NANOTECHNOLOGY FOR SUSTAINABLE ENERGY

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ABSTRACT

Nanotechnology and its applications have captured a worldwide market. Nanomaterials that have been developed using this technology can be incorporated into the devices so that renewable energy can be converted or generated more efficiently. Nanomaterials have the potential to change the way we generate, deliver and use energy.

Hydrogen cells are used in auto industry as a viable power source. Compressed hydrogen tanks are used to supply Hydrogen, and Oxygen is used from the air directly. There is no pollution caused by hydrogen fuel cell autos since the only emission is water.

Organic dyes (dye sensitizers), which are sensitive to light, can absorb a broader range of the sun's spectrum. A dye-sensitized solar cell has three primary parts. On top is a transparent anode made of fluoride-doped tin dioxide (SnO_2:F) deposited on the back typically of a glass plate. On the back of this conductive plate is a thin layer of titanium dioxide (TiO_2), which forms into a highly nanoporous structure with an extremely large surface-area. After soaking the film in the dye solution, a thin layer of the dye is left covalently bonded to the surface of the TiO_2.

Computational material science and nanoscience can play many critical roles in renewable energy research. These include: finding the right materials for hydrogen storage; finding the most reliable and efficient catalyst for water dissociation in hydrogen production; finding a cheap, environmentally benign, and stable material for efficient solar cell applications; and understanding the photo-electron process in a nanosystem, and hence helping design efficient nanostructure solar cells.

Keywords: *Sustainable energy, Nanotechnology, Hydrogen cell, Dye solar cell, Computational nano sciences for renewable energy.*

1. INTRODUCTION

In today's world economy, acquiring reliable, efficient, pollution free, abundant energy is a major challenge. Major energy needs for economic development pertain to transportation, residential and commercial sectors. The World is heavily dependent on the non-renewable resources for our energy needs. Not only will these resources deplete over time, but they are also the major source of pollution, which is another key issue faced by the world economy. To address these challenges, there is a need to devise new technology that helps in reducing the problems and improving the economy.

With the advancement of S&T in the modern world, technology has been reduced and compressed to a nano-scale – to the order of 10^{-9} – in various applications.

Growing energy needs of the world call for increased measures to conserve energy, as well as to optimally utilize the alternative energy resources. This would not only reduce total dependence on fast-depleting fossil-fuels (oil, coal, gas, etc), but will also reduce the toll they take on environment in the form of green house gas emissions. Hence, the use of renewable energy resources (solar, hydro and wind) needs to be encouraged due to their economical viability, environment-friendliness and long-term availability.

2. THE ENERGY RESOURCES OF EARTH

Most of the energy currently used in the world comes from non-renewable sources. Disappointingly, the contribution of solar and wind energy has been very small, even lesser than geothermal. Most of the renewable energy comes from hydro-electric plants and some from biomass.

Increasing efforts and aspirations of the developing countries to come at par with the developed parts of the world in terms of socio-economic growth have resulted in increased energy demands. Figure-1 shows the uneven distribution of energy utilization rate throughout the world. It shows that 72 % of the world population uses less than 2 kW/capita, whereas 6 % of the population uses more than 7 kW/capita (Aldo, 2005).

There is a reasonable correlation between the total energy utilization rate of a country and its corresponding annual gross national production. About 2.2 W are used per dollar of yearly GNP. Thus, to generate each dollar, 69 MJ are needed. These figures, which are based on 1980 dollar rates, vary with time, owing partially to the devaluation of the currency, and partially due to changing economic circumstances. In fact, it has been demonstrated that during an energy crisis, the number of mega joules per dollar decreases, while the opposite trend occurs

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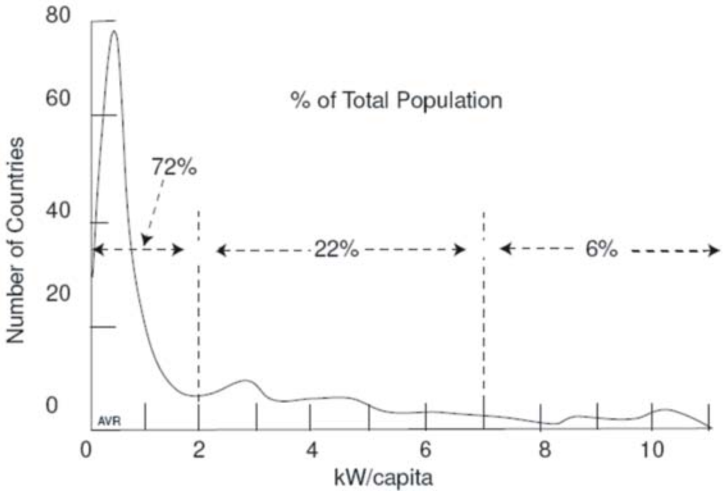


Figure-1: Most Countries use Little Energy Per Capita while a few Developed Ones Use a Lot. (Aldo, 2005)

during financial crises.

