The Role of University Research in Furthering PV Technology

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Classification of Solar Cells

Solar Cell

- Silicon
  - Bulk: Single Crystal, Poly-Crystal
  - Thin Film: Amorphous, Poly-Crystal
  - → Solar Photovoltaic Power Generation Buildings, Cars, Street light, Vessel
- Compound Semiconductor
  - Bulk: GaAs, InP
    - → Signal Beam, IR-Detector Power for Satellites
  - Thin Film: $CuInSe_2$, CdTe
    - → Lamps, Battery Chargers, Solar Toys
- Multi-layer Type
  - Thin Film: a-Si/c-Si, GaAs/Ge
  - → Sunroof, Auto Windows Residential Windows Commercial Curtain
- Dye-sensitized Type
  - TiO_2:Dye
  - → Cellular Phone, PDA Displays, Batteries
- Organic Semiconductor
  - Organic/Inorganic Nano Composites
  - → Power for Military Tent Mobile Military Units

What Determines University Research Areas?

Why do you rob banks, Willy?
"Cause that's where the money is"
Willy Sutton
Bank Robber

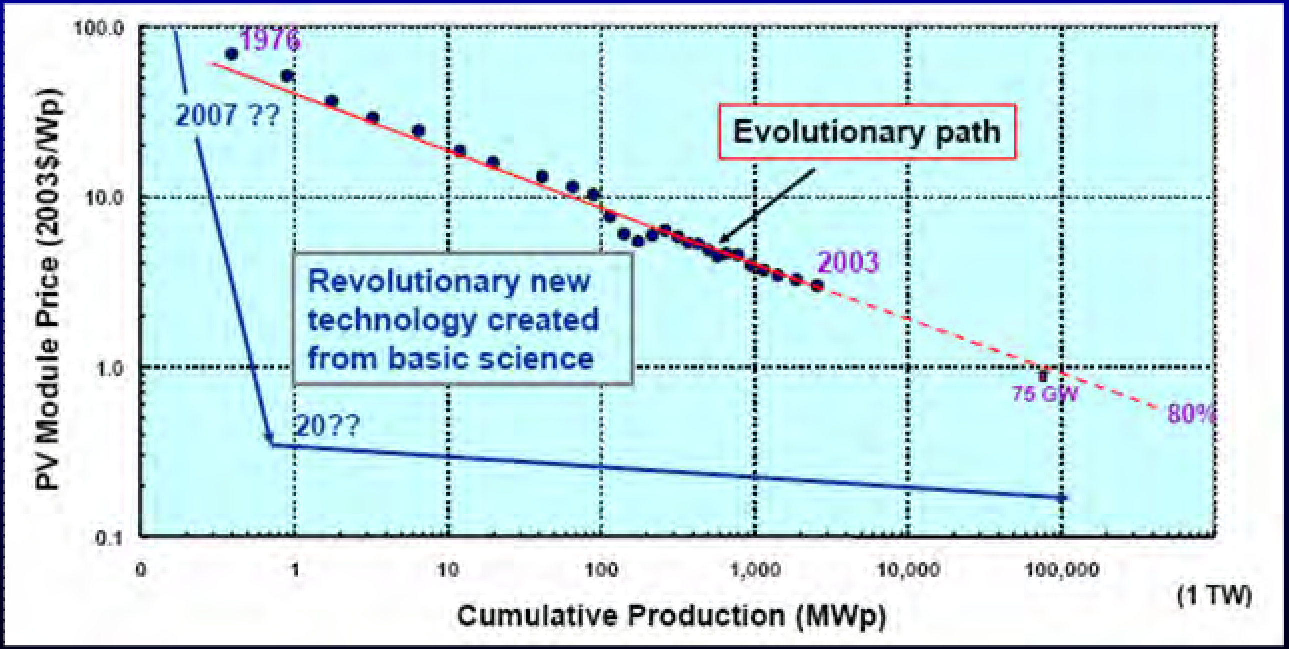
Photovoltaics R&D: DOE Funding Opportunities

PHASES	Material & Device Concepts	Device & Process Proof of Concept	Component Prototype & Pilot Scale Production	System Development & Manufacturing	
SOLICITATION	Solar Energy Utilization	Future Generation PV Devices & Processes	PV Component / System Incubator	University Product & Process Development Support	Technology Pathway Partnerships
FUNDING SOURCE	DOE/O/S, BES	DOE / SETP	DOE / SETP	DOE / SETP	DOE / SETP
DESCRIPTION	New materials and pathways for solar to electric conversion	Novel devices or processes with potentially significant performance or cost advantages	Prototype PV components or systems produced at pilot-scale with demonstrated cost, reliability, or performance advantages	Universities perform targeted materials science and process engineering research in support of industry-led teams developing new PV systems for commercialization in 2010-2015.	PV systems and components ready for mass production delivering energy at target costs
PROJECT LIFECYCLE	3 years	3 years	1.5 years w/ 9 mo. On/Off Ramp	3 Years	3 years
ANNUAL FUNDING LEVEL	\$0.3 - 1.5 Million	≤ \$300K	\$1 - 2 Million	Up to \$300,000/year	\$2 - 7 Million
TEAM LEADS	Universities or Laboratories*	Businesses or Universities*	U.S. Commercial Entity	Universities	U.S. Commercial Entity
ELIGIBLE PARTICIPANTS	All	All	Universities / Laboratories*	Universities	Universities / Laboratories
ENTRANCE CRITERION	Basic science properties conceived/simulated	Materials synthesized; properties observed	Coupon-scale PV cell; process demonstrated in lab; proof of concept demo	Identification of manufacturing process or component improvements possible through targeted research investigations.	Prototype components; pilot production demo; business case established
EXIT CRITERION	Materials synthesized; properties observed	Coupon-scale PV cell; process demonstrated in lab; proof of concept demo	Prototype components; pilot production demo; business case established	Incorporation of research results into commercial manufacturing operations or product designs.	Commercial PV systems and subsystems; scaled production demonstrated >25MW
TOPICS	• Single-crystal, polycrystalline, amorphous, and nanostructured inorganic and organic materials • Electronic structure • Single or multiple junction solar cells	• New devices and structures using materials such as thin-film silicon, microcrystalline/amorphous silicon, polycrystalline metal chalcogenides and oxides, nanocrystalline materials, biomimetic concepts, organic materials, photoelectrochemical cells, dye-sensitized materials, materials with low-dimensional quantum structures • Very-high efficiency epitaxial solar cells or other concepts	• Modules: multiple technologies (including CPV) seeking efficient material use, better performance, or improved manufacturing • BOS Components: higher reliability inverters, CPV trackers, rapid installation features, storage systems • Systems: controls and smart monitoring, integration of components, factory diagnostics	Identifying and developing: • Fabrication processes to improve material properties during manufacture • Improved solar cell materials • Innovative device designs to improve solar cell efficiency • Simpler, lower cost manufacturing processes • New electrical contacting techniques for improved efficiency and reliability • Diagnostic techniques to identify properties and quality of solar cells materials during manufacturing • Improved materials utilization processes • Understanding of chemistry between encapsulants and solar cell materials • Providing careful long-term field testing of modules and systems in support of product improvement	• Partnerships with U.S. industry for projects that focus on development, testing, demonstration, validation, and interconnection of new PV components, systems, and manufacturing equipment • Technology improvements in PV system and component design, integration, and installation will be a focus • Cost reductions, performance enhancements, and reliability improvements are sought for all aspects of PV systems

