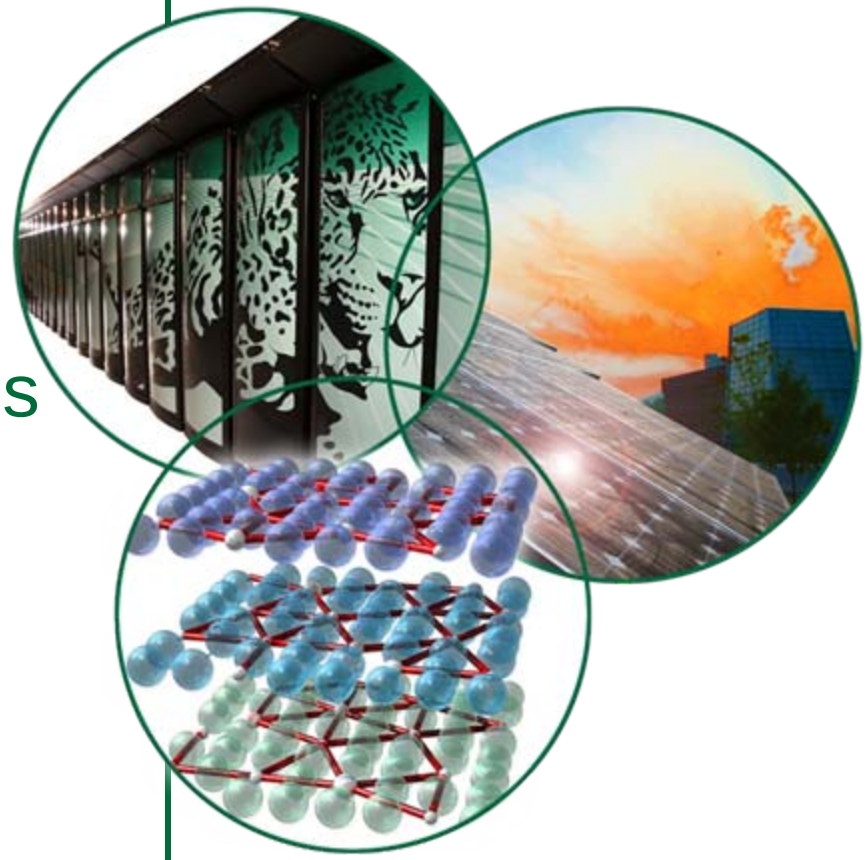
Computational Pathways to the Experimental Design of High Performance Photovoltaic Solar Cells



Sheila N. Baker, ORNL

Fall Creek Falls Workshop
September 23, 2009

U.S. DEPARTMENT OF ENERGY

OAK RIDGE NATIONAL LABORATORY
MANAGED BY UT-BATTELLE FOR THE DEPARTMENT OF ENERGY

Energy – Where do we get it from and why care?

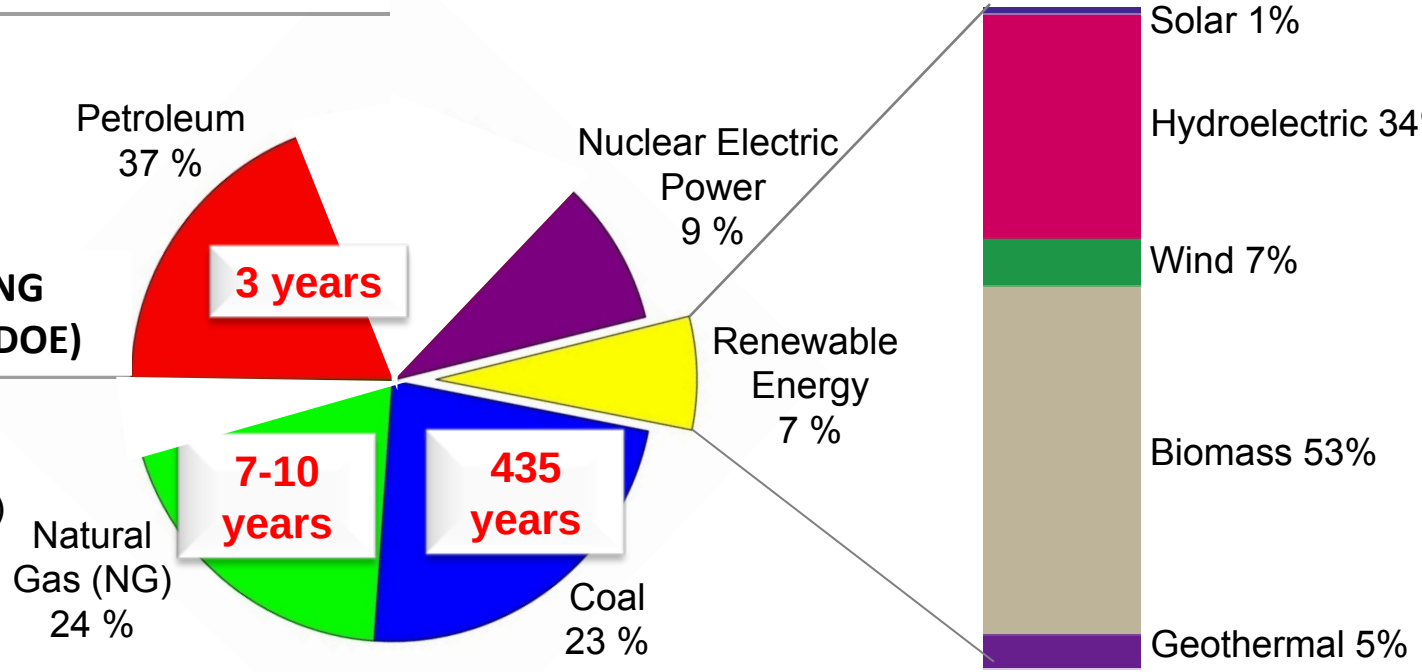
- Fossil fuels are *nonrenewable!* (a resource that cannot be reused or replaced easily. Source: 3rd grade science textbook)
- National Security /Energy Independence

U.S. Dependence on Net Petroleum Imports 58.2% (DOE)

US Reserves
~ 22,014 million barrels
US Consumption
19.5 million barrels/day

U.S. Dependence on NG Imports 17-20% (2007, DOE)

US Reserves
~ 237,726 billion cubic ft
US Consumption (yearly)
23.047 billion cubic ft



US Reserves ~ 491 billion short tons
US Consumption (yearly) 1,128 million short tons

www.eia.doe.gov

Energy – Where do we get it from and why care?

