

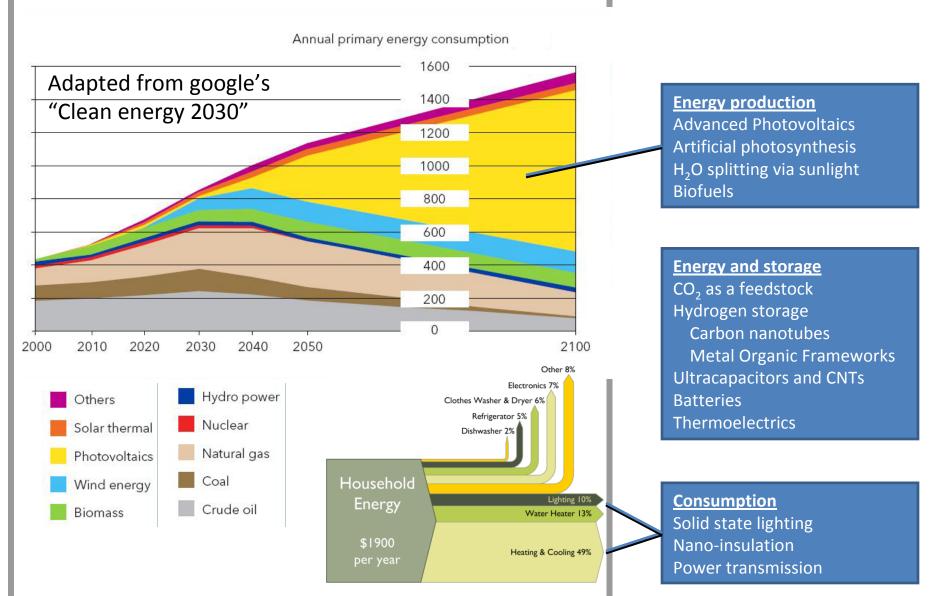
NANOTECHNOLOGY FOR ENERGY CONVERSION, STORAGE AND INCREASED EFFICIENCY

Mihail C. Roco

National Science Foundation and National Nanotechnology Initiative

Seoul, Korea, April 6, 2010

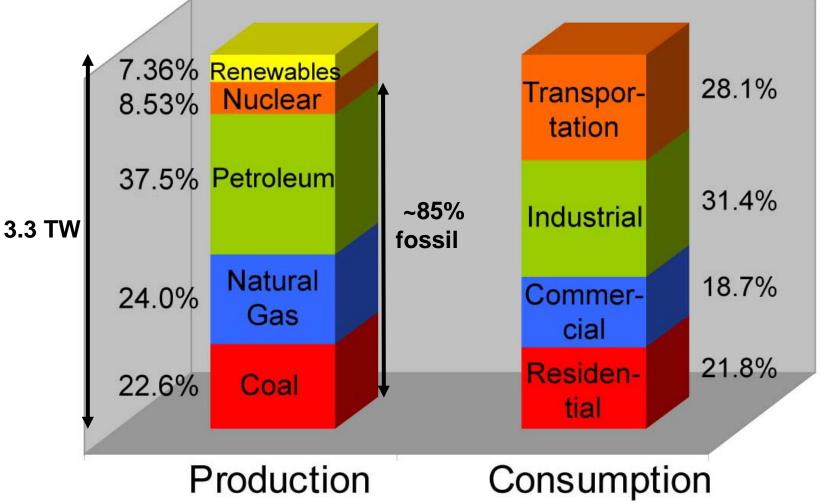
The impact of nanotechnology on our energy landscape | CJ Brinker David Ginger The size of the energy challenge is enormous—we need to look for solutions that have impact on the TW scale



Where does it come from? Where does it go?

We must replace several terawatts of coal, petroleum, and natural gas usage





US population from Google report of US census data: 304059724 Energy data from DOE: http://www.eia.doe.gov/emeu/aer/contents.html Benchmark with experts in over 20 countries in 1997-1999

"Nanostructure Science and Technology"

NNI preparatory Report, Springer, 1999

Nanotechnology Definition for the R&D program

Working at the atomic, molecular and supramolecular levels, in the length scale of ~ 1 nm (a small molecule) to ~ 100 nm range, in order to understand, create and use materials, devices and systems with fundamentally new properties and functions because of their small structure

- NNI definition encourages new R&D that were not possible before:
 - the ability to control and restructure matter at nanoscale
 - novel phenomena, properties and functions at nanoscale,
 - integration along length scales, systems and applications

Nanotechnology Research Directions

Vision for Nanotechnology in the Next Decade

Edited by M.C. Roco, R.S. Williams and P. Alivisatos

Book, Springer, 2000

"Vision for nanotechnology in the next decade" (2001-2010)

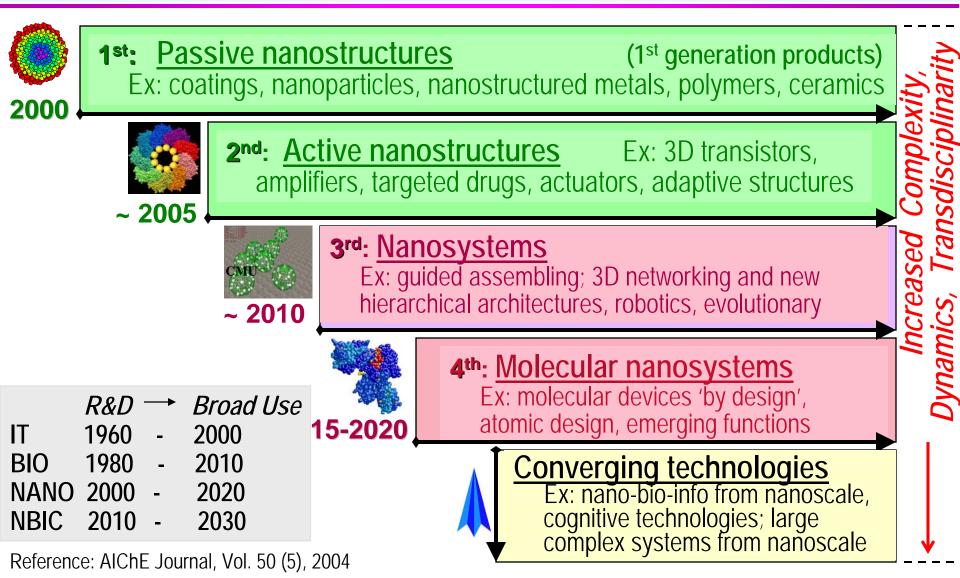
Systematic control of matter on the nanoscale will lead to a revolution in technology and industry
<u>Change the foundations from micro to nano in</u> <u>knowledge, industry, medicine, sustainability, ...</u>
Create a general purpose technology (similar IT)