Further industrialization of the developed countries may not necessarily translate into an increase of the per capita energy utilization rate; the trend towards higher efficiency in energy use may have a compensating effect. Technological innovation has resulted in more efficient use of energy. Examples of this include better insulation in houses and better mileage in cars. Alternate energy sources have somewhat alleviated the demand of fossil fuels. Such is the case of using ethanol from sugarcane for the propulsion of automobiles. It is possible that the development of fusion reactors will, one day, bring back the times of abundant energy.

Introduction of a more efficient device does not immediately result in energy economy because it takes a considerable time for a new device to be widely accepted. The reaction time of the economy tends to be long. For example, in case of a privately owned fleet of cars, a sudden rise in gasoline price has little effect on travel, but it increases the demand for fuel-efficiency. However, car owners do not rush to buy new vehicles while their old ones are still usable. Thus, the overall fuel-consumption will only drop many years later, after a significant fraction of the fleet has been updated. Large investments in obsolete technologies substantially delay the introduction of more desirable and efficient systems. A feeling for the time constants involved can be obtained from the study of the market penetration function.

If, in 2050, all the estimated 11 billion inhabitants of Earth were to use energy at the present day USA level (11 kW/capita), the world energy utilization rate would reach 122 TW, which is a 16-fold increase over the present 7.6 TW. Such a rate is probably one order of magnitude higher than can be supplied unless fusion energy becomes practical and inexpensive.

3. EMERGING TECHNOLOGY

To identify and conserve the new renewable sources, many countries are trying hard to develop new projects to harness the new renewable forms of energy. Nanomaterials and hydrogen fuel cells have the advantage of being smaller and portable. Therefore, they have many more applications.

Today, solar cell technology is in limited use due to the relatively high manufacturing cost of silicon-based technology, and the low power efficiency of organic polymer-based technology. However, research is being done on hybrid cells based on dye-sensitizing organic polymers and a thin transparent conducting oxide layer comprised of nanoparticles. These cells could offer the same ease of manufacturing as organic cells, with improved efficiency.

Currently, although the improved efficiency is promising, it is still far below silicon-based solar cells. This paper also explores the role of nanomaterials in this flexible solar cell technology.

4. NANOMATERIALS

Nanomaterials, which are of the size of a 10^{-9} of a meter, offer different chemical and physical properties of the same materials in normal form. They can be adopted in new technologies (Alsayed-Ali, M. A, 2010). Nanomaterials have the potential use in making more efficient solar cells and catalysts that can be used in hydrogen-powered fuel-cells. In this regard, the utilization and modification of the carbon nanotubes systems to enhance and tune the hydrogen storage capabilities of the nanotubes is important. The introduction of transition metals and hydrogen bonding clusters inside tubes undoubtedly increases their relevance.

Formation and modification of metal-organic frameworks (MOFs), three-dimensional nano-porous constructions made up of carbon atoms, is imperative, so that they can hold as much hydrogen as possible.

Due to small size and excellent conductivity, CNTs (carbon nanotubes), can be used as a foundation of future electronic devices. CNT cables could be used to make electricity transmission lines, giving huge performance improvement over present day power lines.

5. HYDROGEN FUEL-CELL

Hydrogen can be used in a fuel-cell, which basically operates like a battery. The fuel-cell consists of two electrodes and an electrolyte. Hydrogen and oxygen are passed over the electrodes to generate electricity and water. Hydrogen cells are mostly used in automotive-industry. Hydrogen vehicles include hydrogen fuelled space rockets, as well as automobiles and other transportation vehicles. The power plants of such vehicles convert the chemical energy of hydrogen to mechanical energy, to run electric motors, either by burning hydrogen in an internal combustion engine, or by reacting hydrogen with oxygen in a fuel cell. Widespread use of hydrogen for fueling transportation is a key element of a proposed hydrogen economy. Compressed hydrogen tanks are used to supply the hydrogen, and oxygen is used from the air directly. There is no pollution caused by hydrogen fuel cell autos, and the only emission is water. If the hydrogen fuel cell autos become mainstream instead of exception, autos can cease to be a part of the global pollution problem.

Hydrogen fuel does not occur naturally on Earth and thus is not an energy source, but is an energy carrier. At present, it is most frequently made from methane or other fossil fuels. However, it can be produced from a wide range of sources (such as wind, solar, or nuclear) that are sporadic, too diffuse or too cumbersome to directly propel vehicles. Electrolysis of water, integrated wind-to-hydrogen plants, etc. are technologies being explored to deliver low costs and high quantities to compete with traditional energy sources. Earlier research and development on hydrogen energy pertains to auto-thermal steam reforming catalysis of gas and alcohols, gasification, pyrolysis, thermo-chemical cycle, solar PV-electrolyser splitting of water, photo-electrochemical and photo-biological splitting of water and carbon nano-tube hydrogen storage. Previous research and development of fuel cells relates to proton exchange membrane fuel cell (PEMFC) materials, such as alternative electrolyte membranes, low-Pt electrodes, manufacturable bipolar plates and prototyping of PEMFC systems of 200 W to 5 kW portable power generator and fuel-cell motorcycles. PEMFC are promising devices for decentralized energy production, both in stationary and automotive fields, thanks to high compactness, low weight (high power-to-weight ratio), high modularity and efficiency, fast start-up, and response to load changes. The fuel-cell research groups are: fuel-cell process system engineering, fuel-cell electrochemical processes, fuel-cell material and manufacturing, micro direct methanol fuel-cell (DMFC), solid oxide fuel-cells (SOFC), and biofuel cell (BFC). The alkaline fuel-cell (AFC), phosphoric acid fuel-cell (PAFC) and molten carbonate fuel-cell (MCFC) have all been fully developed but were not fully commercialized due to technical and economic reasons. On the other hand, the PEMFC, DMFC and SOFC are still being intensively researched all over the world.