NOTE: The NREL and SNL teams that are part of the SETP program will continue to provide technical support for these activities through the SETP but will not be direct participants

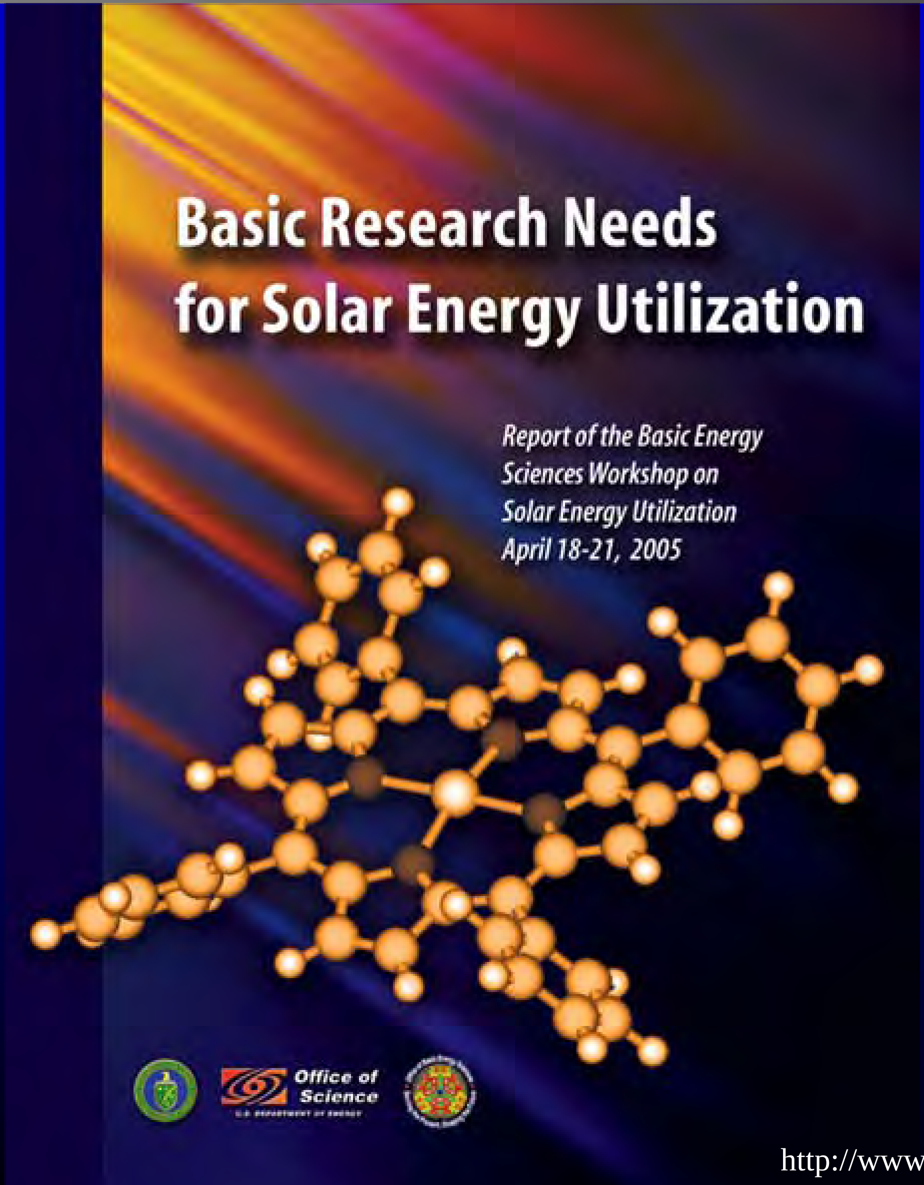
Role of Universities

- **Basic Research**
  - **Fundamental understanding**
  - **New technologies**



http://www1.eere.energy.gov/solar/solar_america/pdfs/d_horwitz_os_bes.pdf

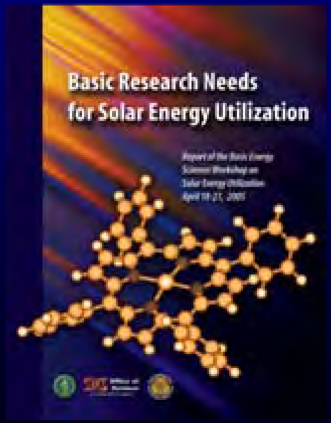
2005 BES Workshop Report



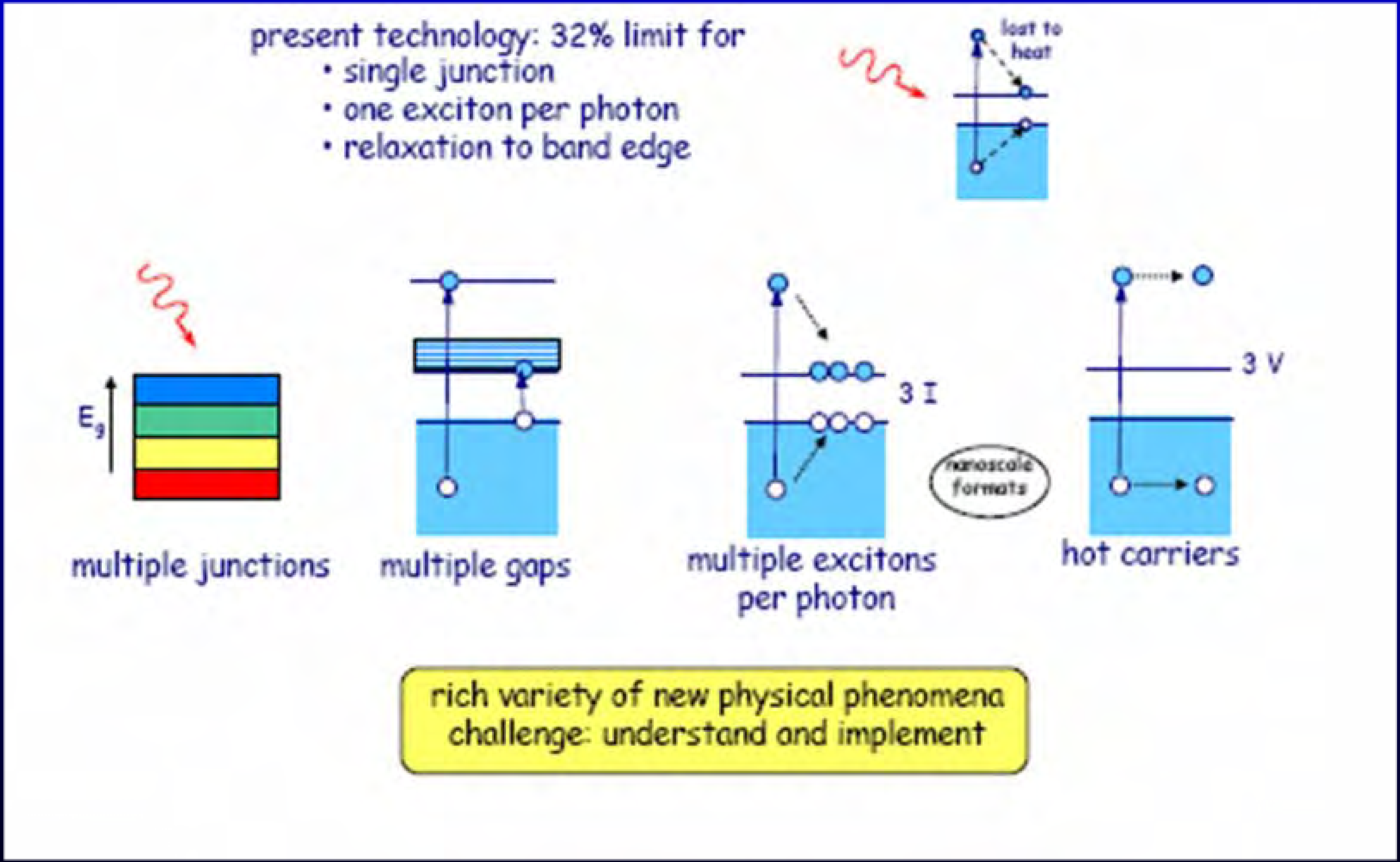