More important than miniaturization itself:

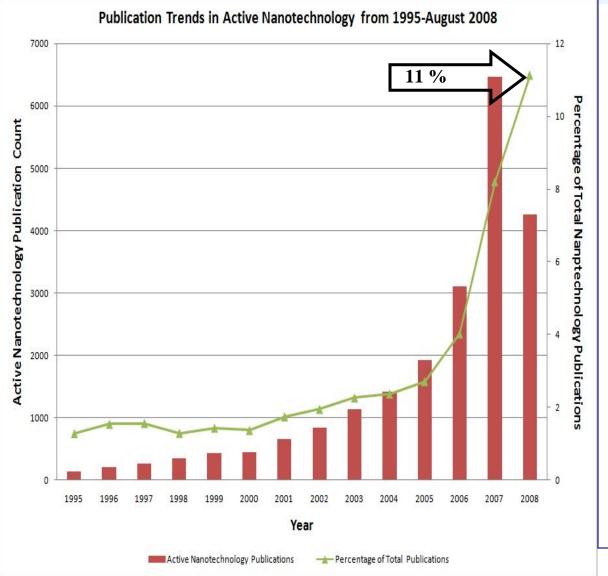
- Novel properties/ phenomena/ processes/ natural threshold
- Unity and generality of principles
- Most efficient length scale for manufacturing, biomedicine
- Show transition from basic phenomena and components to system applications in 10 areas and 10 scientific targets

Introduction of New Generations of Products and Productive Processes (2000-2020)

Timeline for beginning of industrial prototyping and nanotechnology commercialization



A shift to "active nanostructures" after 2006



On active nanostructures

21,000+ articles from WOS/SCI from 1995 to 2008

Exemples:

- Transforming (e.g., self-healing materials)
- Remote actuated (e.g., magnetic, electrical, light and wireless tagged nanotechnologies)
- Environmentally responsive (e.g., actuators, drug delivery)
- Miniaturized device (e.g., molecular electronics)
- Hybrid (e.g., uncommon material combinations, biotic-abiotic, organic-inorganic in chips)

Drug delivery

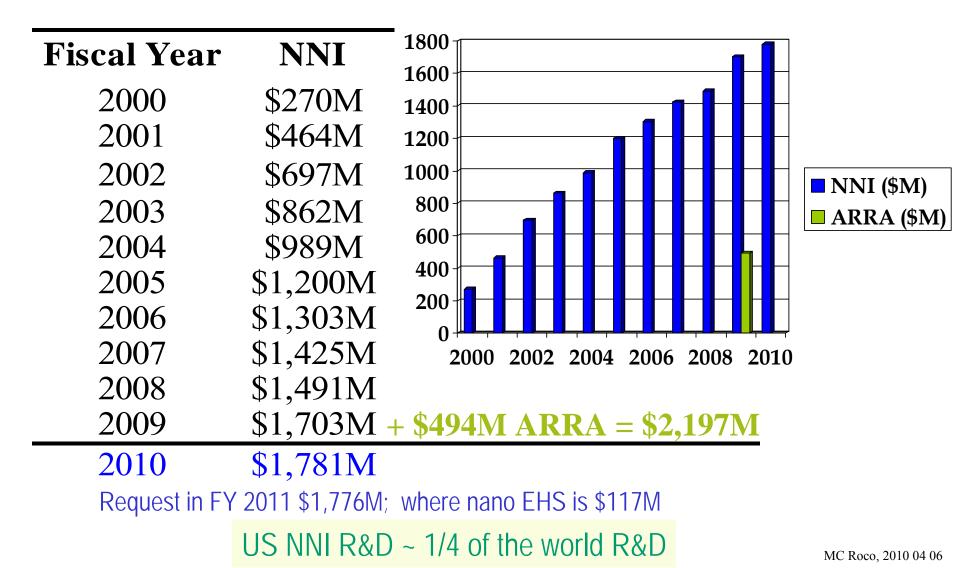
Source: V. Subramanian, J. Youtie, A. Porter, and P. Shapira (2009). Is there a shift to "active nanostructures?" *Journal of Nanoparticle Research*, 2010, Vol. 12(30

Ten highly promising products incorporating nanotechnology in 2010

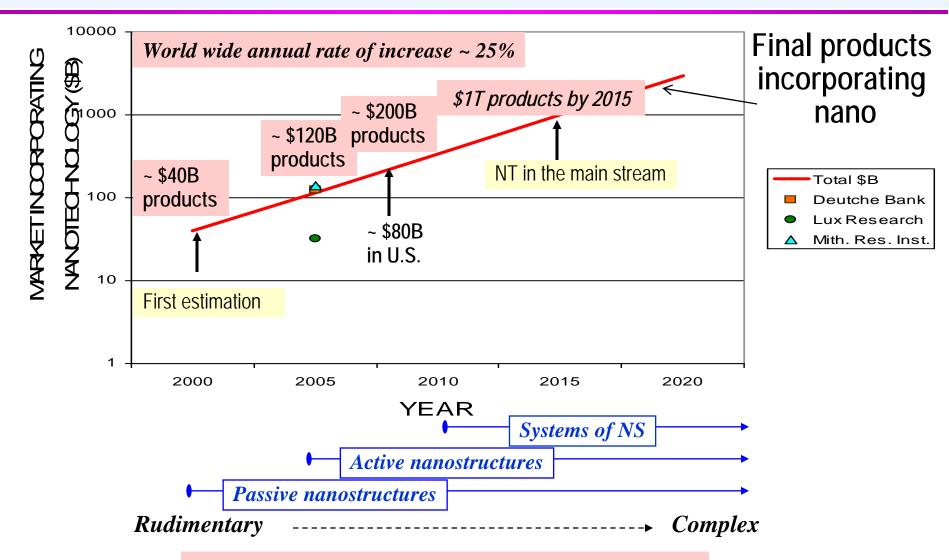
- Catalysts
- Transistors and memory devices
- Structural applications (coatings, hard materials,.)
- Biomedical applications (detection, implants,.)
- Treating cancer and chronic diseases
- Energy storage (batteries), conversion and utilization
- Water filtration
- Video displays
- Optical lithography
- Environmental applications

With safety concerns: cosmetics, food, disinfectants,..