A new type of fuel cell, the microbial fuel cell (MFC) is also now being explored as a sustainable way of providing power. The ideal fuel for PEMFC is hydrogen with low carbon monoxide content to avoid poisoning of the fuel cell; in this way, PEMFC can achieve efficiency of up to 60 %, far higher than the 20-35 % efficiency of an internal combustion engine. The main thrust in PEMFC research is cost reduction of fuel cells by reduction of membrane and electrocatalyst costs; lowering electrocatalyst loading, reducing system complexity; and, by using CO tolerant anodes. PEMFC, system efficiency can be further enhanced through better designing of flow field in bipolar plates, and fuel/air in the stack, as well as through process optimization. The main thrust of SOFC R&D is reduction of the operational temperature by replacement with low temperature electrolytes, anodes and cathodes. Future DMFC R&D will focus on reduction of methanol crossover, watermanagement and reduction in manufacturing costs. The main thrusts of R&D in hydrogen production from fossil-fuels are towards the development of low temperature auto-thermal steam reforming catalysts of alcohols, purification of reformed hydrogen through pressure swing adsorption and membrane processes, as well as membrane reactors, and higher hydrogen storage in carbon nano-tubes.

6. HYDROGEN ECONOMY

There is always a need for clean, efficient, convenient forms of energy, which the user can easily access. Hydrogen is one of the many convenient forms of energy, which have the potential to make an energy system and satisfy the human energy needs (Figure-2).

The hydrogen economy would be an energy system of the coming generations in the near future. Hydrogen, being most demanded, needs technologies for its production, storage, distribution, and utilization.

Hydrogen can be generated using the renewable energy sources which are readily available. One such source is wind energy that is playing the major role in the generation of hydrogen. The hydrogen economy is capable of fulfilling the human needs of the coming generations (Sherif, Barbir and Veziroglu, 2005).

6.1 Characteristics of Hydrogen

Hydrogen in chemistry has the following properties (Veziroglu and Babir, 1992):

- Available in huge quantity;
- Can be stored in solid, liquid or gaseous form;
- Can be converted into other forms of energy efficiently;
- Renewable source made from the product of water or water vapour;
- Easily transportable;
- Hydrogen as an energy carrier is environmentally compatible.

6.2 Hydrogen Production

Several technologies have been developed to produce hydrogen. Some of them have been analyzed to describe the process of hydrogen production. Hydrogen is mainly being produced from fossil-fuels in refineries or industries. The fossil-fuels that are used for hydrogen production are in the form of coal, crude oil or natural gas. These fuels produce carbon-dioxide gas during their combustion. The processes involved are hydro-treating and hydro-cracking. To avoid emission of carbon-dioxide gas, many other technologies are being developed to produce cost-effective hydrogen. Water electrolysis is one of the most efficient methods to produce hydrogen but it needs electricity, which is expensive (Veziroglu and Babir, 1992).

More suitable and effective method of water electrolysis would be with the use of photovoltaics; but photovoltaic cells are costly to produce and install. Thus, even though highly efficient, photovoltaics do not make a good alternative.

Wind energy is the other way to produce hydrogen at a low cost but this energy can be utilized only in the areas where the wind energy is easily and abundantly available. The energy required to produce hydrogen is more than what it is capable of releasing during its utilization as a fuel.

6.3 Hydrogen Storage

Hydrogen can be stored as solid, liquid or gas in the form of glass micro-spheres, chemical hydrides, or cryo-adsorbers.

Liquid hydrogen storage is being used only when there is a high need of hydrogen. Metal hydride storage system has an advantage in terms of storage safety. This process requires system set up and release of heat during the process is another important factor to make this storage system more popular.

In particular, one potential use of hydrogen lies in powering zero-emission vehicles via a proton exchange membrane fuel-cell to reduce atmospheric pollution. The recent discovery of high and reversible hydrogen storage capacity of carbon nanotubes makes such a system very promising. Due to its high surface area and abundant pore volume, porous carbon is considered a good adsorbent. For conventional porous carbon, the hydrogen uptake is proportional to its surface area and pore volume, while a high hydrogen adsorption capacity (4~6 higher wt.%) can be only obtained at very low temperatures, such as liquid nitrogen temperature. The important matters include:

a) How do structural characteristics influence the physical/chemical process?
b) Where does the adsorption occur, in inner hollow cavities and/or other pore space?