- Fossil fuels are *nonrenewable! (*a resource that cannot be reused or replaced easily. Source: 3rd grade science textbook)
- National Security Energy Independence
- Environmental Damage -human responsibility

Energy – Where do we get it from and why care?

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- National Security Energy Independence
- Environmental Damage -human responsibility
- $$$$$, Technological Advances

"There is no reason anyone would want a computer in their home."
—Ken Olson, President, Chairman, and Founder of Digital Equipment Corporation, 1977

"I watched his face (Samuel F.B. Morse) closely to see if he was not deranged, and was assured by other Senators as we left the room that they had no confidence in it either."
—Senator Oliver Smith of Indiana, 1842, after witnessing a first demonstration of the telegraph

"Well-informed people know it is impossible to transmit their voices over wires, and even if it were possible, the thing would not have practical value."
—Editorial in the Boston Post, 1865

Bottom Line – We need Renewable energy resources, Renewable energy resources—such as wind and solar energy—are constantly replenished and will never run out (at least not for 5.5 billion years).

Steven Chu "By 2050, we need to reduce carbon emissions by 80% or more. To reach that goal we will need transformative new technologies."

10 TW of carbon-emission-free power by 2050 (equivalent to power of all energy sources in 1998 combined)

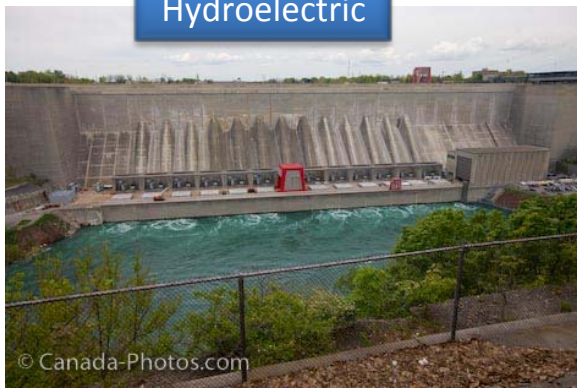
Not just a Challenge, but a *Necessity* for today!

How do we get there?

More energy strikes the world in 1 hour.
Then the entire world uses in 1 year!
Solar is only 1% of renewable energy sources used today,
yet it is largest sustainable source of energy!

- Our options…….

Hydroelectric



Biomass

Nuclear Power

2009 - Presid n
accele es
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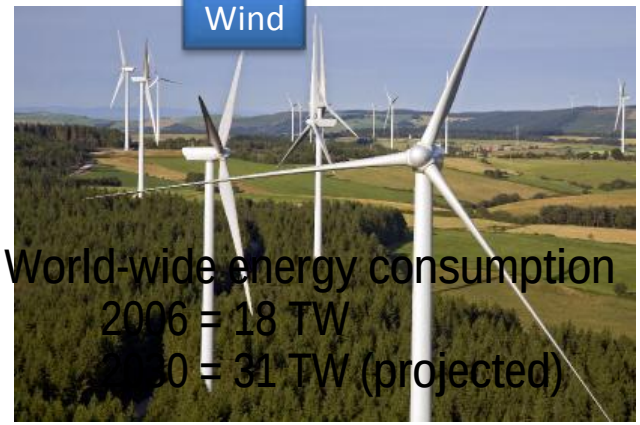
The trick is to *effectiv*

Wind

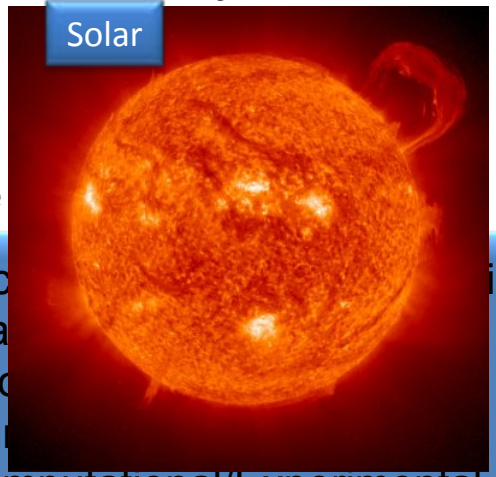


World-wide energy consumption
2006 = 18 TW
0 = 31 TW (projected)

Sun's Energy Production
120,000 TW

Geothermal

Solar



ive
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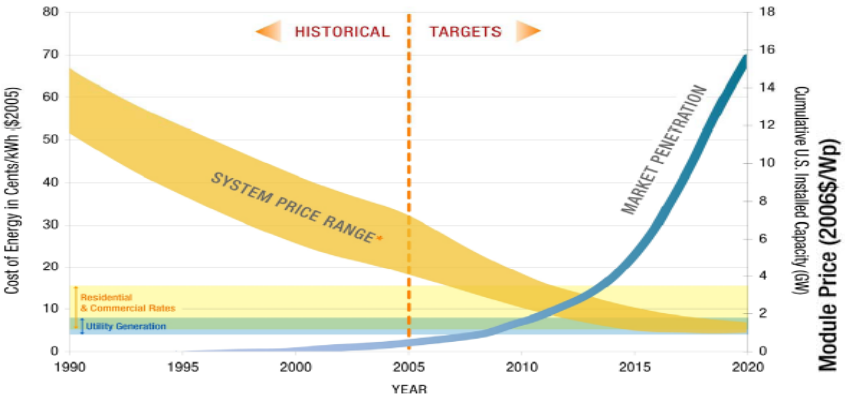
e-a
what needs to
methods for i
Computational/Experimental