http://www.sc.doe.gov/bes/reports/files/SEU_rpt.pdf

Basic Research Recommendations

- New concepts in solar electric
- Organic and hybrid organic/inorganic conversion systems
- Photoelectrochemical solar cells
- Novel nanoscale and self-assembled materials
- Theory, modeling, and simulation



Routes to Increased Efficiency



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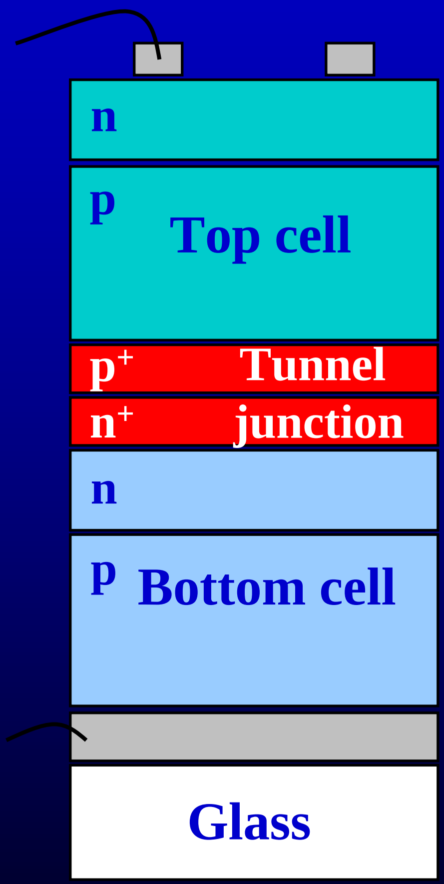
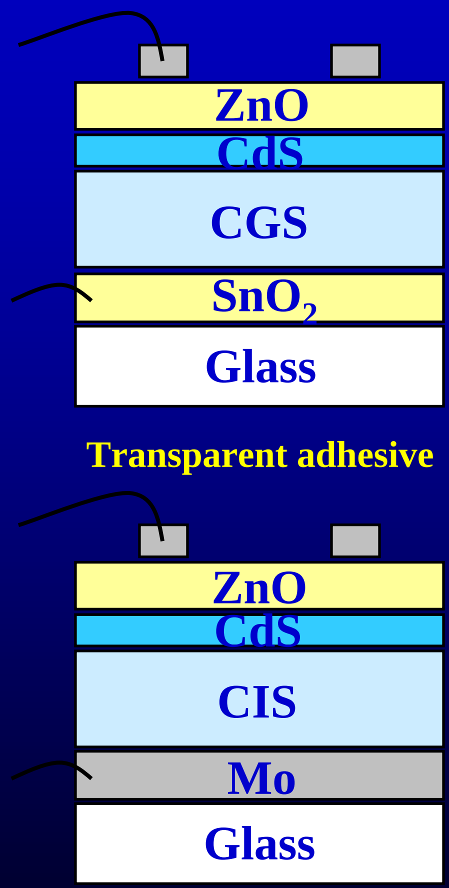
Tandem Cell Structures

