ERC White Paper

The Solar Opportunity

The Problem. Rising living standards of a growing world population will cause global energy consumption to increase significantly. Estimates indicate that energy consumption will increase at least two-fold, from our current burn rate of 12.8 TW in 2005 to 28 - 35 TW by 2050.[1-3] The current approach to energy supply, that of increased fossil fuel exploration coupled with energy conservation, is not scaleable to meet future demands. Moreover, external factors of economy, environment, and security dictate that this global energy need ultimately be met by renewable and sustainable sources from a carbon-neutral source.[1,4-8]

Where will this carbon-free energy come from, and how can it be produced and utilized in an environmentally sustainable fashion?

Sunlight is by far the most abundant global carbon-neutral energy resource. Solar has the significant advantages of wide distribution, it is the most environmentally sound energy source, and solar has the potential to meet the large scale energy needs of the future. More solar energy strikes the surface of the earth in one hour than is provided by all of the fossil energy consumed globally in a year. Sunlight may be used to power the planet by its conversion into electricity and chemical fuel. But there is a problem. A response to the "grand challenge" of using the sun as the future's energy source faces a daunting challenge - large expanses of *fundamental science and technology* await discovery for sunlight-based energy systems to be enabled and a robust *energy policy* must be developed that permits new solar technologies to be implemented in a competitive energy market.

Why an MIT Effort? The solar opportunity represents a high payoff direction with significant reward but there is no escape that the development of this energy source faces tremendous challenges and substantial breakthroughs are needed. Any viable solar energy conversion must result in a 6 fold decrease in the cost-to-efficiency ratio for the production of electricity and a 10-20 fold decrease stored *fuels* and must be stable and robust for a 20-30 year period. To reduce the cost of installed solar energy conversion systems from \$0.25 - 0.40/kW hr to \$0.02 - 0.10/kW hr, a cost level that would make them economically very attractive in today's energy market, will require truly revolutionary technologies that do not exist at the present time. With the current science and technology landscape for solar so wide open, and no obvious "silver bullet" solution to the problem on the horizon, a comprehensive program that tackles the solar energy problem on all fronts should be pursued. Key components of a solar program include:

---

[1] Hoffert, M. I.; Caldeira, K.; Jain, A. K.; Haites, E. F.; Harvey, L. D. D.; Potter, S. D.; Schlesinger, M. E.; Schneider, S. H.; Watts, R. G.; Wigley T. M. L.; Wuebbles, D. J. *Nature* **1998**, *395*, 881-884.

[2] Lewis, N. S. In *Energy and Transportation*; The National Academies Press: Washington, DC, 2003; pp 33-39.

[3] *World Energy Assessment Report: Energy and the Challenge of Sustainability*; United Nations Development Program; United Nations: New York, 2003.

[4] *Basic Research Needs for the Hydrogen Economy*; A Report from the Basic Energy Sciences Workshop on Hydrogen Production, Storage, and Use; U.S. Department of Energy: Washington, DC, 2003.

[5] *Basic Research Needs to Assure a Secure Energy Future*; A Report from the Basic Energy Sciences Advisory Committee; U.S. Department of Energy: Washington, DC, 2003.

[6] *Energy and National Security*; Karas, T. H.; Sandia Report SAND2003-3287, 2003.

[7] The Effect on the National Security of Imports of Crude Oil and Refined Petroleum Products; U.S. Department of Commerce, An Investigation Conducted Under Section 232 of the Trade Expansion Act of 1962, as Amended, November 1999, p. ES-9.

[8] Goodstein, D. *Out of Gas: The End of the Age of Oil;* Norton, New York, 2004.

(1) A comprehensive program in photovoltaics

- Manufacturing processes to make current semiconducting photovoltaics cheaper to produce
- Conceptually new photovoltaics should be explored based on photobiological, organic and inorganic materials
- Use of thermopower PV systems for chemical or electrical generation

(2) Solar photochemical methods for fuel storage

- New catalysts are needed that can be integrated with solar PVs to effect water splitting directly or via the water gas shift reaction
- Assessment and implementation of photobiological methods for fuel forming reactions such as a “Hydrogen-Bug”

(3) An energy policy program that is a guidepost to science and technology efforts.

