding Agencies, OSTP
- Engage senior members of scientific community

Workshop on Integrated Nanosystems for Atomically Precise Manufacturing

- 1-1/2 days, 5-6 August 2015, Berkeley, CA
- Attendees from industry, govt, academia
- Invited speakers:
  - Lloyd Whitman
  - Eric Drexler
  - Chris Schafmeister
  - Alex Zettl
  - Khershed Cooper
- Panel: Jim Tour, Paul Rothemund, John Randall, Olga Ovchinnikova

Key Stakeholders

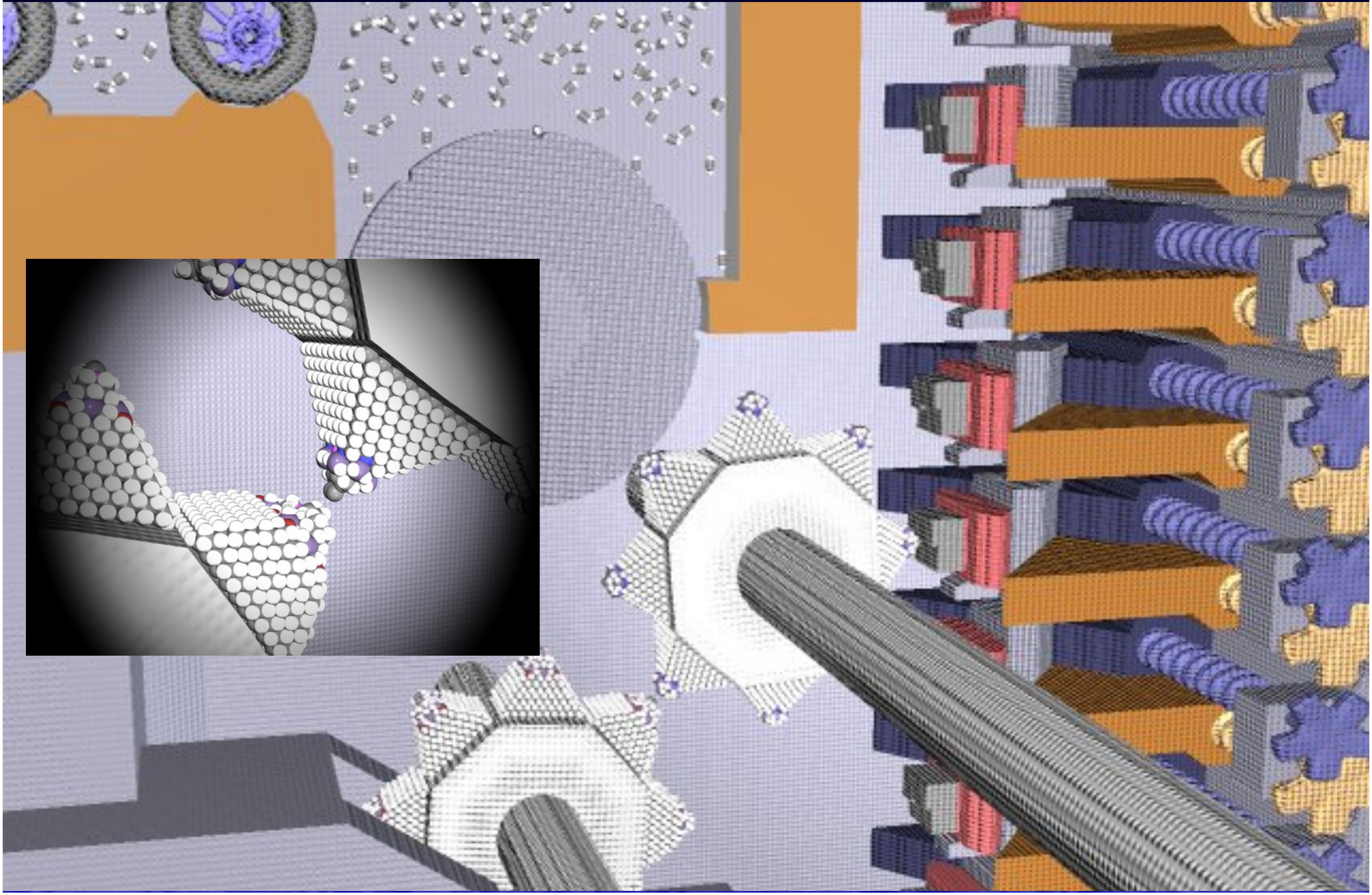
- Visionary Involvement
  - Eric Drexler/Oxford
  - Lloyd Whitman/OSTP
  - Kershed Cooper/NSF
- Technology Demonstration:
  - UC Berkeley (Alex Zettl)
  - Temple University (Chris Schafmeister)
- Research Institutions