2001-2010 Changing national investment FY 2011 NNI Budget Request \$1,781 million



WORLDWIDE MARKET INCORPORATING NANOTECNOLOGY (Estimation made in 2000 after international study in > 20 countries)

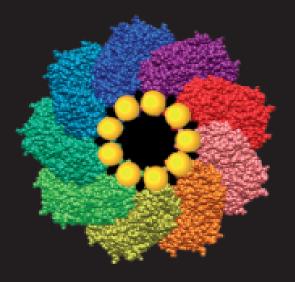


Reference: Roco and WS Bainbridge, Springer, 2001

Nanotechnology: Societal Implications I

Maximizing Benefits for Humanity

Edited by Mihail C. Roco and William Sims Bainbridge





March 2007



January 2009

Mapping Nanotechnology Innovations and Knowledge

Global and Longitudinal Patent and Literature Analysis

technology overview viedge mapping foundation viedge mapping framework TO analysis, 1976-2002 funding & USPTO analysis, 176-2004 funding & USPTO analysis, 176-2004 fo literature analysis, 176-2004 fo literature analysis, 176-2004 ano Mapper system TO, EPO & JPO analysis, 176-2004 ano Mapper system TO, EPO & JPO analysis, 105-2007

USPTO patents of major country groups, 1976-2006.

Nanotechnology papers in Thompson SCI database, 1976-2004

> Hsinchun Chen Mihail C. Roco

2000-2010 Expanding nanotechnology domains

2000-2001: nano expanding in almost all disciplines; by 2009: 11% of NSF awards; 5% papers; 1-2% patents

2002-2003: industry moves behind nano development by 2009: ~ \$200B products incorporating nano worldwide

2003-2004: medical field sets up new goals

2004-2005: media, NGOs, public, organizations -involved

2006-2007: new focus on common Earth resources - water, food, environment, energy, materials

2008-2010: increased relevance to economy – policies - sustainability

The World is NOT Currently Achieving Sustainable Development

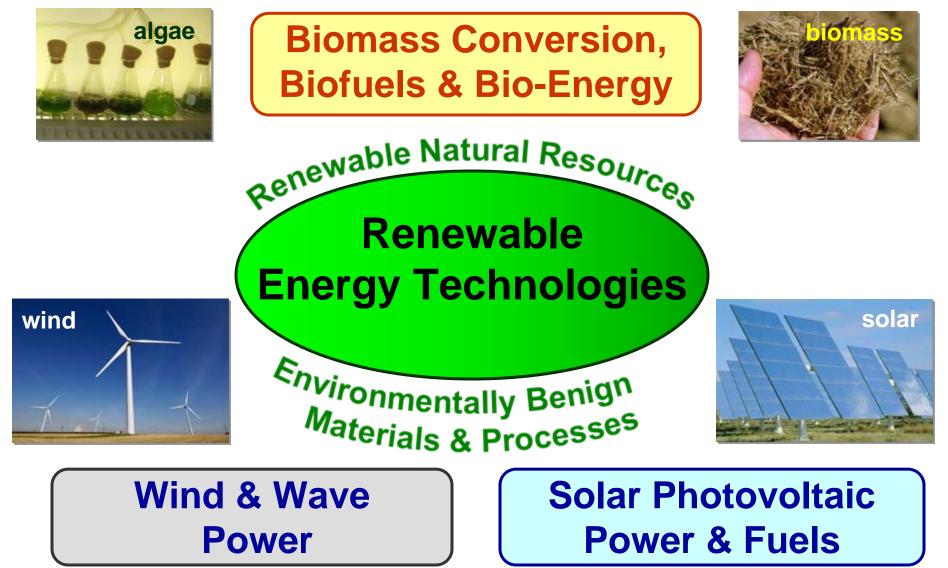
Every major ecosystem is under threat at different time scales: food, water, risk of climate change, energy, biodiversity, mineral resources

Nanotechnology may offer efficient manufacturing with less resources, less waste, better functioning products

Need for global governance of converging technologies



Renewable Energy Emphasis Areas using nanoscale processes



MC Roco, 2010 04 06

Nanotechnology Impact Areas in Energy

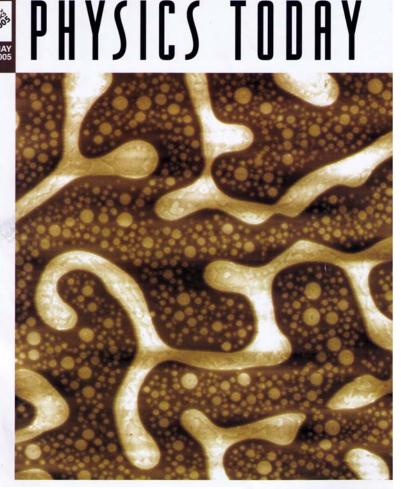
- solid-state lighting (LED)
- Iow-power displays
- fuel cells
- battery materials
- solar power
- catalysis
- weight reduction
- propellants and explosives
- hydrogen storage
- nanoscale energy (ATP motors, etc.)