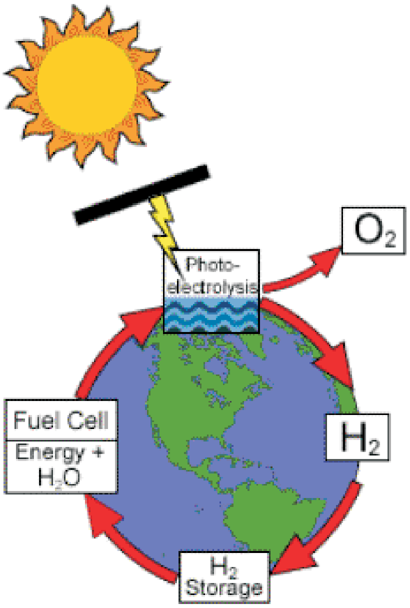


Figure-2: Clean, Cyclic Process of Generation of Hydrogen

c) In the adsorption of hydrogen onto carbon nanotubes, what interaction, chemical or physical occurs between the hydrogen and the carbon?
d) What are the adsorption mechanism and capacity?

Methods of hydrogen storage for subsequent use involve many approaches, including high pressures, cryogenics, and chemical compounds that reversibly release H_2 upon heating. Metal-organic framework (MOF) compounds consist of metal-oxide clusters connected by organic linkers. MOFs are a relatively new class of nano-porous material that show promise for hydrogen storage applications because of their tunable pore size and functionality.

6.4 Hydrogen Transport and Distribution

Hydrogen transportation by pipeline can be done up to 200 km from production to utilization sites but for effective transportation, high-capacity reciprocating compressors are used. The pipelines used for hydrogen transportation require large diameters and more compression power. Due to low volume of hydrogen and lower pressure losses, less recompression stations are required that need to be placed far apart. It has been estimated that transportation of hydrogen is cheaper compared to transportation of electricity. However, hydrogen distribution from industrial production plants to small-scale users has some limitations related to difficulties in hydrogen storage and transport. For its chemical and physical properties, indeed, the development of a hydrogen infrastructure seems to be not feasible in short term, while the concept of decentralized hydrogen production seems to be more reasonable; in this way, a hydrogen source, such as methane, is distributed through pipelines to the small-scale plants, placed near the users. The in-situ produced hydrogen is fed directly to the energy production system, avoiding hydrogen storage and transportation. In this sense, a compact fuel processor, capable of generating a hydrogen rich stream from an easily transportable fuel, may widely be used in the future.

6.5 Hydrogen Utilization

Hydrogen is being greatly used as a fuel in the internal combustion engines. The greater advantage is that it is cleaner and its use causes less pollution compared to gasoline. Hydrogen-use in jet engines and turbines produces only one pollutant, nitrogen oxides. Use of hydrogen in biomedical technology is becoming popular in the form of micro steam generator. Catalytic burners in household appliances are coming up with the use of combustion of hydrogen only.

6.6 Hydrogen Safety

Every process has its own risks and benefits. Similarly, hydrogen can be a risk if proper care is not taken from the beginning of the process of production till the process of utilization. Hydrogen has the smallest molecule and so has a higher tendency to leak through small openings. Also, due to low ignition energy of hydrogen, the flame becomes nearly invisible that could be a dangerous issue, as it becomes hard to detect if there is a fire. Liquid hydrogen also creates the risk of cold burns. In spite of all the safety hazards, hydrogen has a very good safety record and is actually a safer fuel than any other gas.

7. DYE-SENSITIZED SOLAR CELLS BASED ON TiO_2 NANOPARTICLES

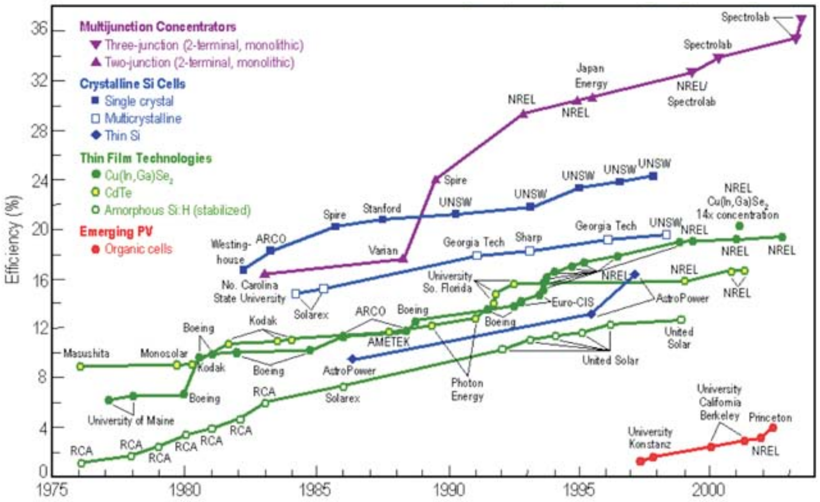
Today, due to the increasing global demands on energy, it is imperative that a renewable energy source be determined that is cost-effective and reliable. Solar cell technology has shown much promise over the years to replace the use of fossil-fuels. However, with the current technology, the cost per watt is rather high due to the high cost of manufacturing of silicon-based solar cells. The cost per watt can be lowered in two ways: i) lower the manufacturing cost; or ii) increase the amount of power output for the same cost. The latter is related to efficiency of the device. In other words, energy efficiency is the amount of energy output vs. the amount of energy coming in. In Figure-3, we can see the timeline of energy efficiencies of different types of solar cell technology. The current best is around thirty-six per cent. Clearly, a more efficient way of converting sunlight into energy needs to be researched in order to make solar cell technology economically viable.