  LBNL
  UC San Francisco
  California Institute of Technology
  Stanford University
  UC Riverside
  Rice University
  ORNL
  Batelle
- Private Sector
  - Zyvex Labs
  - Covalent, LLC

Why Integrated Nanosystems?

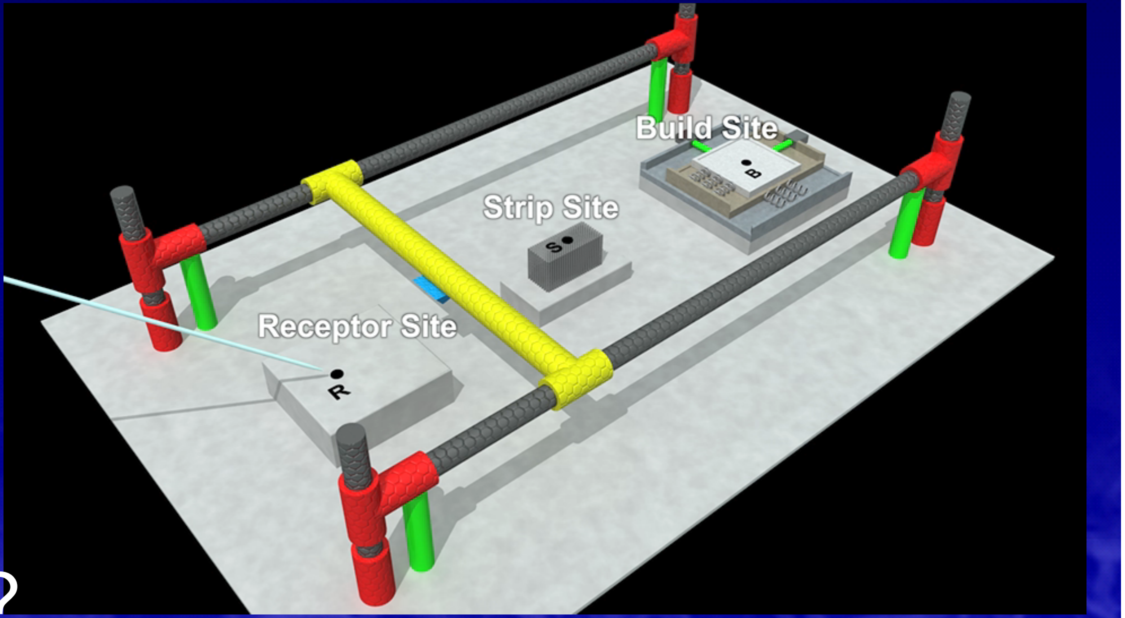
- Condensing matter from solution, vapor, or melt fundamentally cannot produce atomically precise structures.
- Left with self-assembly of atomically precise building blocks, or with positional assembly
- Compelling vision for a scalable high throughput system based on positional assembly presented by Drexler (Nanosystems (1991) and elsewhere)
- Recent advances point to a potential approach

Long Term: need manufacturing system with complete control of trajectories and orientations



Workshop on Integrated Nanosystems for Atomically Precise Manufacturing

Threw down gauntlet



Q: to achieve long term vision for atomically precise manufacturing should we build a simple demonstration machine?

What's needed to do this?

Why a demonstration nanosystem?