Monolithic, two-terminal device



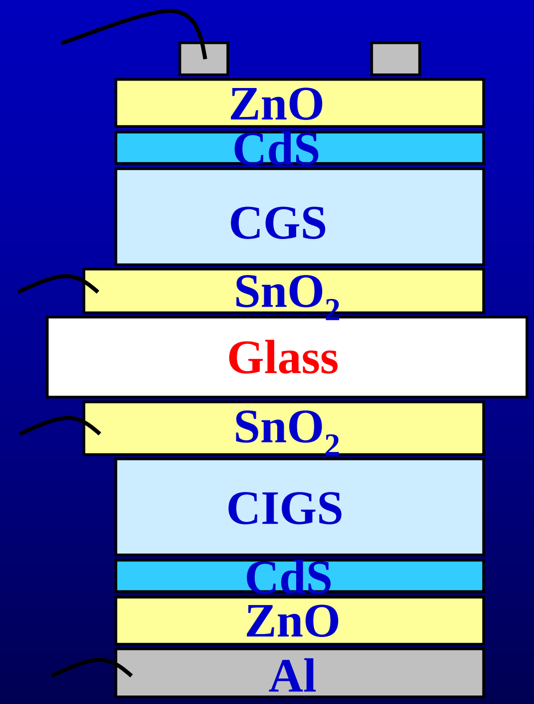
- Growth temperature limitation
- $E_{g,\ tunnel} \geq E_{g,\ top}$

Mechanically stacked, four-terminal device



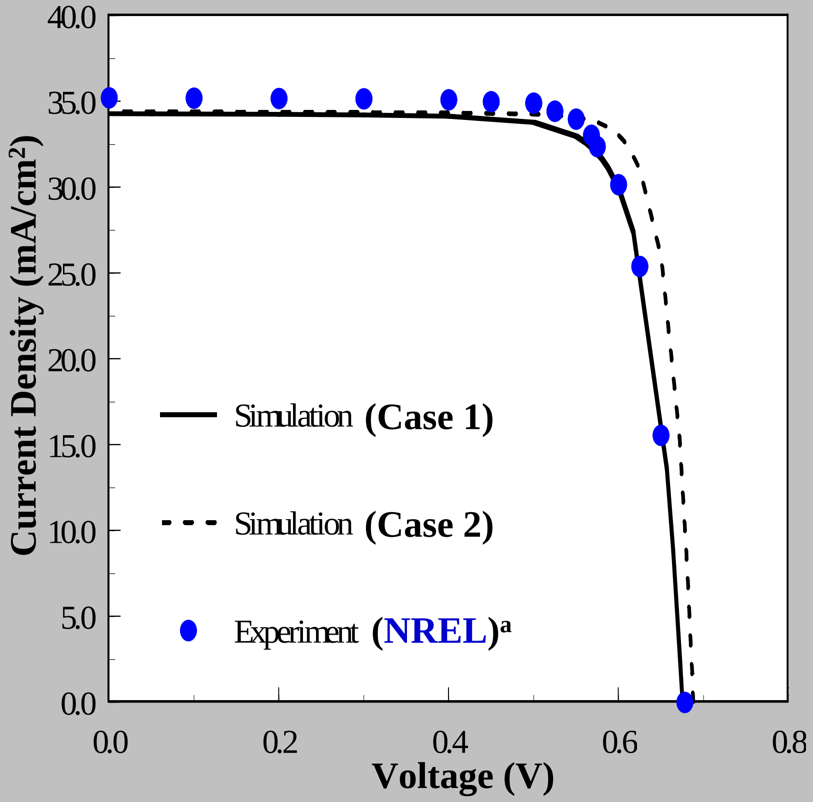
Individual cells are fabricated independently