Most traditional solar cells rely on a semi-conductor (typically silicon) for both light absorption, and charge transport. A fairly new, promising method separates these functions. Organic dyes (dye sensitizers), which are sensitive to light, can absorb a broader range of the sun's spectrum. When a photon hits the dye, an electron in the dye becomes excited and is injected into the conduction band of a nano-crystalline semiconductor oxide, where charge transport takes place. Electrons lost from the dye are regenerated by a redox electrolyte, usually an inorganic solvent. These components are sandwiched between substrates of transparent conducting oxide. It appears that the enormous surface area per unit volume of nanoparticles can increase the photon-to-current ratio.

Future studies are focusing on controlling the order and shape of the particles to increase the photon-to-current ratio even more. Although the mechanisms and processes of the dye sensitizer, electrolyte, and conducting substrate are worthy of study, we have tried to review the material properties of TiO_2 nanoparticles, and explore the mechanisms that make it a promising material in improving the efficiency of dye sensitized solar cells (DSC) (Michael Grätzel, 2004).

7.1 Theory of Operation for Dye-Sensitized Solar Cells

Dye-sensitized Solar Cells (DSCs) shown in Figure-4, rely on processes similar to photosynthesis. In



Source: *NREL: www.nrel.gov/ncpv/thin_film/docs/kaz_best_research_cells.ppt*

Figure-3: Timeline of Solar Cell-Efficiency according to Different Methodology (Kazmerski L., 2006)

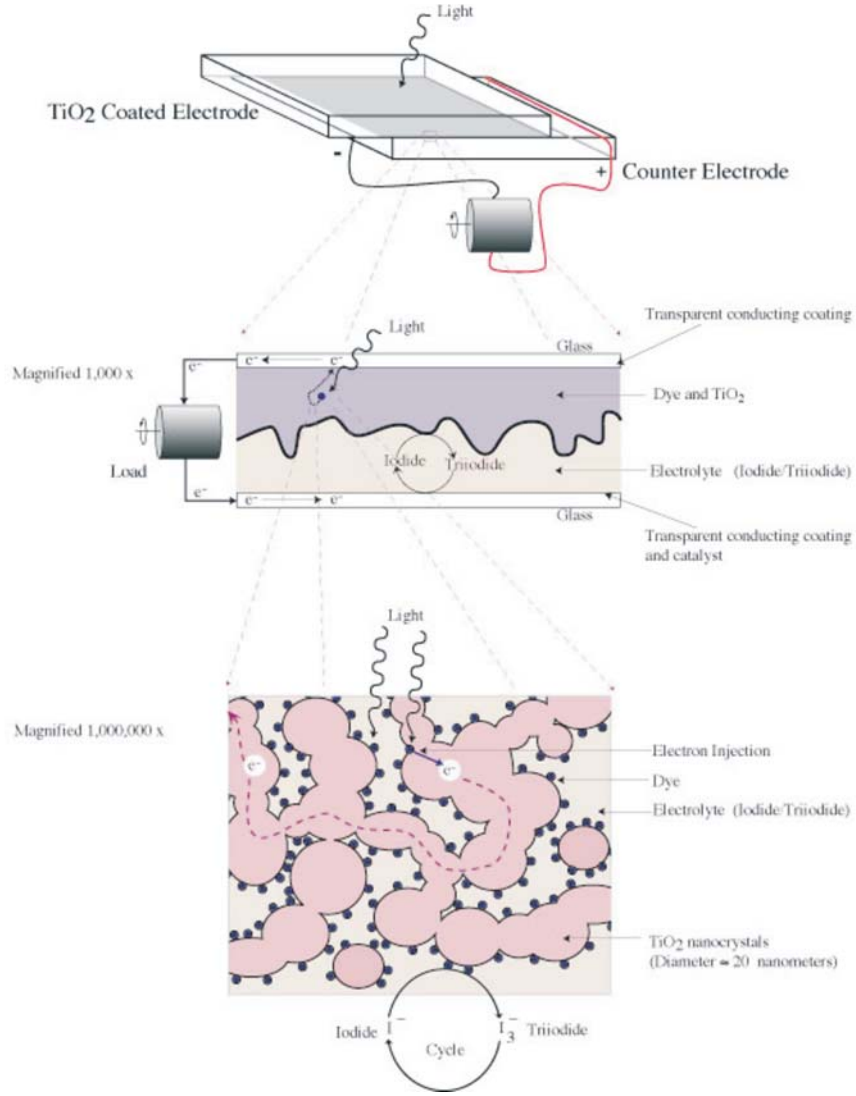


Figure-4: Schematic Diagram of a Dye-Sensitized Solar Cell (Wikipedia, 2006)