• • • • •

Example: Polymer solar cells are intrinsically nanostructured devices

In a bulk heterojunction solar photovoltaic a nanostructured donor/acceptor interface is used to dissociate excitons while providing co-continuous transport paths

Hierarchical assembly – can we control molecular to nanoscale structure over large areas, in scalable processes?



Review by Malliaras and Friend

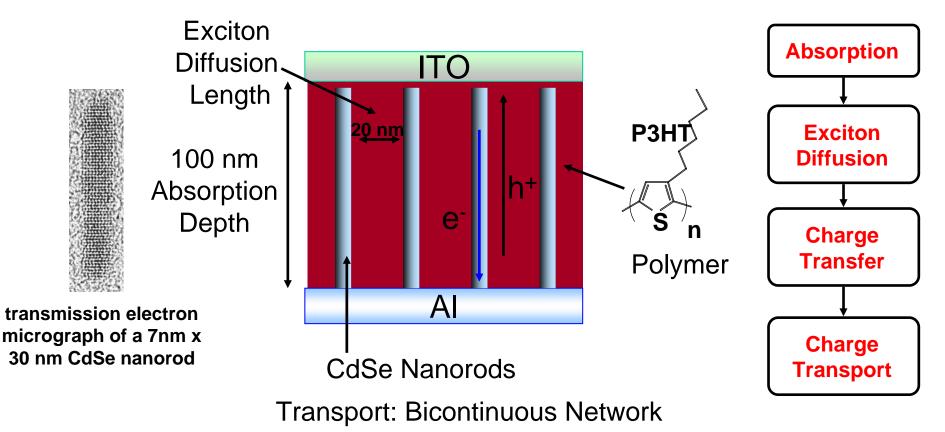
The growth of organic electronics <u>Trajectory</u> 2000 Efficiency <1% Lifetime= ~hours crazy to discuss as viable technology

2010 Efficiency ~8% (certified lab scale) Lifetime= unknown: months-years? Industrial startups

2020 Efficiency 10-15% (in production) Lifetime= years+ Successful, transformative technology

Polymer/Nanorod Structures for Novel Solar Cells

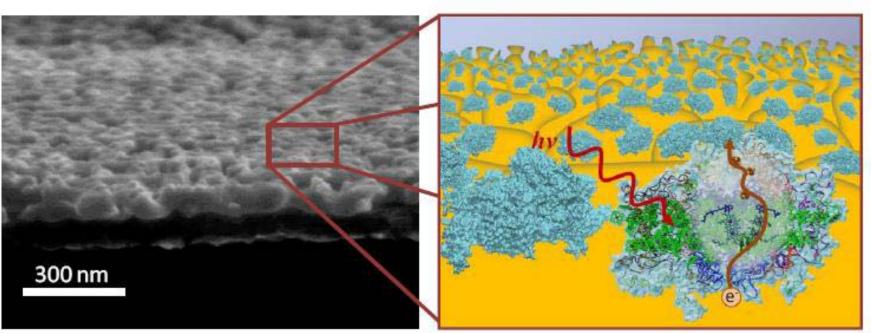
- Nanoscale volume of rods reduces amount of inorganic semiconductor needed
- Potential for low cost, ultra-light weight, and flexible cells
- Nanorods can be tailored to absorb certain wavelengths via quantum size effects



P. Alivisatos et al., LBNL/UC-Berkeley

Biomimetic Solar Cells

P. N. Ciesielski, A. Scott, C. J. Faulkner, B. J.Berron, D. E. Cliffel, and G. K. Jennings,—Functionalized Nanoporous Gold Leaf Films



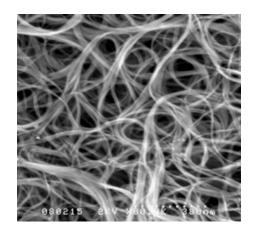
Scanning electron micrograph of a ~100 nm thick nanoporous gold electrode

Nanotechnology to Improve Lithium-Ion Battery Storage Capacity

Landi, B.J., Rochester Institute of Technology, 2009

Three time increase in battery performance through the addition of single wall carbon nanotubes (SWCNT) in the anode, cathode, and carbonaceous materials of Lithium-Ion batteries.

Applications to automotive batteries and space



Single wall carbon nanotubes created by laser ablation



SWCNT paper that is used to make an anode MC Roco, 2010 04 06

Battery Materials for Ultra-fast Charging and Discharging

- Kang, B. and G. Ceder. Nature 458: 190–193, 12 March 2009. NSF Award # 0819762
- Lithium (Li) batteries: In order to speed the diffusion of Li ions from the cathode surface into the bulk of the crystal - use LiFePO4 and a processing scheme that leaves a glassy, fast ion conductor on the surface, thereby leading the lithium ions rapidly to the proper "tunnels" for more efficient movement into the material.

Film of (LiFePO4) that allows quick charging and discharging of lithium ion batteries.



Photovoltaics : Nanoparticle co-sensitizers for increased efficiency. NSF SBIR Award to Konarka, Inc

From Light to Power

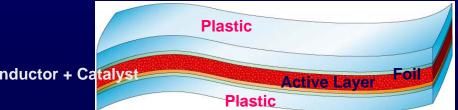


Polymer photovoltaic products in a variety of form factors for commercial, industrial, military and consumer applications

- Uses photoactive dyes & conducting polymers
- High-speed manufacturing processes
- Low temperature environment
- Uses low cost materials
- Highly scaleable

Schematic of Dye Sensitized Titania Cell

Total thickness 0.01 inch



- Mass customization from a single source
- World solar PV market: CAGR > 35%
- 20+ patents pending

Transparent Conductor + Catalyst

NSF SBIR Award to T/JTechnologies, Inc.