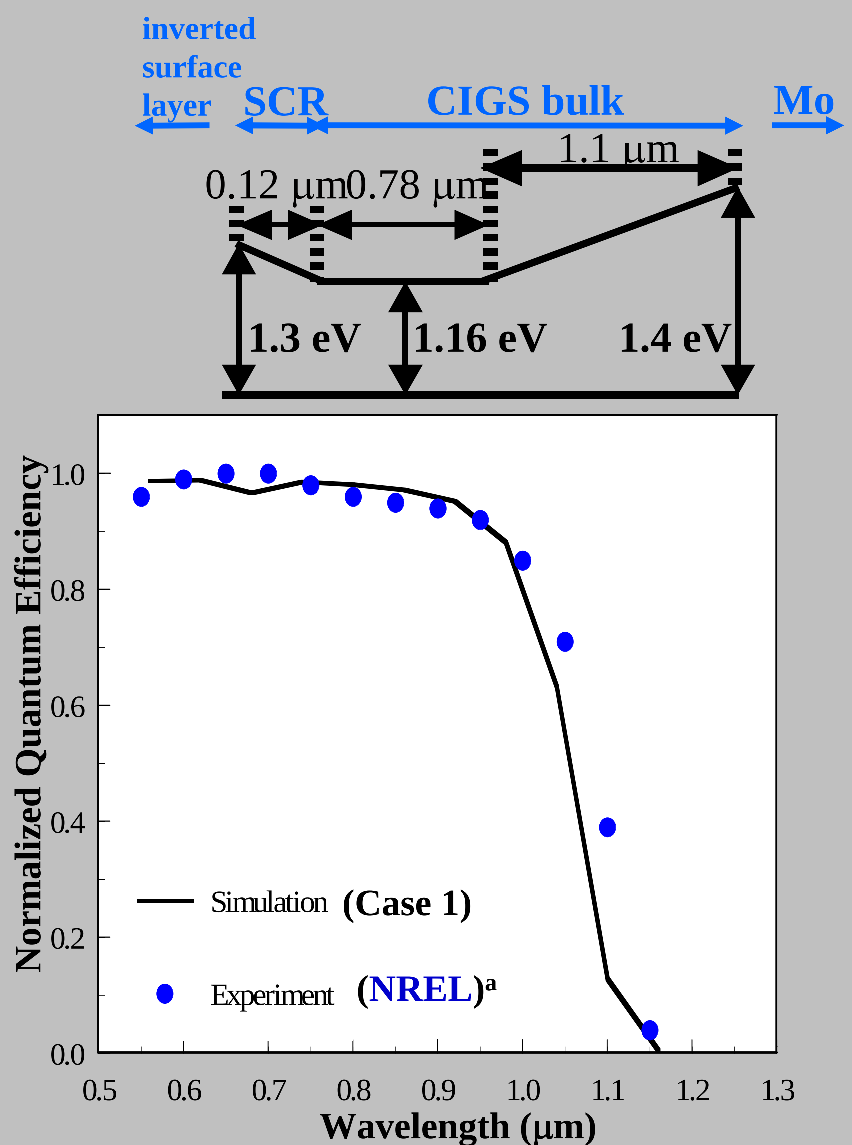
Bifacial, four-terminal device



- Non-mechanically stacked
- Single substrate

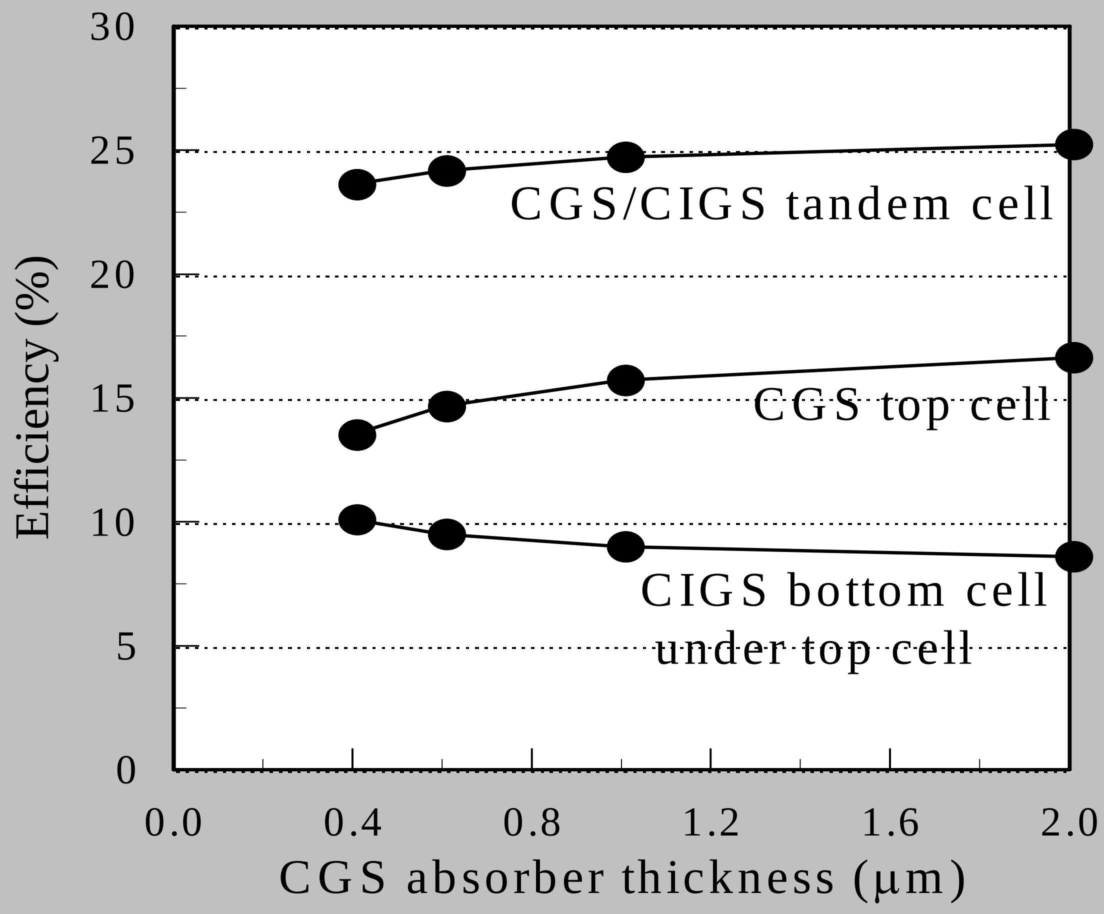
Comparison of Simulated and Reported *Photo- J-V* and Quantum Efficiency