photosynthesis, light is converted into chemical energy. Chlorophyll and other pigments can eject electrons through photo-induced charge separation when struck by photons. The main component of a DSC is a semi-conducting material with a wide band gap. One such material is titanium dioxide (TiO_2). This is deposited as a thin layer onto a transparent conducting oxide (TCO) substrate using a sol-gel technique. The TiO_2 layer is also in contact with a monolayer of polymer dye, which has commonly been a ruthenium complex, also known as N3 (Kazmerski L., 2005). Exposure to sunlight causes electrons in the dye to become excited. This phenomenon is called photoexcitation. The electrons are then ejected from the dye and into the conduction band of the semi-conducting oxide layer. Regeneration of the lost electrons is handled by a redox process within an electrolyte, commonly an iodide and tri-iodide couple, which is in contact with the dye. The final component is a layer of TCO. The voltage generated is related to the difference between the redox potential of the electrolyte and the Fermi level of the electron within the solid. The electron that was ejected from the dye diffuses through the TiO_2 layer and into the conductive oxide electrode where it can be used as current.

7.2 Properties of TiO_2 Nanoparticles

The crystal structure of common forms of TiO_2 is tetragonal. Initially, mesoporous films of fractal dye

Figure-5: Scanning Electron Micrograph of a Mesoporous TiO_2 Film (Wikipedia, 2006)

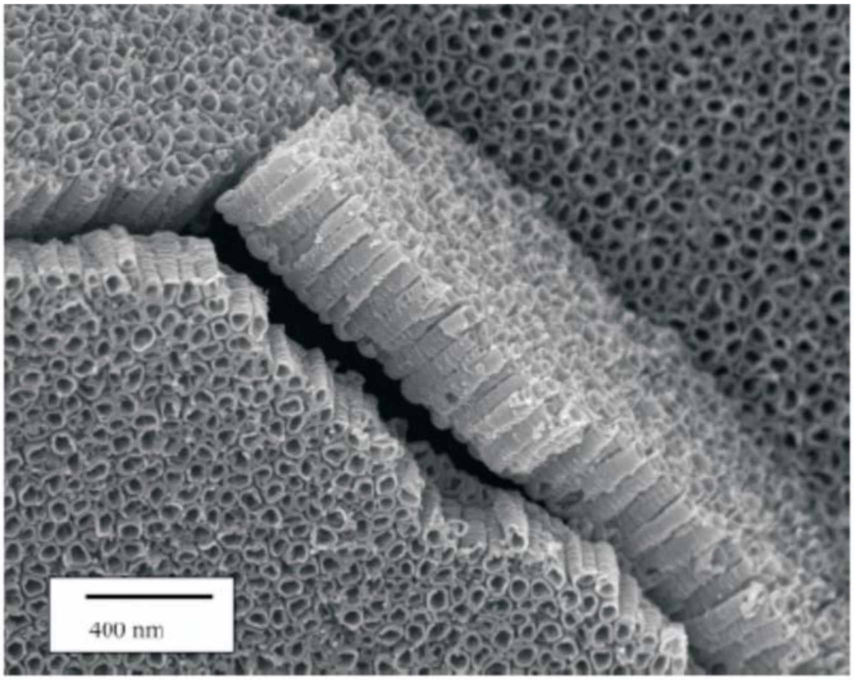


Figure-6: FESEM Images of Highly Ordered TiO_2 Nanotube Arrays (Gopal K. M., et al., 2006)

derivatized TiO_2 (Figure-5), with a surface roughness factor of 150, were used as the semi-conducting material in contact with the polymer dye. As seen in the micrograph, there is more surface area as compared to a flat surface. Adsorption of the mono layer dye sensitizer on a flat surface will result in a limited amount of coverage. By increasing the contact area between the semi-conductor and the dye, the amount of light harvesting is increased. The increased injection of electrons from the dye to the semi-conductor film improved the efficiency but more was needed. In order to further improve the efficiency of light harvesting, nanoparticles of TiO_2 were utilized. Nanoscale properties can be exploited to increase the amount of electrons captured. One very important property of nanomaterials is the morphology. The size and shape of the nanocrystallites, as well as the surface topography is a key to increasing the efficiency of capturing electrons, as can be seen in Figure-5. Continuing studies are looking at controlling the size and shapes of these nanocrystallites. Control of the morphology of nanomaterials primarily takes place during synthesis.