Technology: High Rate, High Capacity Anodes for Rechargeable Li Batteries Based on Metal Oxide Nano Composites and



Lithium Ion Batteries

Outside Investment

NASA Contract: \$2,200,000 Acquired by A123 Company

Goals:

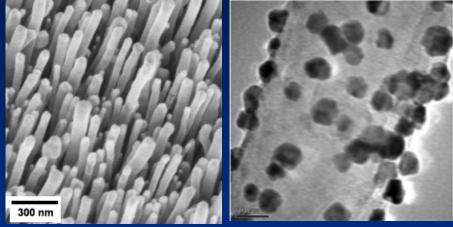
- Reduce irreversible capacity to <15%
- >300 mAh/g reversible capacity
 - >10C at 80% rated capacity and 80% DOD
- Achieve projected material costs of <\$10/kg</p>

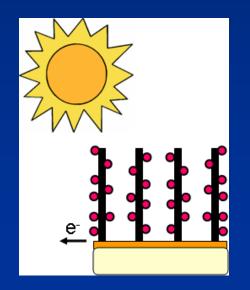
Commercialization Strategy:

- System payoff: 30-50% reduction in large format lithium-ion battery size
- •Develop a cost-competitive battery suitable for HEV, UPS, military and aerospace applications
- •Strategic Partnerships for joint development of new materials: materials production and battery manufacturing

Chemical and Biochemical Surface Functionalization of Group IV Materials Robert Hamers, University of Wisconsin-Madison CHE-0613010

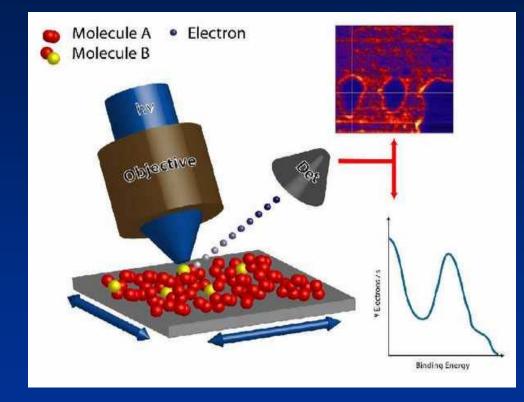
Carbon nanofiber materials offer extremely high surface areas and individual fibers can conduct electricity. Hamers and his group are developing new energy related chemistry technologies based on vertically aligned carbon nanofibers (VACNFs). They have discovered ways to grow nanometer scale catalysts such as platinum onto the VACNFs in unprecedentedly high densities. Catalysts can accelerate chemical reactions, and since the platinum nanocrystals are in electrical contact with the carbon nanofiber, the VACNF forest can collect sunlight and generates electricity. Alternatively, the forest can generate hydrogen fuel (sunlight + water $=> H_2 + O_2).$





Development of a Spatially Resolved Photoionization Microscope for Chemically Selective Mesoscale Spectroscopy in Organic Photovoltaic Cells Francis Oliver Monti, University of Arizona CHE-0618477

Organic solar cells have the potential to make solar energy conversion widely economically viable, thereby reducing dependence on fossil fuels. This group has successfully developed a complete experimental platform for the study of organic photovoltaic devices. The platform includes a novel approach to ultrafast, simultaneous data acquisition from eight detectors in parallel to obtain spatially resolved chemical and electronic information at near micron length-scales. Enabling the collection of imaging data on a submicron length-scale allows data to be gathered that will help guide the development of more efficient organic solar cells.



Schematic of a scanning photoionization microscope to investigate the electronic structure of heterogeneous interfaces in organic photovoltaic cells. ACC-F Variable Band-gap Block Co-Polymers Made from n-type Organoborane Polymers and p-type Thiophene Polymers for Photovoltaics Diane Hinkens, South Dakota State University CHE-0836082

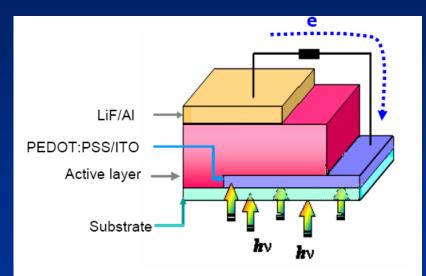
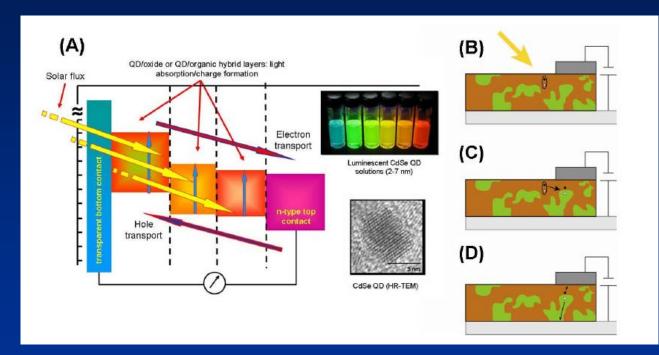


Figure 4. Schematic diagram illustrating the photovoltaic device architecture. Four different active layers will be used: (1) p-type polymer / n – type polymer; (2) p - type polymer / C60; (3) n - type polymer / C60; (4) p - n block polymer / C60.

Dr. Hinkens will synthesize and study the properties of new types of variable band gap block copolymer materials for phtovoltaic applications. Hinkens will work with scientists at Argonne National Laboratory. In her plan for broadening participation, she will develop handson activities describing photovoltaic materials for inclusion in the mobile science laboratory "Science on the Move" that travels across South Dakota, reaching small rural schools as well as schools on Native American reservations. In addition, she will develop a photovoltaic laboratory for the Chemistry Van of the Chicago Science Alliance -- which supports science teachers in the Chicago Public Schools.

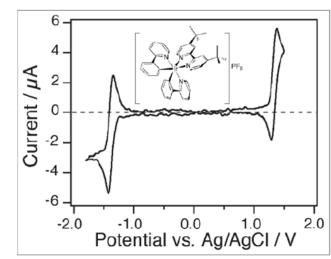
ACC-F: Investigating the Energy Levels of Semiconductor Nanocrystal-Polymer Hybrid Materials

Andrea Munro, University of Arizona CHE-0836096



Dr. Munro will synthesize and study the properties of semiconductor nanocrystals (CdSe) embedded in a polymer matrix. Dr. Munro will work in collaboration with scientists at the National Renewable Energy Laboratory. In her plan for broadening participation, she will develop hands-on materials with associated curriculum to be used by teachers of grades K-6 in the Tucson and Sunnyside school districts. Some of these materials may be modified for use in the University of Arizona Biosphere II for outreach to the general public.