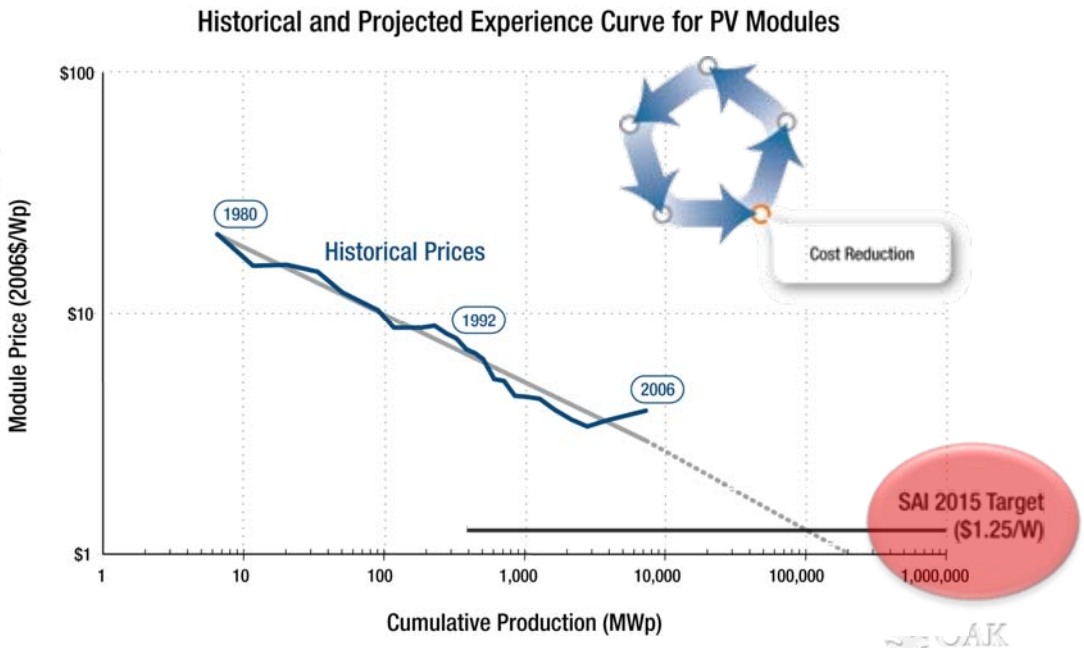
So, why not use solar

- Current technologies are inefficient – only using a small portion of the sun's rays and suffer from conversion losses
- Sun doesn't illuminate all of the earth 100% of the time.
  - Need for storage
- Expensive compared to cost of current electricity.

Best PV systems on market now are $3-5/Wp



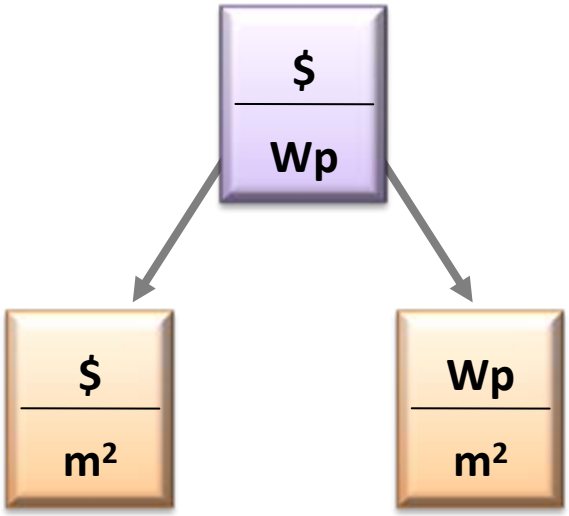
Market Sector	Current U.S. Market Price Range (¢/kWh)	Cost (¢/kWh) Benchmark 2005	Cost (¢/kWh) Target 2010	Cost (¢/kWh) Target 2015
Residential	5.8-16.7	23-32	13-18	8-10
Commercial	5.4-15.0	16-22	9-12	6-8
Utility	4.0-7.6	13-22	10-15	5-7