[a]M.A. Contreras *et al*., **18.8%** CIGS cell

The Effect of CGS Top Cell Thickness on CGS/CIGS Tandem Cell Performance

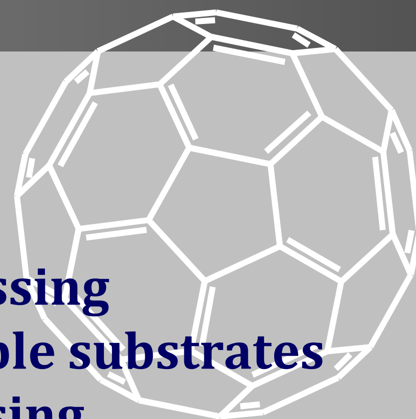


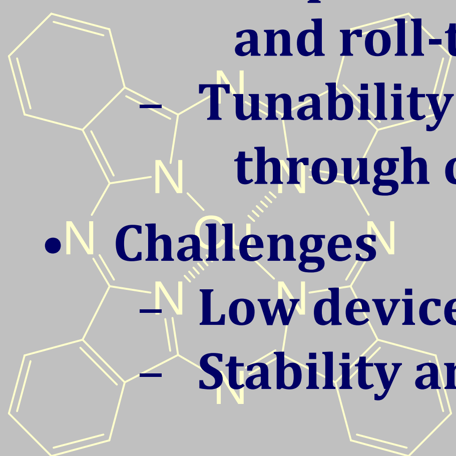
The simulations suggest that a mechanically stacked CGS/CIGS tandem structure could achieve η ~ 25% using a high performance CGS top cell (η > 16%) and an optimized CIGS bottom cell.

Basic Research Recommendations

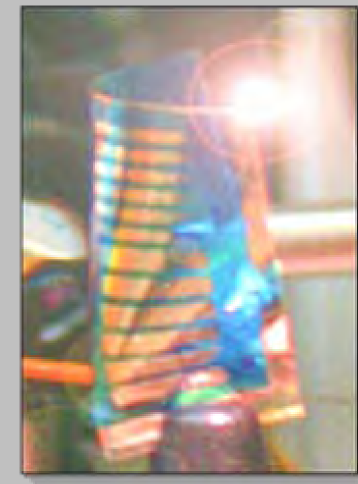
- **New concepts in solar electric**
- **Organic and hybrid organic/inorganic conversion systems**
- **Photoelectrochemical solar cells**
- **Novel nanoscale and self-assembled materials**
- **Theory, modeling, and simulation**

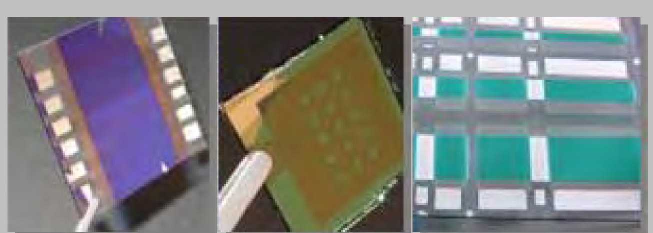
Organic Photovoltaic Cells

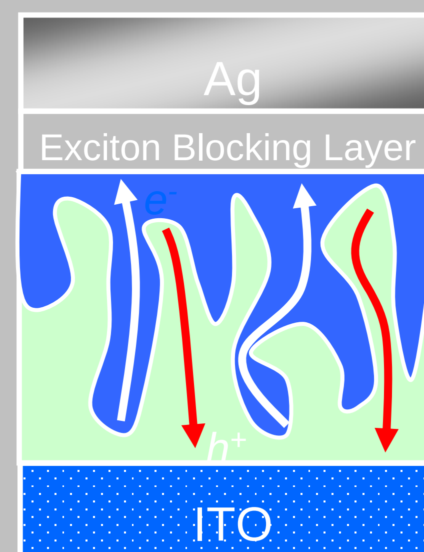




- Advantages
  - Low material cost
  - Low temperature processing
  - Compatibility with flexible substrates and roll-to-roll processing
  - Tunability of material properties through chemical synthesis
- Challenges
  - Low device efficiency (5-6% now)
  - Stability and reliability issues







Basic Research Recommendations

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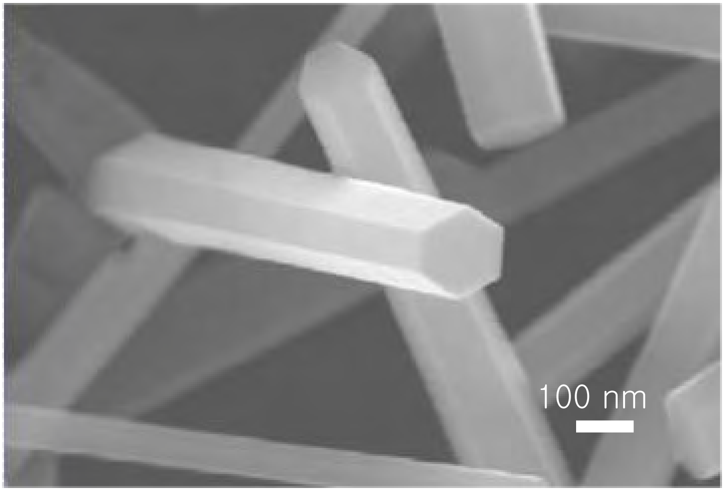
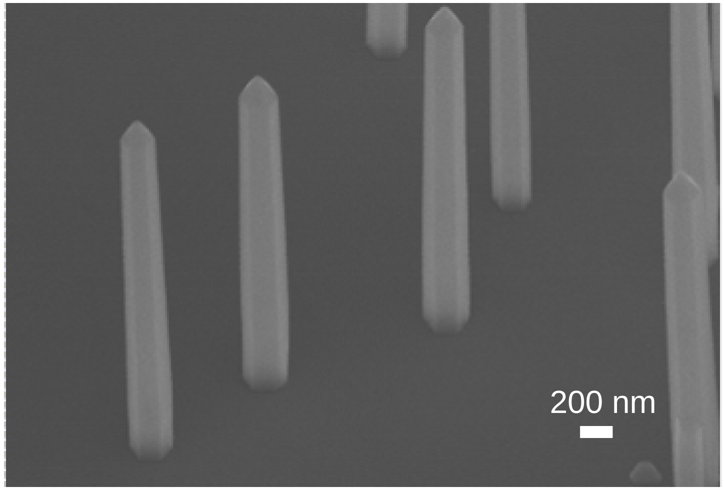
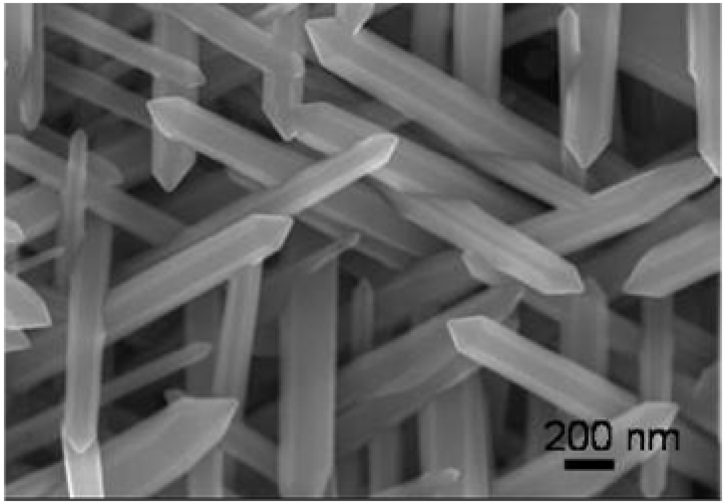
Unseeded, Template-free InN Nanorod Growth