- Assessment of the viability and strategies for implementation of various technologies that are being developed for short- and long-term energy markets
- Market and economic evaluation of short- and long-term impact of new science and technology discoveries

The above program requires strong efforts in science, engineering and policy and requires a partnership of knowledge among scientists spanning a range of disciplines of chemistry, materials science, physics, biology, mechanical and chemical engineering and economics. All sectors are well-represented at MIT. Working in concert, we believe that there is a high probability that MIT can make a major contribution in the development of solar power for the future global energy needs.

A Proposed Initiative. This white paper seeks to provide a roadmap to produce the underlying science, technology and attendant economic policy needed to permit future generations to use the sun as a renewable and sustainable energy source and to advance the time at which this is realized on a large scale.

1. Photovolatics. To achieve low solar (electrical or chemical) cost to power ratios, at least four approaches are possible. These are presented from the most technology intensive endeavors (1.1) to the most basic research intensive endeavors.

1.1. A focus on crystalline silicon as the substrate material is warranted owing to its abundance, high efficiency, environmental stability and huge technology base in both PV and microelectronics. Current and new manufacturing technologies of crystalline silicon for low cost solar cells should be a study focus of engineering science at MIT. Several issues need to be addressed including an understanding of the factors limiting carrier lifetime (the parameter controlling efficiency) over the full range of PV substrates. The effect of manufacturing methods on PV performance need to be defined with in-line measurements and PV performance enhanced with process control. Key process technologies critical to PV manufacturing should be explored in the areas of: metallization, passivation and defect engineering; the development of novel, high lifetime substrate technologies that allows for totally continuous processing through cell making; and new approach to the glass superstrate that eliminates the need for aluminum framing and eases the demands on interconnection.

1.2. The development of new chemical and materials methods to make polycrystalline and nanocrystalline semiconductors perform as if they were expensive single crystals. Numerous research approaches should be pursued. Some of these include: Nano-structured PVs. Materials consisting of a network of interpenetrating regions can facilitate effective charge separation and collection, thus relaxing the usual constraint in which the photogenerated carriers exist long enough to traverse the entire distance of the cell. Multiple bandgap PVs of nontraditional materials. Present photon conversion devices based on a single bandgap absorber, including semiconductor photovoltaics, have a theoretical thermodynamic conversion efficiency of 32% in unconcentrated sunlight, but the conversion efficiency can be increased, in principle, to 45 - 65% if carrier thermalization can be prevented (overcome the Shockley-Queissner limit). Multiple bandgap absorbers in a cascaded junction configuration can result in high photoconversion efficiencies, particularly when cells are designed to sustain the operating conditions (e.g. elevated temperatures) associated with highly concentrated sunlight. It is expected that mature high concentration PV systems can provide 10%-20% more energy than standard PV systems with the same installed power rating.

1.3. In addition to making evolutionary changes to existing PV technologies, an aggressive high risk program is needed to develop nascent technologies based on inorganic, organic and photobiological PVs. Building upon recent success in developing record efficient molecular organic PVs and the recent advances in the controlled assembly of hybrid organic/inorganic nanostructures, organic and hybrid PV cells could possibly exceed 10% power conversion efficiency, while offering a potentially inexpensive manufacturing paradigm (e.g. casting from emulsions, printing, and use of flexible substrates for production of large area, thin film cells). To guide the PV nanostructure assembly, biologically derived and genetically engineered systems can be used to control crystal structure, phase, orientation and nanostructural regularity of inorganic materials. Genetically modified photosynthetic complexes from plants and bacteria can also convert incident light into photocurrent. Although the present power conversion efficiencies are low, the projected maximum reaches 40%. Finally, the SQ limit discussed in Section 1.2 may be overcome by utilizing multilayer junctions of semiconductor quantum dots, quantum wells and related nanostructures, and new inorganic materials and photoassemblies. Such materials could channel the excess energy of electron/hole pairs into photovoltages and photocurrents, with the design guided by refined detailed understanding photon absorption, charge creation and charge separation processes.