Metrics Involved in lowering cost

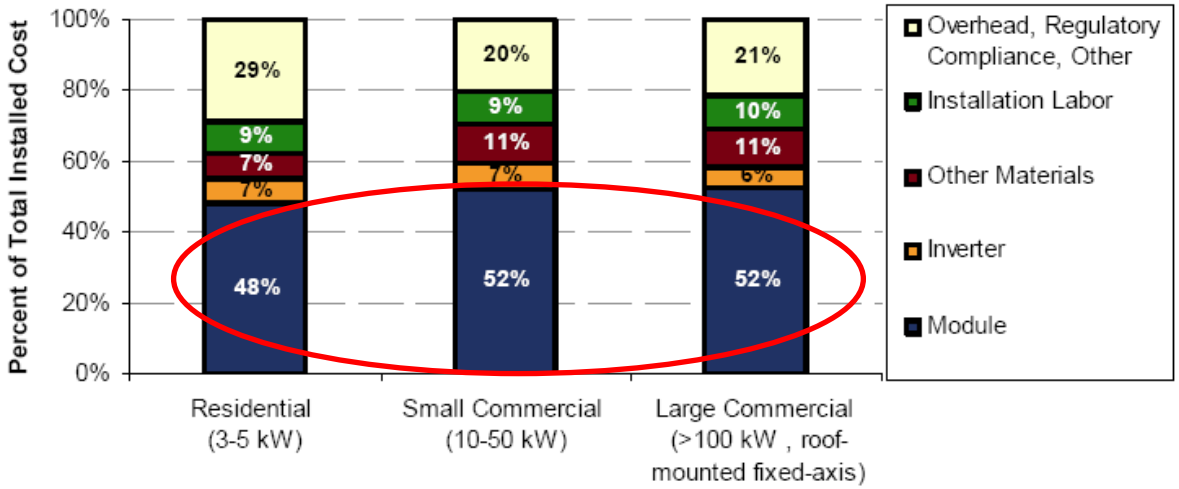
< $1/Wp

Two ways to get there



Manufacturing costs

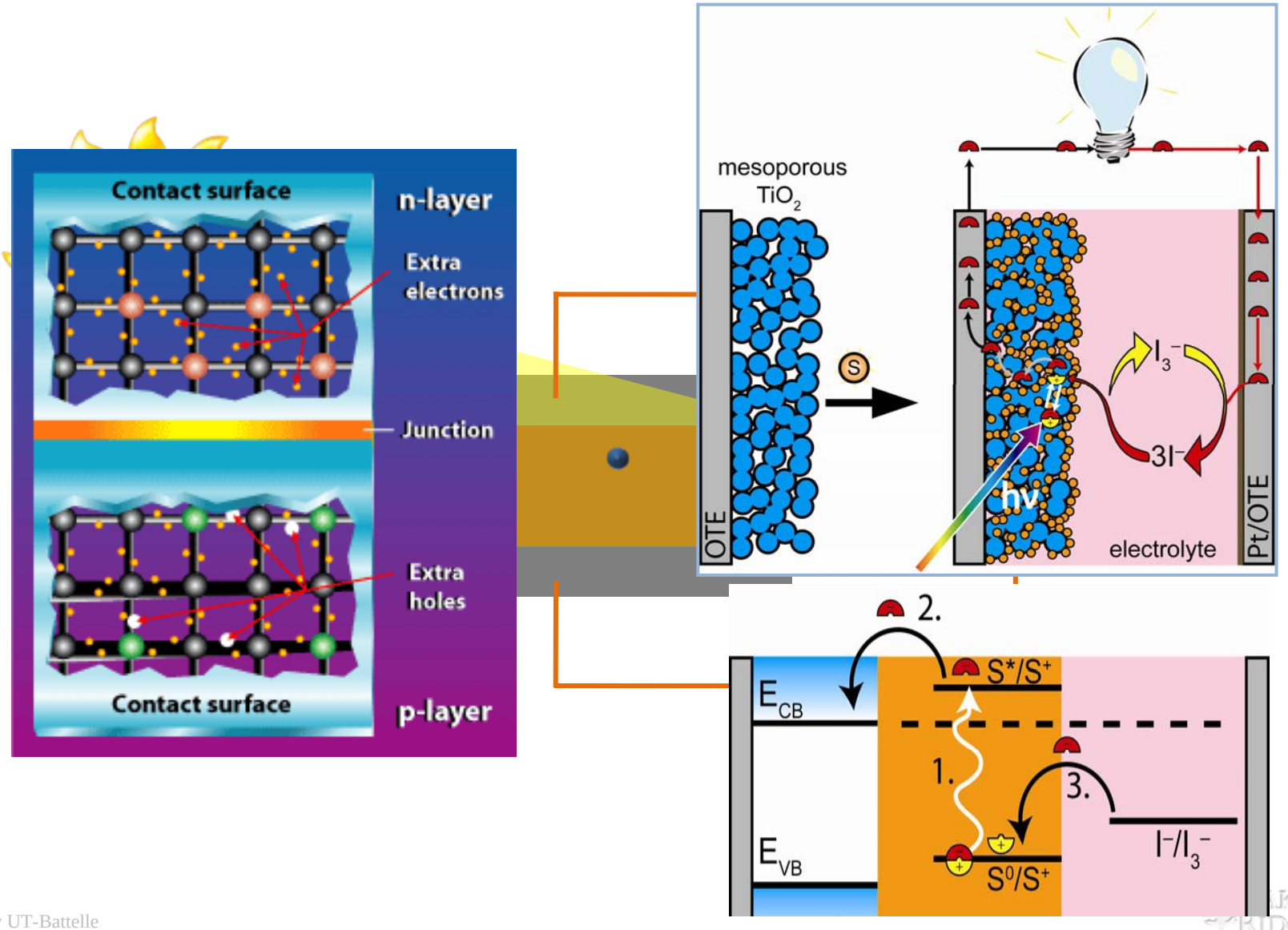
Efficiency



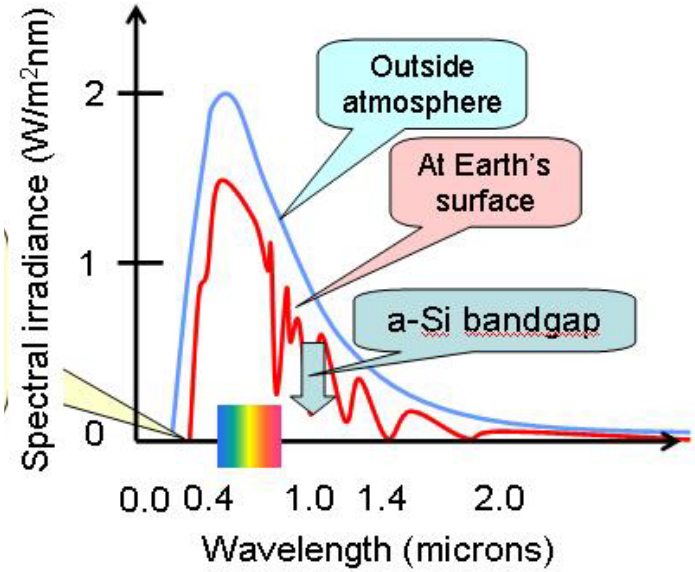
NEED:

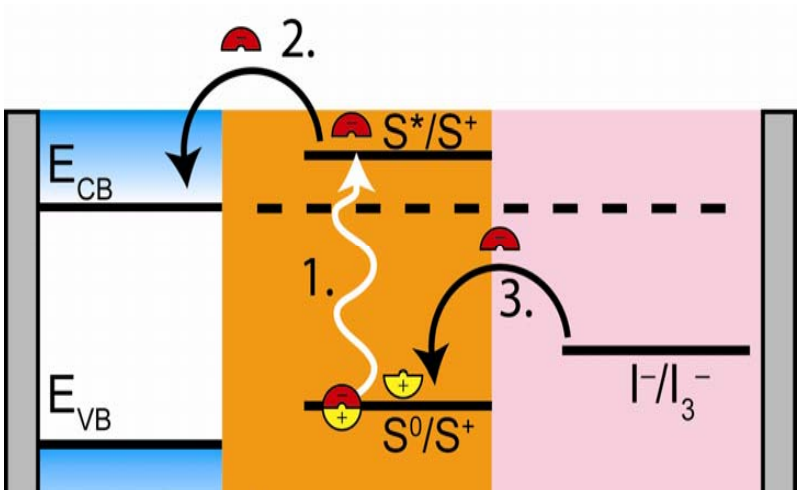
LOW COST AND HIGH EFFICIENCY

How do PV cells work?

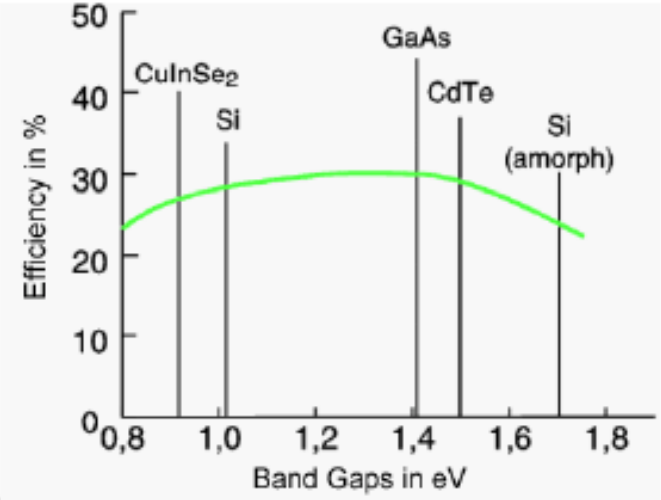


How do PV cells work?