- Focus attention on an important technology space
- De-risk the concept for funding agencies
- Decisive step toward long term vision
- Design, analysis, and fabrication of nanosystems will show us:
  - Technical barriers
  - New advances needed
  - Provide platform for future scaling

DOE AMO Workshop Mission

Solicit feedback on developing integrated nanosystems for atomically precise manufacturing.
Identify barriers and needs to accelerate pathways for demonstration systems.

Industry Vision and Goals

5 Year Vision

- Integrated multicomponent systems
- Commercial binary devices
- Prototype catalytic positional assembly
- Concept development for medical, environmental, computing, energy, and other applications
- Improved functionality – assembly methods, speed, materials
- Improved measurement technologies

Goals to Achieve Vision

- Technology acceptance by scientific and public community
- Incentivize data publishing and open library of parts and toolkits for nanosystem community
- Open architecture-driven development to support collaboration
- Demonstrations to show scalability and applications

Top Barriers and Needs

Design

- Better design algorithms that combine top-down and bottom-up with focus on modularity, and in-situ scale diagnostics

Measurement

- microanalytic devices, real-time super resolution sensors/microscopy and probes, at scale

Demonstration

- Instrumented test bed for APM to measure progress

Fine Positional Control

- Ability to quickly and precisely position probes in three dimensions

Collaboration

- Government support and interconnection to outside world

Actionable Demonstration Approach

Team Sponsor and Institute

- Recognize current nanoscale community
- Broader industry informed (not just semiconductor)
- Parallel approaches (pick/place and self-assembly)

Scale

- Around $10 MM/year

Process

- Tool, protocol sharing

Outcome

- Demonstration process or product.
- Public benefits and risks identified

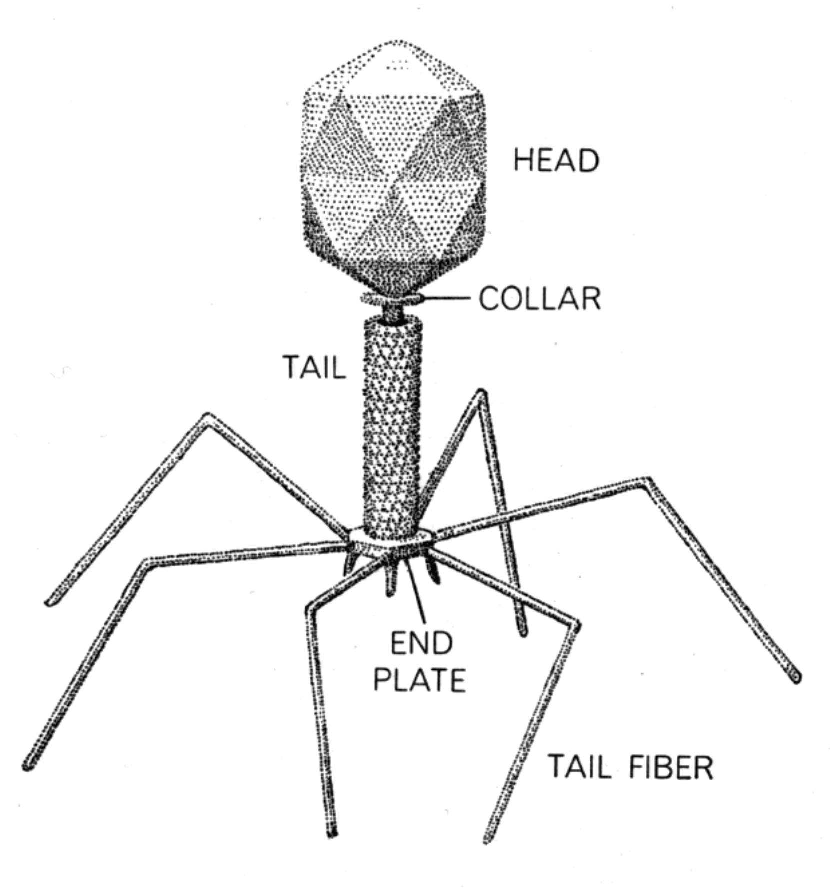
Milestones (3-5 years)

- Demonstrated APM building block, (100 nm precise).
- Current property performance improved x 5