1.4. Thermophotovoltaic (TPV) power generation mimics solar PV as it directs the low-energy photons of radiative thermal heat sources to low-bandgap PV cells to generate electricity. The radiation emitter can be heated to 1000-2000 ^{o}C by fuel combustion or by concentrated solar radiation. Potential TPV applications are many: in hybrid vehicles, in central utilities for increased fossil fuel plant efficiency, and for home furnaces. With an appropriate thermal storage scheme TPVs in conjunction with solid state thermoelectric (TE) materials could provide a 24-hour source of power. Thermoelectrics produce electricity from lattice vibrations (phonons) generated by heat sources. Recent theories and experimental results suggest significant improvement in nano-designed TE material sets. Consequently, TE materials research coupled with deeper understanding of electron and phonon transport mechanisms is expected to yield TE conversion efficiency of up to 35%.

2. Solar Photochemical. Solar energy is intermittent and must be stored and dispatched to be useful on a large scale, thus chemical fuels must be produced to provide a useable primary energy system from this intermittent source. To do this, several basic chemistry, (bio-) engineering, materials and theory problems need to be addressed:

2.1. The activation and use of small molecules of energy consequence, including H_2, H_2O and O_2, CO_2, N_2 and CH_4. Their study involves the synthesis of new compounds/catalysts and the experimental kinetics describing the mechanism of activation. These catalysts can be interfaced with PVs for fuel forming reactions. In addition, work in this area will also find utility in a parallel fuel cell initiative, if one is developed.

2.2. Overarching multi-body theories to describe the basic mechanistic commonalities that lie at the root of small molecule activation with a predictive power akin to that of Marcus theory for one-electron transfer reactions. Some of the theory topic areas for small molecule activation are: *multielectron* processes in which *electron and proton inventories* are involved and *atoms* are *transferred* during *bond making/breaking processes*.

2.3. The synthesis of new semiconductor nanocrystals containing p-n, homo-, and heterojunctions and their study for light-driven charge separation and the development of novel methods for compartmentalizing oxidizing and reducing sites by nanostructure design, and of nanoscale pore architectures that steer reaction intermediates to desired fuel products.

2.4. The fundamental mechanisms of ion/electron transfer at solid/solid and solid/gas interfaces are not known. A detailed understanding developed for reactions on the molecular level will need to be translated to surfaces of photovoltaics and/or solids of photoassemblies. In addition, this same knowledge is needed in the engineering of fuel cell and some energy storage (e.g., batteries) initiatives. Hence, this fundamental science can cross several energy initiatives at MIT.

2.5. Active sites of biological catalysts of energy consequence such as hydrogenases, oxygenases and photosynthesis and functional model systems based on these clues from nature as to desirable catalyst motifs. Catalyst design can rely on a strong structural biology effort at MIT. Stepping beyond biology as a framework for energy conversion, the fusion of fuel forming biosystems with various photosynthetic apparatus is a promising line of research. Some ideas include fusing hydrogenase enzymes with Photosystems I and II for the generation of a “Hydrogen Bug”. Also, the genetic engineering of photosynthetic systems for direct fuel forming processes is an intriguing line of future research.

3. Energy Policy. Accelerated development and deployment of advanced solar technologies calls for innovative policy instruments that stimulate innovation and align with industry organization along the supply chain. Significant interventions have been made in Japan and Germany:

- In Japan, a government-led roadmap for PV is highly detailed, with the overall goal to achieve 50% of residential power supply from PV by 2030. It is built upon the particular strengths of Japanese industry and has a scope encompassing the entire PV supply chain. In addition, the government is both developing the market and encouraging capacity additions through financial incentives. The combined impact of these policies has been impressive, with Japan producing more than 50% of global solar cells/modules, generating impressive financial returns, and having the largest installed base.
- In Germany, the government requires that utilities pay a large subsidy to residential households that install and generate solar power, with the costs distributed over the ratepayer base. The government also provides significant support for R&D. Germany surpassed Japan in 2004 as a market for new installations.

While these public subsidies have clearly had the intended effect of stimulating deployment, it is far from clear how long such approaches can be sustained and whether they will lead to the desired long-term outcome of very large scale deployment of cost-competitive technologies. In the US, policy with respect to solar power development and deployment has been inconsistent and occasionally counterproductive. A fresh look is needed that brings together RD&D policy, technology and innovation policy, and the economics and management of technical change.