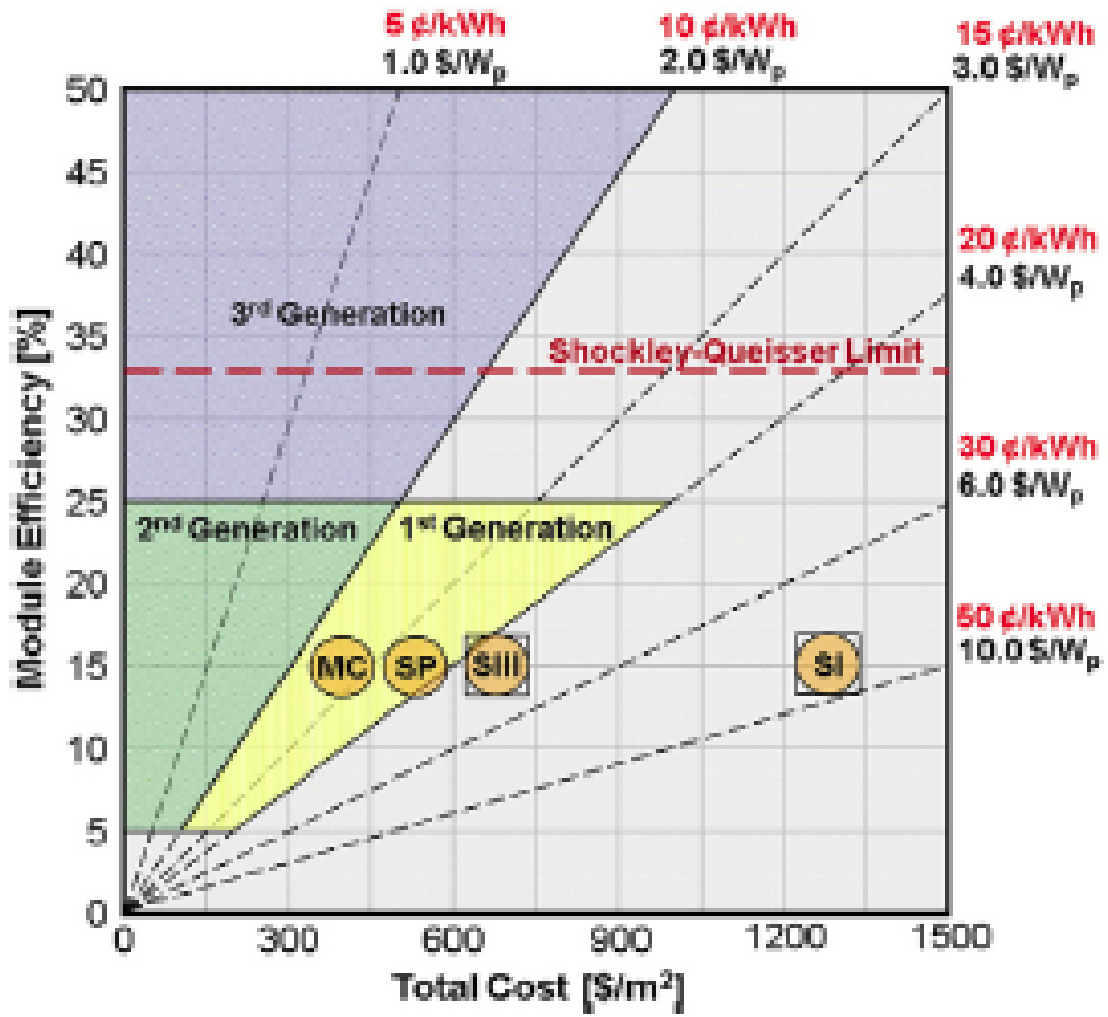




Shockley-Queisser Limit ~ 31%
Optimum Band Gap
= 1.3 to 1.6 eV



PV Technologies



3rd-Generation

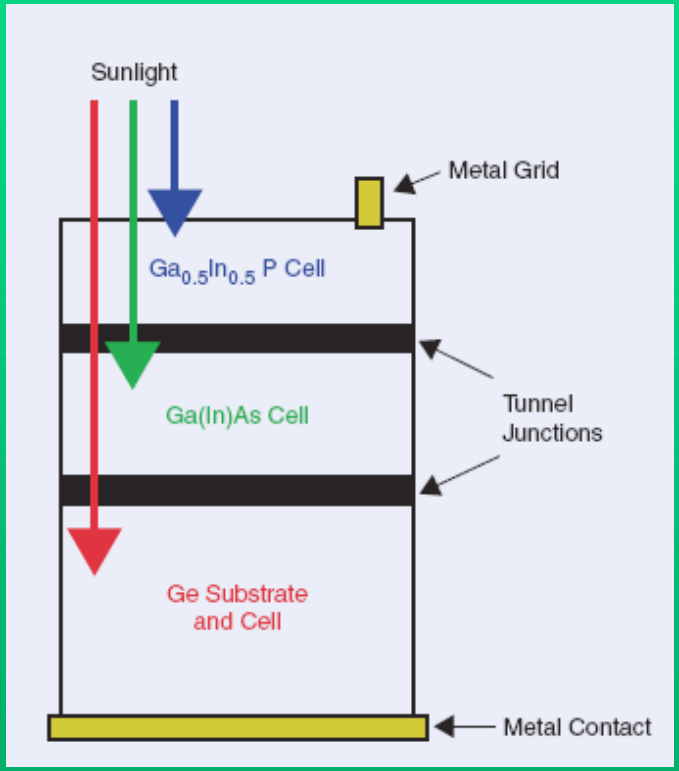
- Utilize photoconversion physics that can increase power conversion efficiencies beyond record 1st generation devices
- Multiple junction
- Multiple excition generation
- Optical frequency shifting
- Hot carrier solar cells

Hillhouse and Beard, Current Opinion in Colloid and Interface Science, 2009, 14, 245-259

How do we get to 50% or greater efficiency in PV cells?