Cultural Issues

- Yes, people still remember Smalley saying this is impossible
- Funding *matters: the minds of program managers*
- "Familiarity breeds contempt"
- No consensus on whether large atomically precise products are possible
- Basic lack of understanding in scientific community of what is atomically precise, and what is a nanosystem

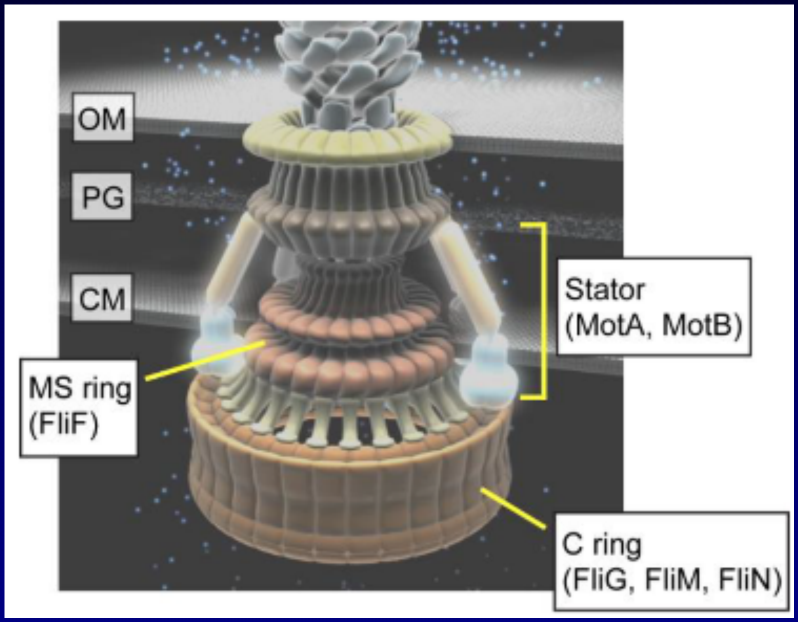
Basic lack of understanding: atomically precise, nanomachine



For example:

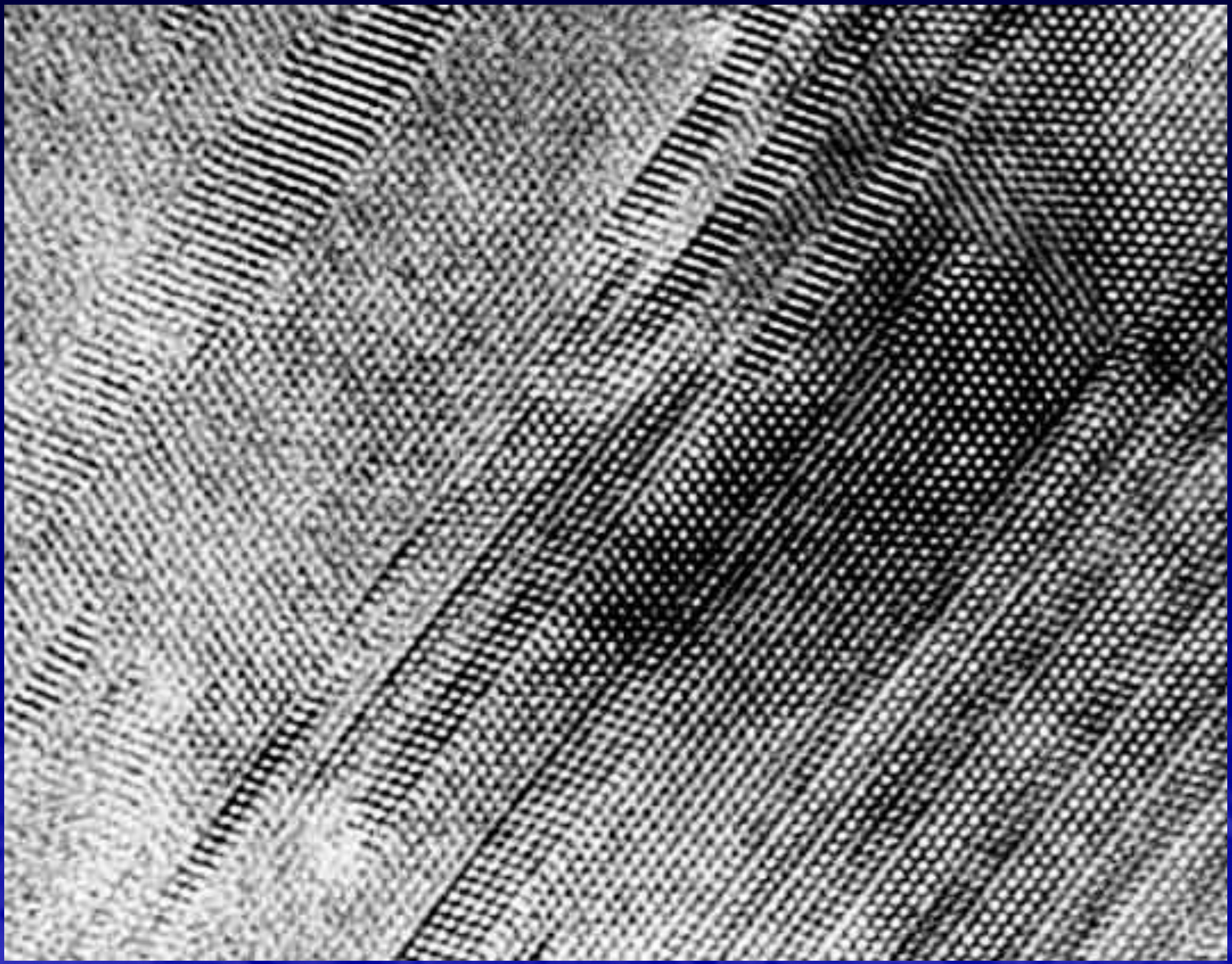
T4 phage is an atomically precise nanomachine