Needs. Assessment of expertise at MIT:

1. Direct PVs

1.1. Strong with cadre of engineers that could undertake this task as long as sufficient funds are provided to stimulate an effort. MIT already boasts connection to leading efforts in the PV manufacturing area.

1.2. Strong faculty presence in PV measurement. A limited expertise of integrating nanoscience with PV design. However, there is enough related expertise in PVs, organic and hybrid organic/inorganic nanostructured materials and crystals at MIT that sufficient funding should catalyze an effort on campus with current faculty members driving such an initiative.

1.3. On the design side of new materials, MIT has a critical mass of expertise in making and measuring of organic PVs. Also we have adequate expertise to pursue bio-engineered PVs. A related effort on light capture in photonic band gap structures can be exploited to facilitate the design of high cross-section PVs and TPVs. Conversely, excepting some related metal oxide work, MIT has no strong effort in design of novel inorganic materials and nanostructures for PV applications and catalysis (e.g., tandem nanostructures, Grätzel cells, inorganic oxide photoassemblies). *Need faculty hire spanning disciplines of inorganic chemistry, chemical engineering and materials science.*

1.4. MIT strongly positioned in TPVs with currently a strong and organized effort as a result of recent proposal to NSF on the subject.

2. Solar Photochemical.

2.1. Strong effort in chemistry with recent successes on the photocatalytic production of hydrogen, catalytic CO_2 and N_2 reductions. There is also ongoing work on water splitting to H_2 and O_2 and CH_4 oxidation catalysis. *The faculty position proposed in Section 1.3 will be essential to this group of scientists for the development of integrated PV/catalyst systems for fuel forming processes.*

2.2. The MIT theory community spanning chemistry, physics and several departments in engineering is formidable. Money is needed to stimulate faculty interest to take up energy problems in this section and research described in Section 1.

2.3. The hire in Section 1.3 should complement the present campus efforts in design of new PV architectures.

2.4. MIT is weak in heterogeneous mechanisms and catalysis. This area of expertise, which was heavily present in Chemical Engineering years ago, has subsequently been lost. A single effort in chemistry presently exists that might be capitalized on. *A faculty hire is needed here, spanning chemistry, chemical engineering and materials science.*

2.5. MIT is very deficient in photobiological energy efforts. We do have strength in structural biology of systems of energy consequence and a small base of expertise in areas tangential to photobiology and bioenergy. Efforts of note are work on carbon metabolism pathways in cyanobacteria, genetic codes of unusual photosynthetic systems and experience with diverse microbes that transform energy in novel ways. Generally, however, MIT's overall effort in bioenergy systems is weak, especially for projects that rely on the development of conceptually new bioenergy systems. *A key hire in bio-engineered photobiological systems (e.g., H_2 producing algae) to augment these efforts would be appropriate spanning environmental engineering, bioengineering and biology.* Side note: biomass energy conversion might be considered as a possible research subject in this white paper. However, MIT is so deficient in the areas of photosynthesis and bioenergy research, that a few key faculty hires would unlikely make the Institute competitive in the fundamental science of biomass conversion (e.g., genetically engineered plants, etc.). So biomass conversion was not included in the current version of this white paper; it might be developed as part of this effort if there is an engineering cohort at the Institute that would be interested in developing a subgroup in this area of research.

3. Energy Policy

There is already a faculty group, working with an ESD doctoral student, bringing together expertise in RD&D policy, PV manufacturing and technology, and the management of technology innovation for research and analysis on the introduction of solar power at large scale.

Financial support. The above program comprises 20 faculty members. A simple calculation of minimally 60 graduate students and 20 postdocs, to support the faculty size effort, translates to ~ 7.5 - 10 million per year.

Governance/Organizational Structure. The development of separate space that fragments groups of individual faculty members is not desirable. Research programs benefit from a cohesive structure and a local MIT lab culture should be maintained. What is needed is a dynamic governance system that brings together the different solar research/policy efforts. More generally, the proposed effort would benefit from a coordinated directorate/structure that unites the different MIT energy efforts.