- Improve light absorption

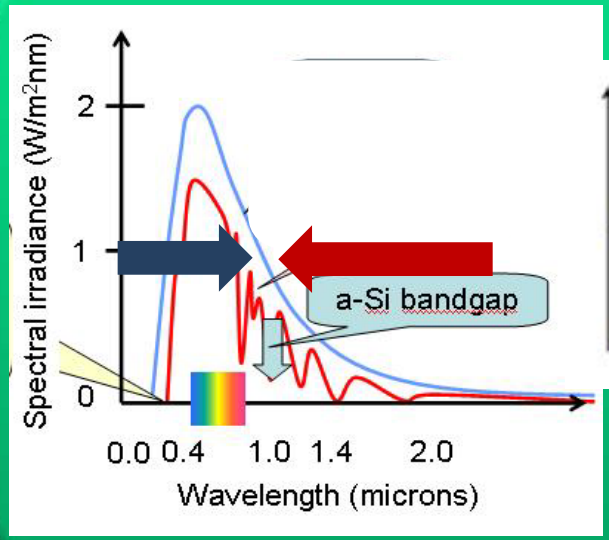
1) Multi-junction cells

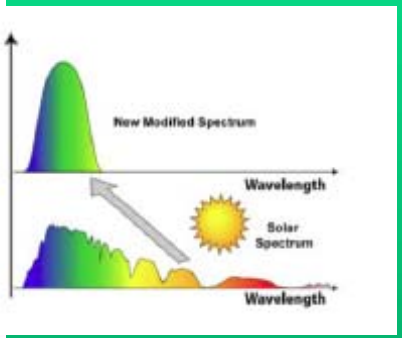


55.9, 63.8, 68.8% efficiencies

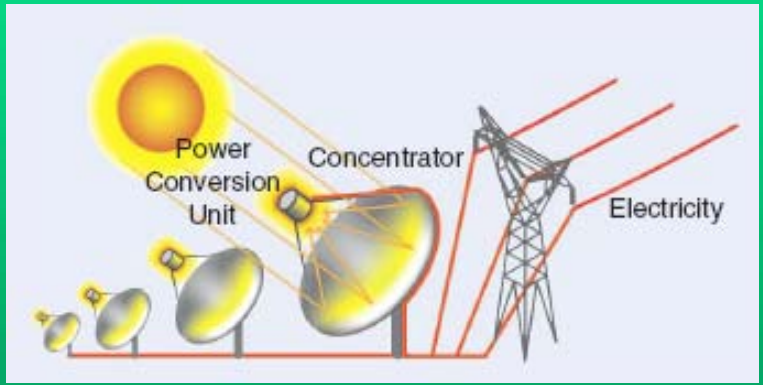
Green , 2006 Third-generation Photovoltaics:Advanced Solar Energy Conversion, Springer

2) Optical frequency shifting





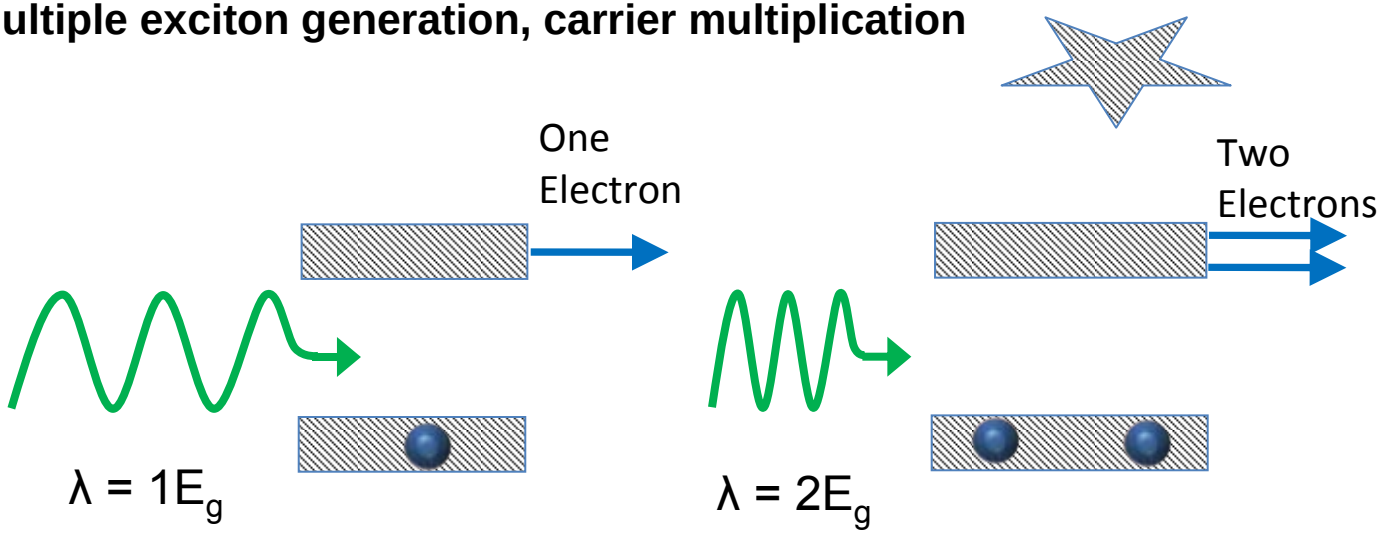
3) Concentrators

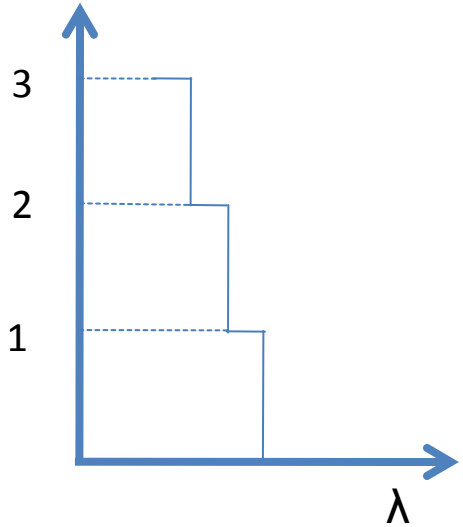


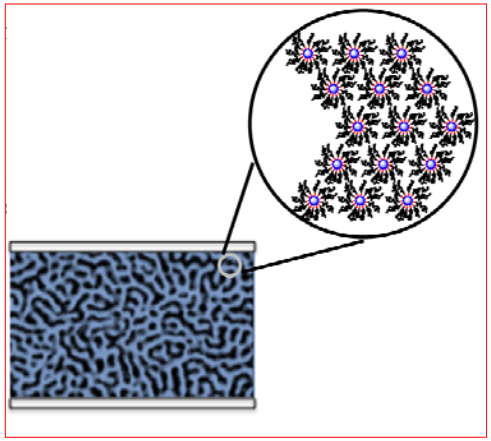
How do we get to 50% or greater efficiency in PV cells?