Bacterial Flagellar Motor is an atomically precise nanomachine

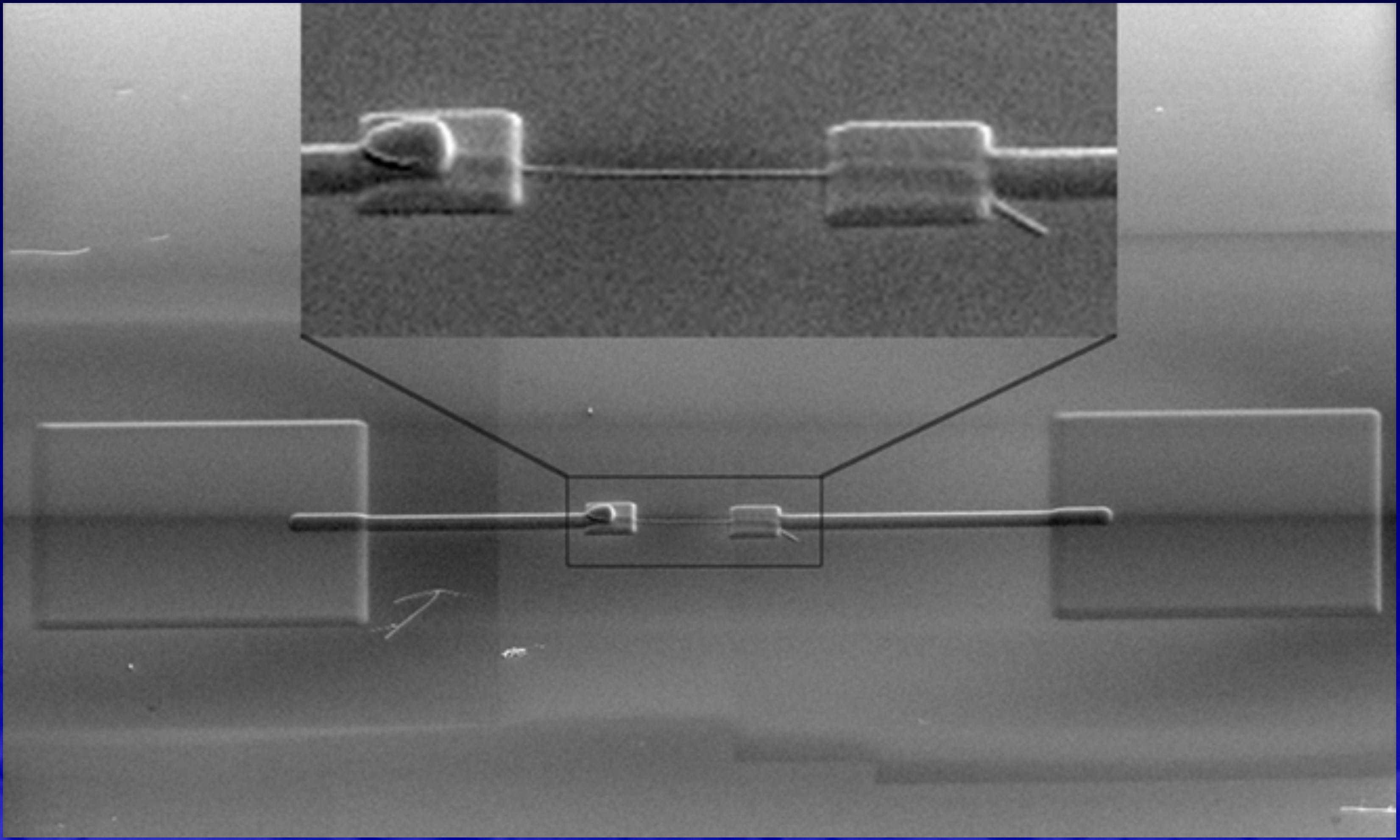


Driving Force	Proton or sodium gradient
Number of Protons per revolution	~ 1000
(energy per proton)	~ 2.5 x 10^{-20} J (6kT)
Maximum rotation rate	300 Hz (protons) 1700 Hz (sodium)
Torque at stall	~ 4 x 10^{-18} Nm
Maximum power output	~ 10^{-15} W
Efficiency	50-100% (stall) ~ 5% (swimming cell)
Number of steps per revolution	~ 50 per torque generator

Atomic Layer Deposition isn't atomically precise anything



Nanoelectronics



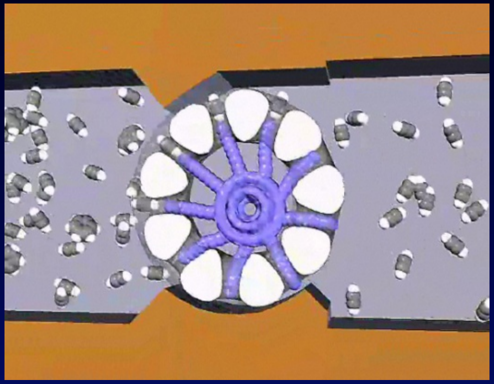
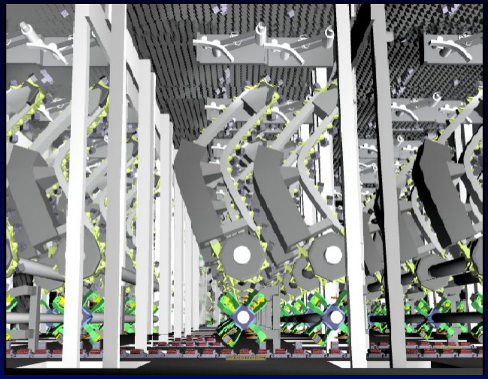
Foresight Mission is highly relevant

Much work is still needed on the education front!

Summary

- Explained AMO's mission for energy efficiency and cross-cutting manufacturing technologies
- Provided quantitative illustration of how APM is aligned with our mission in improving EE
- Articulated short and long term goals to develop APM
- Outlined strategy for accomplishing those goals
- Described $3.4M in funding efforts
- 2105 Berkeley Workshop on Integrated Nanosystems for Atomically Precise Manufacturing
- Some thoughts about ongoing challenges: changing the culture and mindset

U.S. DEPARTMENT OF ENERGY

Thank You