CAREER: Synthetically Tuned Luminophoric Materials: 3D Displays, Solar Energy Conversion and Beyond Stefan Bernhard, Princeton University CHE-0449755



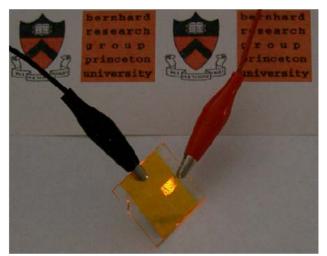


Figure 3: The libraries will be screened for complexes with redox behavior similar to the cyclic voltamogram depicted above. Efficient electro-luminophores possess a gap between the 2 redox waves that exceeds the energy of the excited state and exhibit excellent reversibility for both redox couples (left) An electroluminescent device in air prepared in 30 min employing gilding techniques (right).

Parallel synthetic techniques and parallel screening techniques for photochemical and electrochemical properties will target photoconversion efficiency and stability of photoactive materials. Rigid cage structures will be utilized to inhibit non-radiative decay processes. Combinatorial techniques will be employed to screen the excited state properties of new coordination based materials for both light emitting diode and solar energy conversion applications. Ionic transition metal luminophores will be investigated for light emitting diode development, chiral metal complexes with mesogenic tails will be employed to generate dissymmetric emission (circularly polarized luminescence). Materials with long lived excited states will be identified and examined for electron transfer quenching with redox mediating reagents to explore photolytic cleavage of water using high throughput analysis of gaseous products. An outreach program at Princeton High School that exposes students to optoelectronics will be extended to additional schools, and visits to elementary schools will be expanded to urban New Jersey sites.

CAREER: Rationally Assembled Nanoparticles for Multi-Electron Transfer Processes Sherine Obare, University of North Carolina at Charlotte CHE-0811026

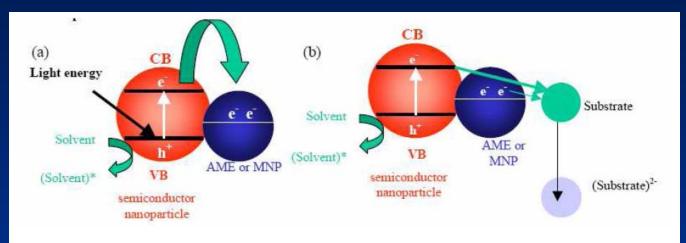
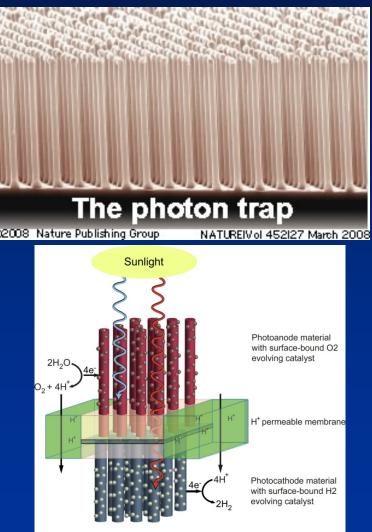


Figure 1. Proposed mechanism (a) Semiconductor irradiation promotes an electron from the valence band (VB) to the conduction band (CB). The holes in the valence band react with the solvent to produce the oxidized solvent (solvent *). Electrons transfer from the conduction band to the interface. (b) Reactive electrons from both the semiconductor and the metal are transferred to the substrate.

The goal of this work is to design, synthesize and characterize nanoscale multi-electron transfer catalysts. Using stopped flow kinetic measurements, coupled with radical clock methods, the complex flow of electrons in these transfer catalysts are being examined. The work provides a unified framework for multi-electron transfer at the nanoscale, which will impact both fundamental scientific understanding and applications in solar energy conversion, electrocatalysis, and photonics. A well integrated program to incorporate this research into the education of graduate, undergraduate, and high school students is underway, and will result in the dissemination of information about nanomaterials and nanoscience and engineering to the general public.

Center for Powering the Planet Harry B. Gray, California Institute for Technology CHE-0802907

- Grand challenge- efficient and economical conversion of solar energy into chemical fuel (H₂, O₂)
- Focus on developing the components for a solar water splitting system
 - membrane-supported assembly that captures sunlight and transports charge,
 - two-electron catalyst that reduces water to H₂ and
 - four-electron catalyst that oxidizes water to O₂.
- Involves 16 academic researchers across 10 institutions with NIST, NREL, and Brookhaven as partners



Renewable Energy Materials Research Science and Engineering Center

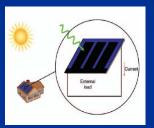
- MRSEC at the Colorado School of Mines (CSM), Sept. 2008, PI: Craig Taylor
- Focus on renewable energy applications: photovoltaic materials and fuel-cell membranes
- Education of the next generation of energy professionals
- \$9.3M over 6 years: DMR and OMA
- Collaborations
 - NREL
 - 20 industrial companies













Examples 3rd generation –nanosystems integrated with microtechnology Solar Energy Cells with focused energy

Consortium led by the University of Delaware has developed a highperformance crystalline silicon solar cell platform (focusing the light) that has achieved 42.8 percent solar efficiency in 2007 at standard terrestrial conditions.

Working under way to achieve 50 percent efficiency (production planned by 2010) http://www.azonano.com/news.asp?newsID=4546

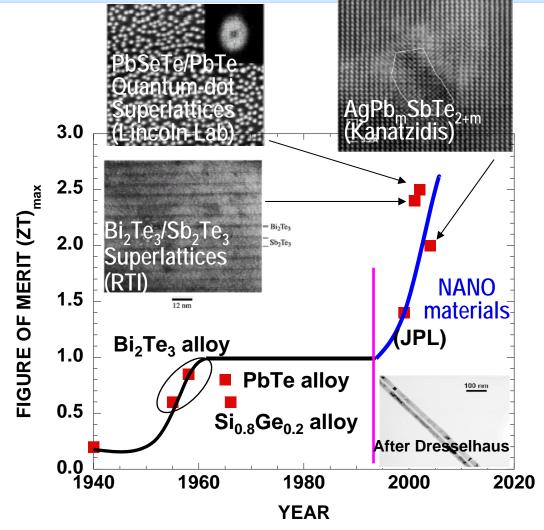
"Nano-generator" fabric with zinc oxide nanowires

Converts low-frequency vibrations into electricity: nanowires in the fabric generate electricity by rubbing together when set in motion by disturbances such as heartbeats and footsteps (currently 80 milliwatts per m² of fabric). Zhong Lin Wang, Georgia Tech.