8. WHAT IS NEXT?

A lot of investigation is being done on each component of dye-sensitized solar-cells these days. Increasing the efficiency of light harvesting, finding a more stable electrolyte, and improving the performance of the dye sensitizer are key topics. With regard to the semi-conducting oxide and light harvesting, researchers are trying to create more ordered rod-like crystallites. It is thought that a way to increase the amount of light harvesting is to have the rods aligned parallel to each other creating channels (Wikipedia, 2006). These channels would be perpendicular to the TCO electrodes. Highly ordered TiO_2 Nanotube arrays integrated into the DSC design (Gopal, et al., 2006) have been studied. Figure-6 shows images of the nanotube arrays from different angles. By assembling in this fashion, the nanotubes provide an excellent path for electron percolation, and thus increase the electron lifetime, and efficiency of charge carrier transport. The fabrication process begins with an Radio Frequency (RF) sputtering process of Titanium. This film is deposited on a glass substrate coated with a fluorine-doped tin oxide. An anodic oxidation step is next, followed by a 450ºC anneal in oxygen ambient. Prior to the annealing step, the nanotube arrays are not fully transparent. The resulting films show superior electrical performance as compared to nanoparticles. For example, open circuit voltage decay measurements were performed to look at the recombination effects. Figure-7 shows the response-time versus open-circuit voltage. The plot for the nanotubes clearly show longer response times, which correlate to longer electron lifetimes, which means less recombination of electron-hole pairs. This will ultimately translate to higher energy output. These results are very promising, and it is predicted that photocurrent efficiencies could approach the ideal limit of 31 % by lengthening the nanotube length (Gopal, et al., 2006). Although this is very encouraging, when dealing with structures that have a high contact area, the interface dynamics between the dye and the oxide must also be well understood.

Continued investigation into the interface dynamics of highly ordered nanotube arrays, as well as optimization of the other components are the focus of relevant future endeavours. The studies mentioned herein show that researchers are close to creating a DSC with viable cost-efficiency.

9. COMPUTATIONAL NANOSCIENCE AND MATERIAL SCIENCE FOR RENEWABLE ENERGY

Computational material science and nanoscience can

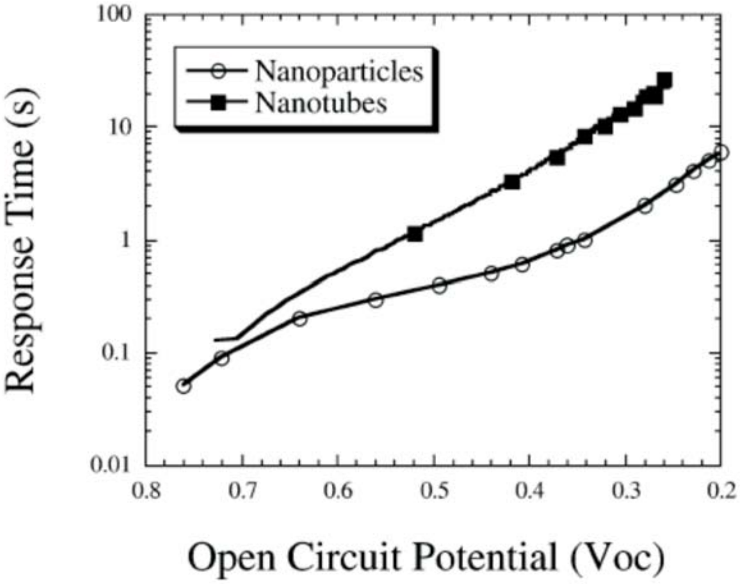


Figure-7: Response Time vs. Open Circuit Voltage for Nanoparticles and Nanotubes (Gopal K. M., et al., 2006)

play many critical roles in renewable energy research. These involve finding the right materials for hydrogen storage, a reliable and efficient catalyst for water dissociation in hydrogen production, cheap, environmentally benign and stable material for efficient solar cell application; and understanding of the photo-electron process in a nanosystem to help design efficient nanostructure solar cell. In all these areas, the possible exploratory parameter spaces are huge. This, at one hand, provides ample opportunity and potential for device-improvement, but on the other hand presents a tremendous challenge to find the best material and design. Exa-scale computation can thus help this optimization process, by either doing a direct numerical material by design search, or by understanding some fundamental processes in nanosystems.

In computational material science and nanoscience, there are three major challenges:

i) to develop the appropriate numerical approximation and model for accurate calculation of the corresponding physics properties;
ii) to integrate the diverse models and computational approaches and programmes to calculate different parts and aspects of a complex system, hence to enable the simulation of the whole system and process; and
iii) to calculate the large-scale systems (nanosystems containing tens of thousands of atoms) and dynamically for a long period of time (nanoseconds or microseconds).

The computational physics and chemistry community have been making efforts to address the fresh challenge since the invention of quantum mechanics. Although the many-body Schrodinger's equation is well known and describes exactly almost all the phenomena in material science; the direct accurate solution of that equation is almost impossible. This is because a system with N electrons needs to be described by a many-body wave function in N dimensional space (Alsayed-Ali and Zakaria, 2010). That makes the needed numerical co-efficients scale as N^N. A direct solution of such a problem might only be possible by future quantum computer. The most common approximation is to re-describe the 'many-body' wave function and the Schrodinger's equation with N single particle wave function. This is exemplified by the currently popular density functional theory (DFT), where a direction calculation scales as N^3, instead of N^N. DFT can describe many properties accurately, including atomic structures and binding energies. Thus, it is very useful in the search of hydrogen storage material and catalysis. Although it gives the approximate value of band gap with some corrections, it still can be used to study the optical properties and electron-phonon interactions. Thus, it can also be used for solar cell simulations. Other methods, like the couple cluster method in quantum chemistry, and GW method in material science can provide more accurate calculations for chemical binding and band structures, respectively. The search for more accurate and fast ways to calculating approximations will never end. But the continuation of search and the need for better methods/numerical models should not prevent us from using the models we already have. Actually, the current approximations (e.g., DFT) are already useful to carry out the simulations listed above for renewable energy research.