- Improve light absorption

3) Multiple exciton generation, carrier multiplication





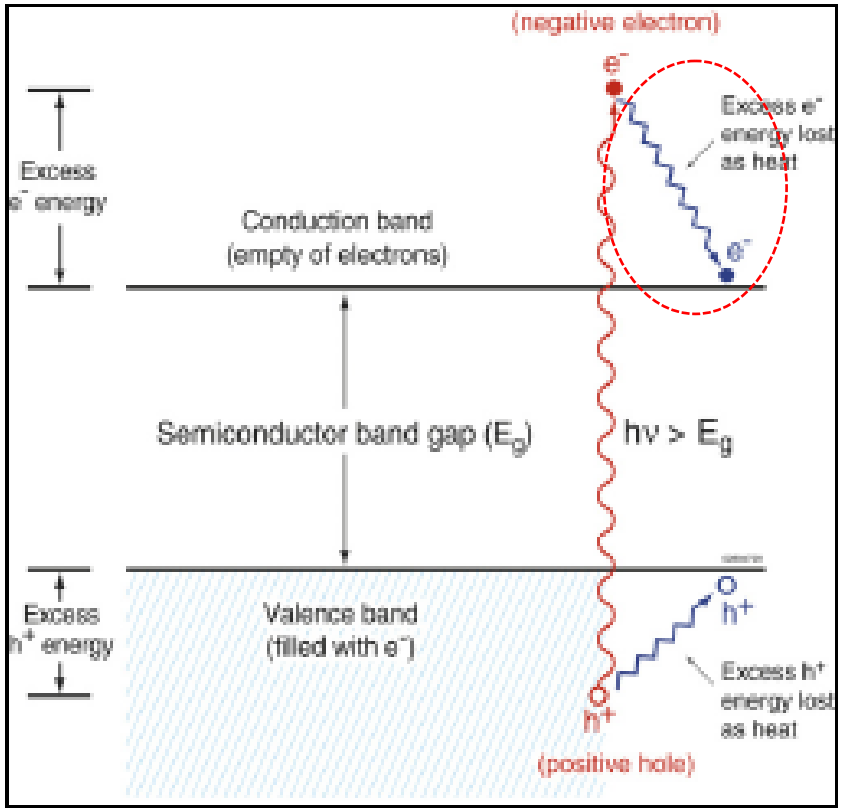


Variations in MEG efficiency observed depending on nanocrystal size and surface treatment

Nano Lett. 2009, 836-845

How do we get to 50% or greater efficiency in PV cells?

- Reduce Thermal Losses - Hot carrier cells



fs-ps timescale
Finite velocity ~10 nm

Eliminate Auger cooling = slow process down

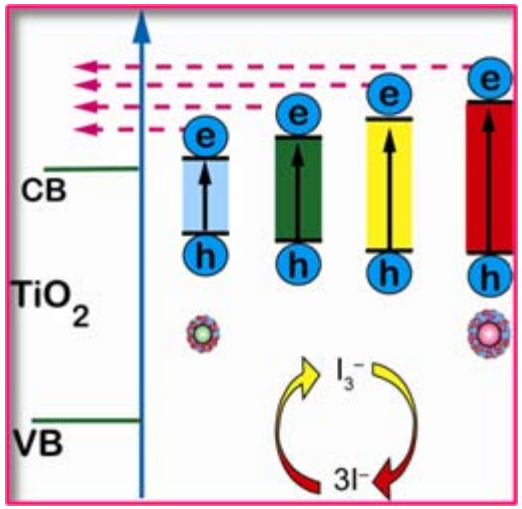
Time-dependent density functional theory studies
J. Phys. Chem. C 2007, 111, 4871-4878.

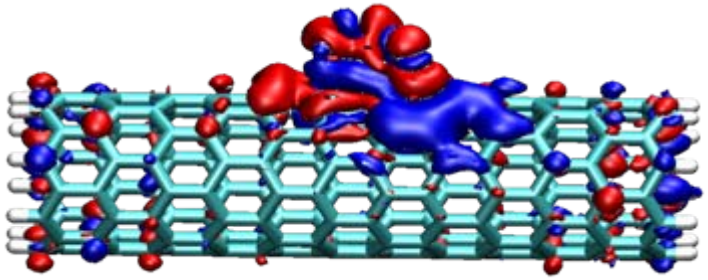
Size, surface chemistry impact rate

Proper surface modification (core/shell/shell) slowed rate to ns
Science 2008, 322, 929-932.

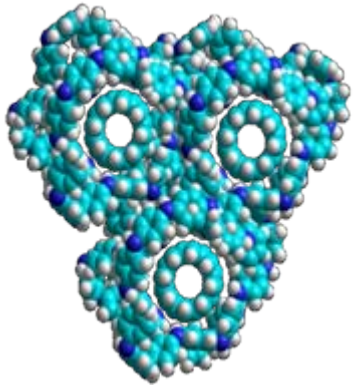
How do we get to 50% or greater efficiency in PV cells?