Example 3rd generation – nanosystems integrated with microtechnology

Direct thermo-electric energy conversion

COLD SIDE N HOT SIDE Electron flux versus phonon flux

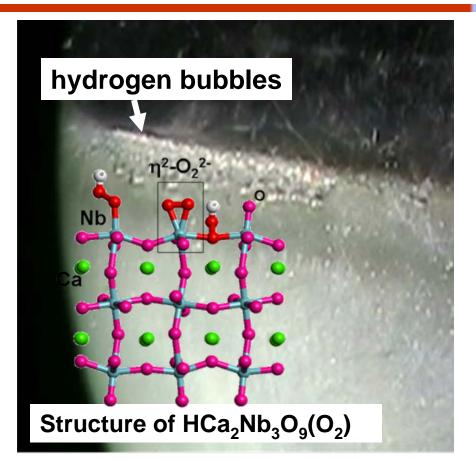


Using nanostructures promises figures of merit up to ZT = 10 Chen, MIT)

MC Roco, 2010 04 06

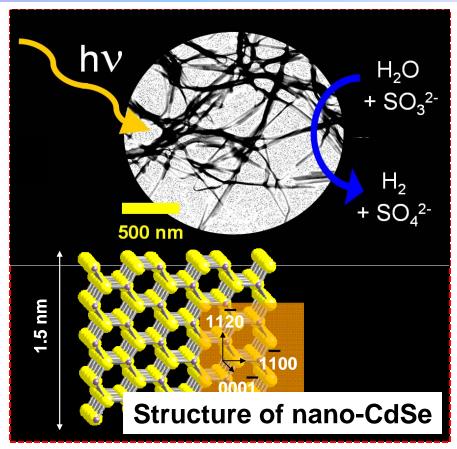


Solar Fuels: Modular Construction of Nanostructured Catalysts for Solar H₂ Generation from Water Frank E. Osterloh - University of California-Davis



New Catalyst: Catalyst-Bound Peroxide Identified as Deactivating Reagent

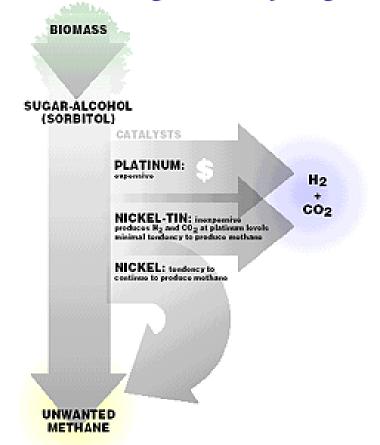
CBET 0829142



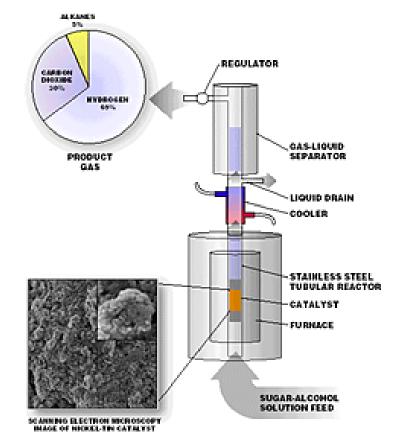
New Phenonema: Quantum Size Effect Activates nano-CdSe for Photocatalytic H₂ Evolution under Visible Light

Hydrogen from Biomass via a Nanostructured Catalyst

The goal was to find a catalyst to convert sugar alcohol to high-value hydrogen fuel.

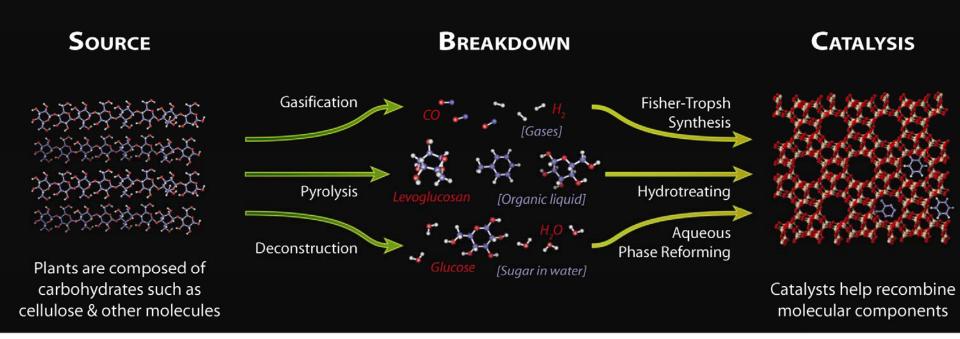


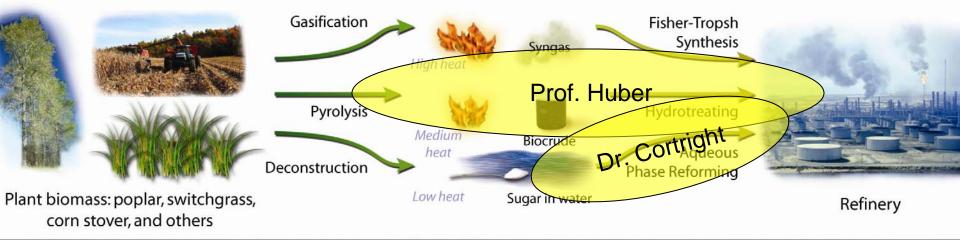
J. Dumesic et al., University of Wisconsin at Madison



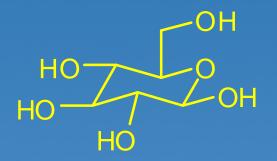
Raney-NiSn catalyst for renewable production of hydrogen for fuel cells by aqueous-phase reforming of biomass-derived hydrocarbons

Green Gasoline: A Renewable Petroleum Alt



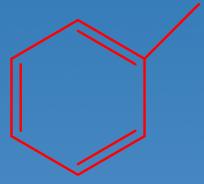


Green Gasoline by Catalytic Fast Pyrolysis



Woody Biomass: wood waste, agricultural wastes (corn stover, sugarcane waste), paper trash, energy crops.