For the second challenge, the main focus should be on software development and integration. It also presents a computational hardware requirement more on capacity side than on capability side. Most experimentally measured physical properties are results of combinations of different physical processes (e.g. the solar cell efficiency and a nanosystem synthesis). At present, there are different methods and codes to calculate each individual property and process. But there lacks to a flexible tool to integrate them together, or to easily replace one model/algorithm in one part of a calculation by another.

For the third challenge, it calls both for algorithm development and for exa-scale computer. Due to the $O(N^3)$ scaling for DFT, even with petascale computers, one can probably only calculate the electronic structures of a system with 50,000 atoms for a given atomic configuration. If many time steps are needed to simulate a process, this direct approach will become unfeasible. Thus, linear scale approaches (to the size of the system) become necessary. Fortunately, due to the near-sight feature of quantum mechanical effects, such linear-scaling algorithms based on domain decomposition are possible, and effective for the large systems discussed here. With the linear-scale algorithm and the exa-scale computer, we should be able to simulate a whole nanostructure device, e.g. from photon-absorption exciton generation, to exciton-dissociation and carrier collection in a nanosize solar cell. This simulation can be done by following a time-dependent Schrodinger's equation (e.g. time-dependent density functional theory, TDDFT), and, at the same time, doing a Newtonian dynamics for the atoms. Although there are still some uncertainties as to how exactly this may be done (for quantum state collapsing), such a simultaneous dynamical simulation for the electrons and atoms will help to reveal the electron-phonon interaction, the non-radiative carrier decay and cooling, as well as the under carrier transport and collection. These processes are critical for solar cell applications, and are poorly understood so far. To carry out such a simulation for an experimental sized nanosystem is a tremendous challenge. First is the size scale as described above and the second is the long-time scale. The typical carrier dynamics takes tens of nanoseconds, while the typical time step needed for a TDDFT is usually in the order of 10^{-3} fs (which is a thousand times shorter than a time step for atomic molecular dynamics due to the small mass of an electron). Thus, the number of time-steps is in the order of 10^{10}. Right now, one can do tens of fs simulations for small systems containing about a hundred atoms (e.g. on the Earth Simulator) based on the direct TDDFT formalism. Thus, there is a gap of about 10^5 in time scale and 10^2 in size scale. It is likely that both algorithm development (both in the linear-size scaling and in accelerating or approximating the dynamics) and larger exa-scale computer are needed to close this gap. But the benefit will be tremendous for understanding the photon-electron process in solar cell applications. The lack of such understanding is the current bottleneck in developing more efficient nanostructure solar cells.

10. CONCLUSIONS

The hydrogen fuel cell system is a green advanced power system for the future that is green, sustainable, clean and very environment-friendly. Priorities in energy research are the cheaper fuel-cell technology and renewable hydrogen production using water splitting photo-electrochemical cell. The main focus of R&D for sustainable hydrogen-production after fossil-fuel depletion is biomass pyrolysis, biohydrogen and photolysis of water into hydrogen and oxygen in solar photovoltaic-electrolyser system, direct solar photoelectrochemical reactors and solar photo-biological fermentors.

The increased injection of electrons from the dye to the semi-conductor film improved the efficiency, yet further improvement was needed. In order to further improve the efficiency of light harvesting, nanoparticles of TiO_2 were utilized. Nanoscale properties can be exploited to increase the amount of electrons captured. One very important property of nanomaterials is the morphology. The size and shape of the nanocrystallites, as well as the surface topography is a key to increasing the efficiency of capturing electrons.

Computational material science and nanoscience can play many critical roles in renewable energy research. An important prospect is to find the right materials for hydrogen storage. More and more experimental and theoretical results continue to appear, and more and more reproducible evidence proves that carbon nanotubes and MOFs (nano-porous materials) are potential hydrogen storage carriers. In order to use carbon nanotubes as a practical hydrogen storage medium, the mass production and utilization of carbon nanotubes are of current interest. Controlling the type and size of the tubes is expected to allow tuning the material for hydrogen sorption at desired temperatures and pressures. Nanoscience research also involves finding the most reliable and efficient catalysis for water dissociation in hydrogen production; the cheap, environmentally benign and stable material for efficient solar cell application; and understanding of the photo-electron process in a nanosystem to help design efficient nanostructure solar cell. In all these areas, the possible exploratory parameter spaces are huge.

The conclusion obtained from the above discussion is that we should increase the use of renewable energy sources and reduce the use of non-renewable resources. Existing renewable resources are well-established and proven. It has been seen that available renewable energy resources are helping in the production of the other forms of energy that makes energy system stronger and economical. The new upcoming technologies in renewable energy resources are very promising but a lot more research and infrastructure is required before they can be adopted.

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