- Improve Charge Transfer



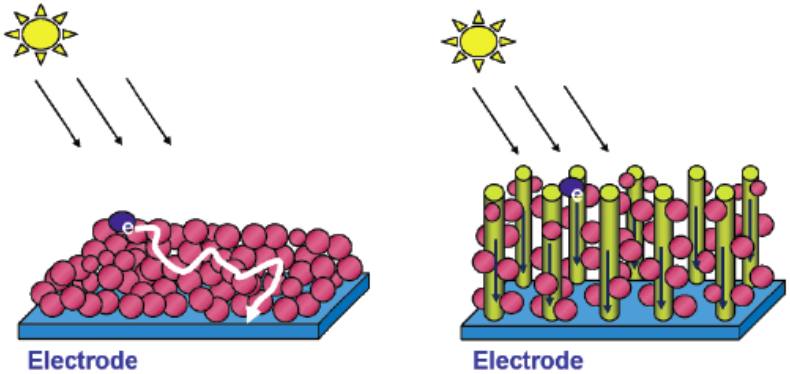


Charge transfer at an interface

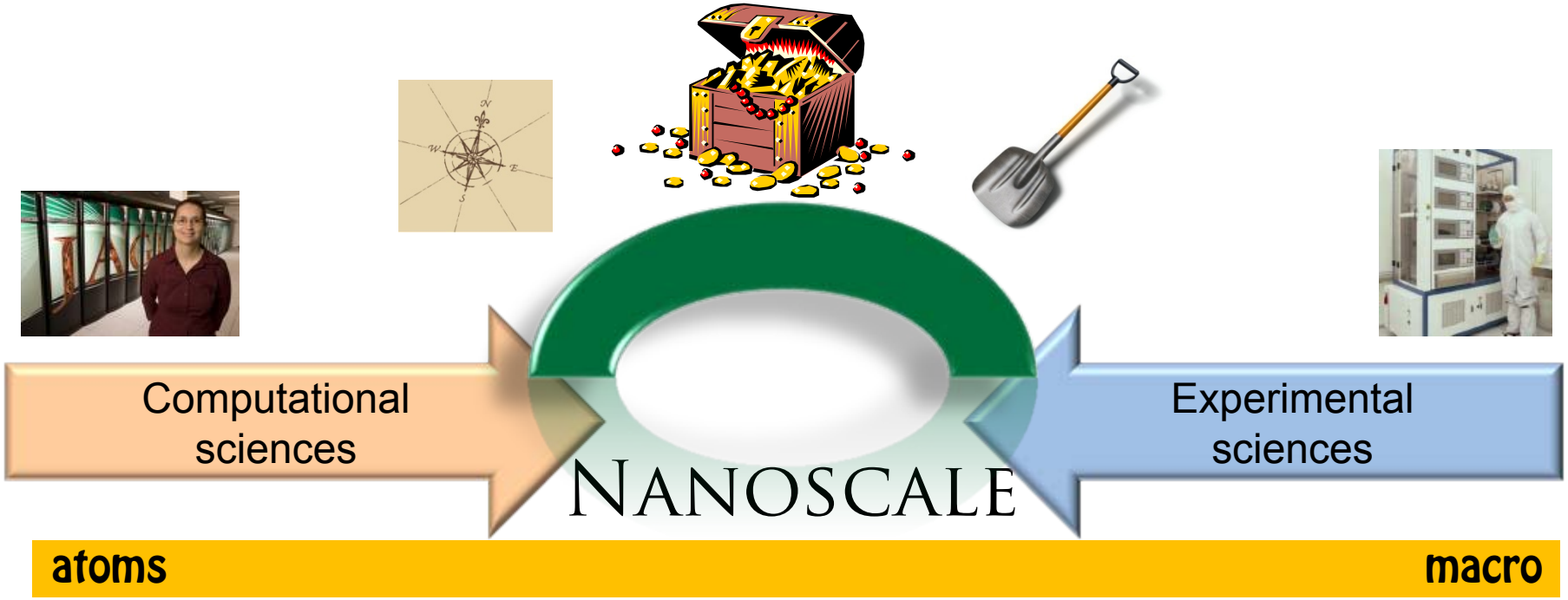


Polymer-carbon nanotube heterjunctions

- Improve Carrier Transport



Path to high efficiency, low cost PV



Nanocrystals present tantalizing possibilities to modify electro-optical properties:

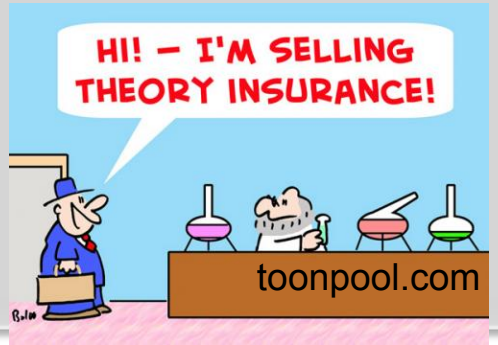
Light absorption - exciton generation

Exciton dissociation

Electron and hole transport

Charge transfer across nanocontacts

Simulations can help one understand and design such materials with confidence



Computational roles –requires computing power

- In order to improve PV quickly, large scale computation *must* play an important role..
- Due to the recent advance in computational power and new algorithms, it is now possible to calculate the electronic structures of nanosystems with tens of thousands of atoms with ab initio accuracy (photon absorption, exciton generation, exciton dissociation, carrier transport and carrier collection.)

Challenges that May be Addressed with Advanced Computing and Mathematics Capabilities

- Modeling of mesoscale structure (lengths of 100's nanometers) and time scales of micro to milli-seconds
- Interface modeling requires high level quantum many-body description (strong confinement effects)
- Exciton generation, migration, and dissociation require new time dependent quantum approaches

- The most difficult challenges are the carrier dynamics and the atomic structures of the surface and interface.
  - –carrier dynamics might involve both coherent and incoherent electron movements. As a result, expensive time-domain simulation might be necessary.
  - –More details on how the surface electronic structures which can determine the carrier dynamics must be fleshed out experimentally and computationally

Need Teams of Scientists….

- **Combination of chemistry, materials science, physics, computational modeling, engineering, industry, business partners, etc**

"…..basic and applied science flourish side by side, so that each contributes to the nourishment of the other. We have learned from our experiences that the key to progress in science and technology is highly gifted and dedicated people working in an environment that fosters ***cross-fertilization, involving a broad spectrum of sciences and technologies, ideas, concepts and such skills, as well as dreams and aspirations*****.** Such an environment cannot, for long, exist in a single-purpose, narrowly focused institution."

Hans Bethe and coauthors in a 1992 Los Alamos National Laboratory Newsbulletin guest editorial.

But the greatest marvel is not the size of the enterprise, its secrecy, nor its cost, **but the achievement of scientific brains in putting together infinitely complex pieces of knowledge held by many men in different fields of science into a workable plan.** And hardly less marvelous has been the capacity of industry to design, and of labor to operate, the machines and methods to do things never done before so that the brain child of many minds came forth in physical shape and performed as it was supposed to do. …. What has been done is the greatest achievement of organized science in history. It was done under high pressure and without failure.

Statement from President Truman on August 6, 1945

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Acknowledgements

- Vincent Munier, ORNL
- Bobby Sumpter, ORNL

Thank you for your time