Green Gasoline: Xylenes and Toluene

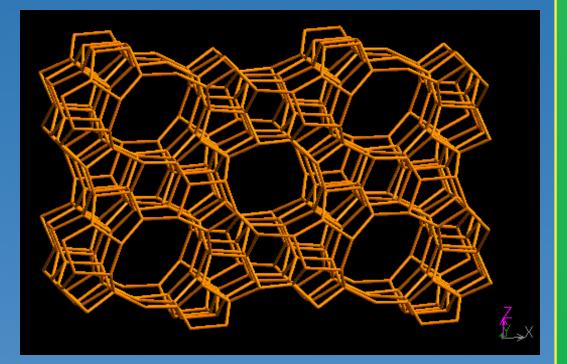
By Products: Water, Carbon Dioxide



Carlson, Vispute, and Huber, Green Gasoline by Catalytic Fast Pyrolysis

Enabling Science: Zeolites

- Zeolites are workhorse of petrochemical industry.
- Zeolites have well defined pores (shape selective).
- Reaction is controlled by pore structure and catalytic sites.



Zeolites: the jewel of nanotechnology.





Most proposed biomass crops are wild, undomesticated species

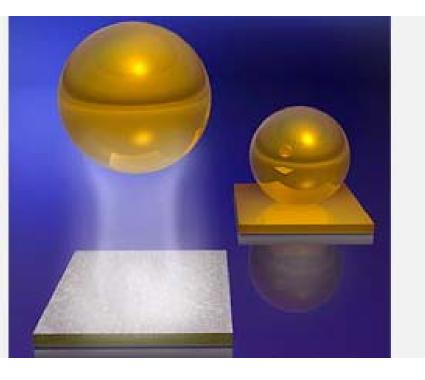


Photo credit: Jake Eaton, Potlatch Corporation



Discovery of Nanoscale Repulsion

Federico Capasso, Harvard University

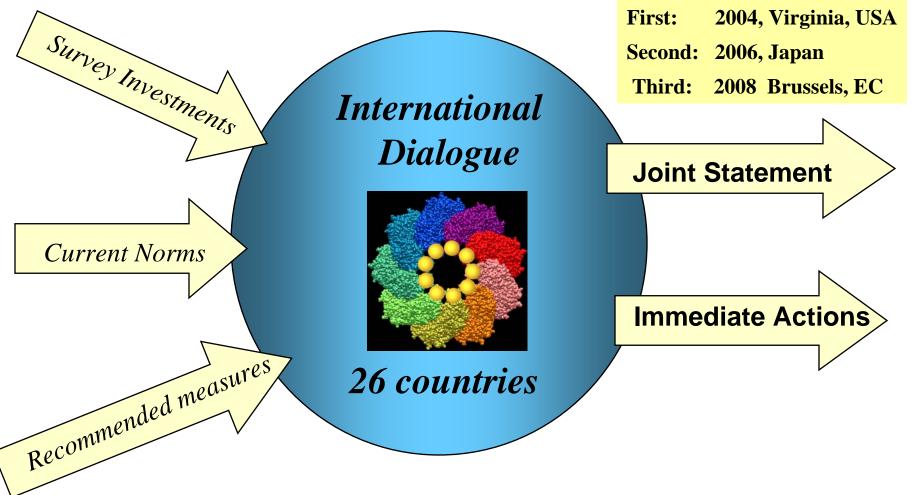


<u>A repulsive force arising at</u> <u>nanoscale was identified similar</u> <u>to attractive repulsive Casimir-</u> <u>Lifshitz forces.</u>

As a gold-coated sphere was brought closer to a silica plate a repulsive force around one ten-billionth of a newton was measured starting at a separation of about 80 nanometers.

For nanocomponents of the right composition, immersed in a suitable liquid, this repulsive force would amount to a kind of quantum levitation that would keep surfaces slightly apart

<u>Inclusive governance</u> - Ex: International Dialogue on Responsible Nanotechnology R&D since 2004



June 2004, Virginia

http://www.nsf.gov/home/crssprgm/nano/dialog.htm

MC Roco, 2010 04 06

Follow up activities after the First International Dialogue on Responsible Nanotechnology R&D (2004)

Coordinated activities after the June 2004 International Dialogue

- October 2004 / October 2005 Occupational Safety Group (UK, US,.)
- November 2004 OECD / EHS group on nanotechnology begins
- December 2004 Meridian study for developing countries
- December 2004 Nomenclature and standards (ISO, ANSI)
- February 2005 North-South Dialogue on Nanotechnology (UNIDO)
 - International Risk Governance Council (IRGC)
 - "Nano-world", MRS (Materials, Education)
 - Interim International Dialogue (host: EC)
- October 2005 OECD Nanotechnology Party in CSTP
- June 2006

May 2005

May 2005

July 2005

- 2nd International Dialogue (host: Japan)
- 2006 Int. awareness for: EHS, public participation, education
- 2007-2009 new activities

OECD, Chemicals Committee, WPMN

2005- (http://www.oecd.org/env/nanosafety/)

OECD: Working Party on Nanotechnology (WPN)

Working Party on Nanotechnology, 2007-(http://www.oecd.org/sti/nano)

- A. Statistics and Measurement
- B. Impacts and Business Environment
- C. International Research Collaboration
- D. Outreach and public engagement
- E. Dialogue on Policy Strategies
- F. Contribution of Nanotech to Global Challenges