SEM

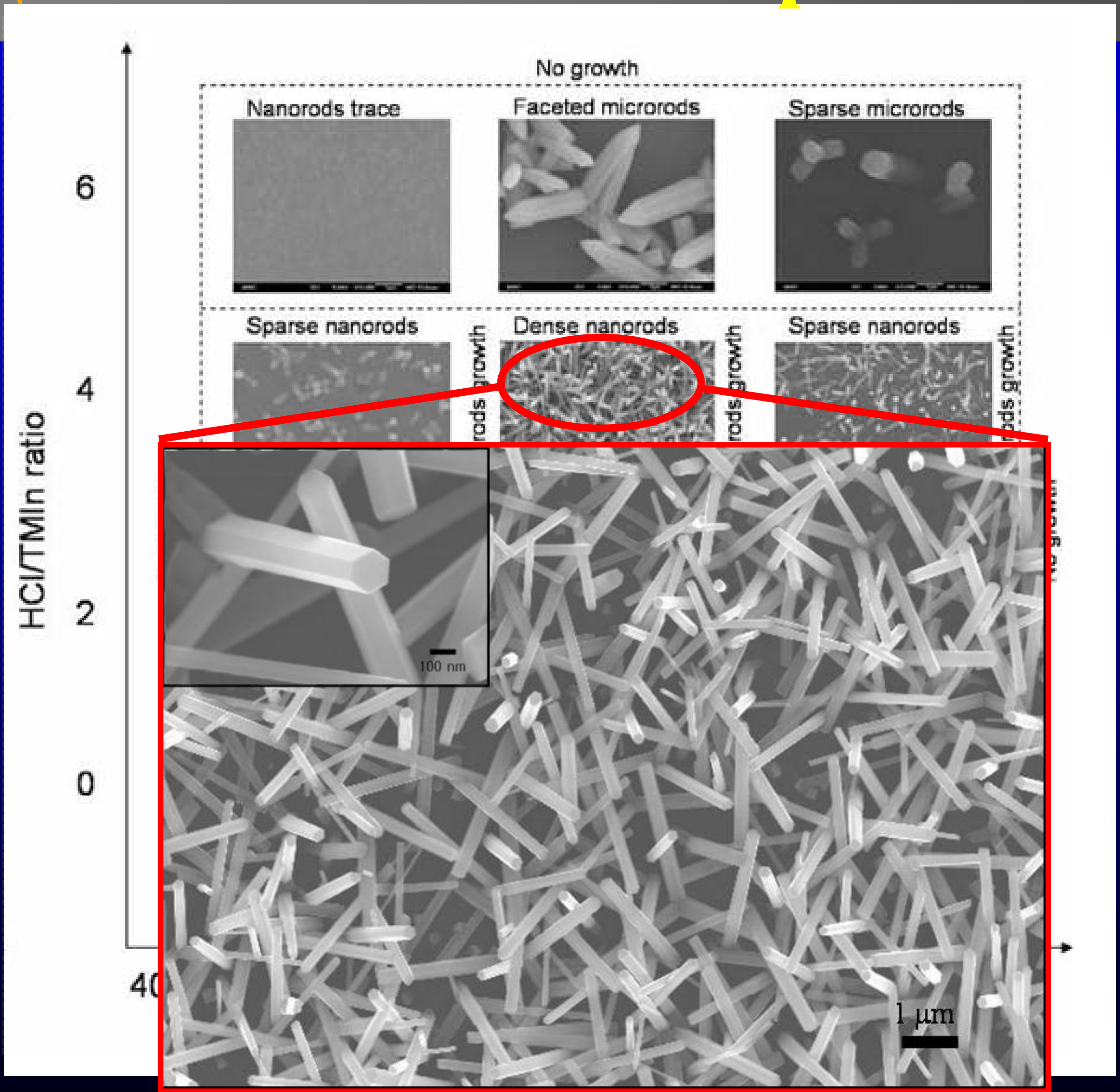






T = 600 ˚C	∅ ~ 100 – 300 nm
HCl/TMIn = 4	L ~ 1 μm
V/III = 250	Flat or sharp edge
Substrates:	Random or aligned
Si(111), GaN/c-Al_2O_3	No liquid indium
Growth time = 1 hr	observed

Effect of HCl/TMIn and Growth Temperature



InN nanorods by H-MOVPE:

HCl/TMIn vs T

V/III= 250

Substrate: c-Al_2O_3

Optimal Conditions:

T = 600 °C

HCl/TMIn=4

V/III=250

Role of Universities

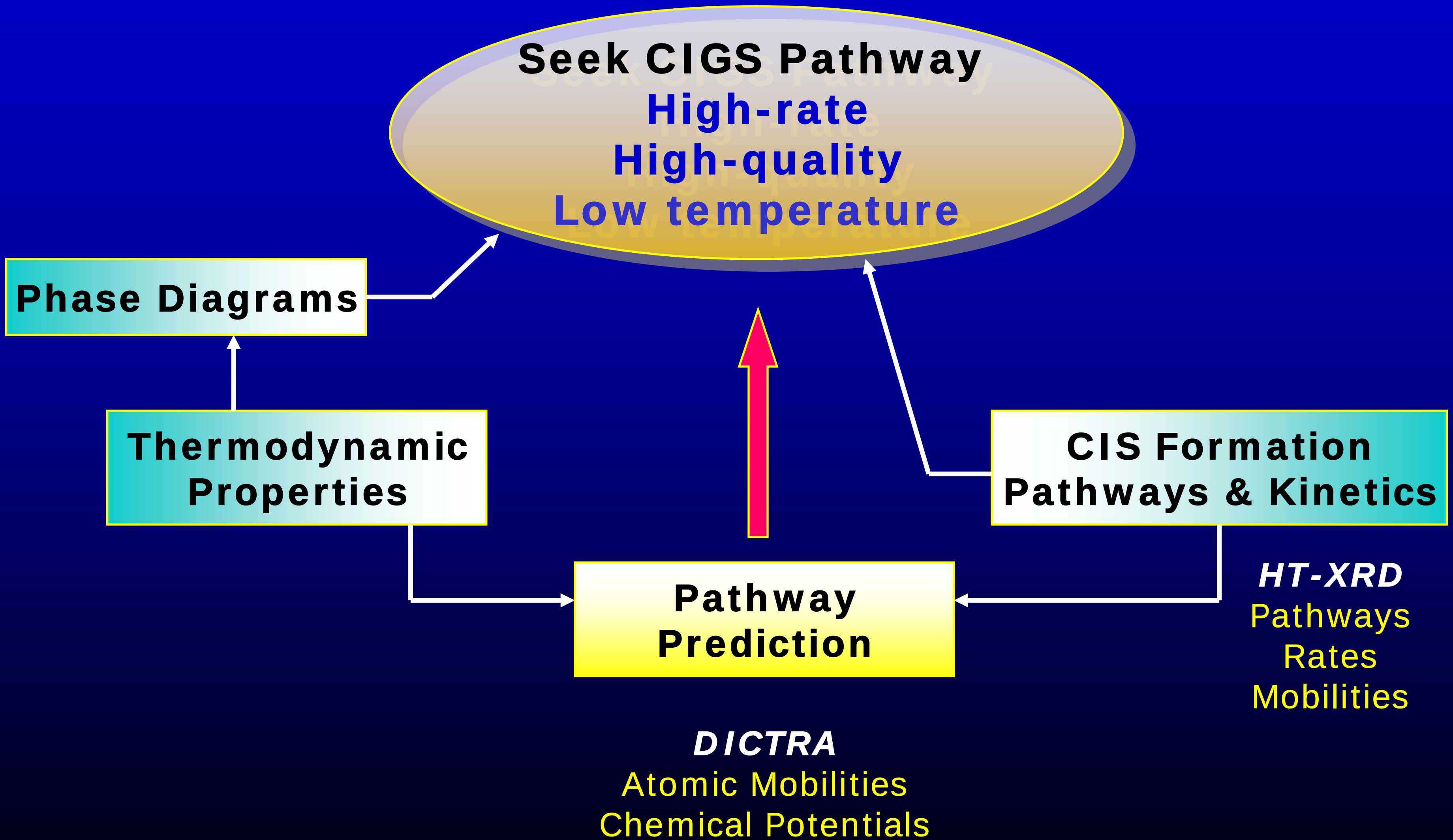
- ***Applied Research***
  - **Experiment with lab-scale processes and prototype production to assist in the transition of PV technology**

http://www1.eere.energy.gov/solar/solar_america/pdfs/d_horwitz_os_bes.pdf

Key Issue: Cost Reduction - $\$/W_p$

- **Materials Costs (~50%)**
  - **Material efficient deposition**
  - **Lower substrate cost (e.g., BIPV)**
    - » **Lower temperature**
- **Processing Costs**
  - **Capitalization largest cost**
    - » Process intensification
    - » Increase process yield (e.g., process control)
    - » Increase throughput (e.g., scale-up, reduce absorber thickness, high rate deposition/rapid reaction pathway/lower temperature)
- **Increase Cell Efficiency**
  - **For advanced technologies: Module level < Champion cell ~ Predicted**

Approach


Seek CIGS Pathway
High-rate
High-quality
Low temperature
Phase Diagrams
Thermodynamic Properties
CIS Formation Pathways & Kinetics
Pathway Prediction
HT-XRD
Pathways
Rates
Mobilities
DICTRA
Atomic Mobilities
Chemical Potentials

Approach to Developing Phase Diagrams

DATA → **Critical Evaluation, Model Selection & Assessment** → **Equilibrium Phase Diagrams**

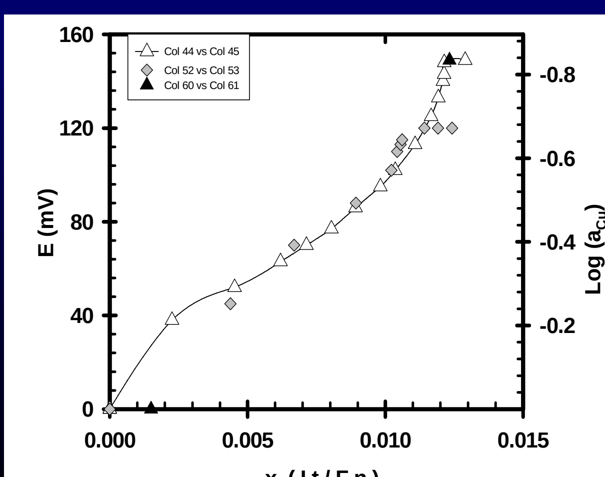
Thermochemical & Equilibrium ↔ **DATA**

Structure ↔ **DATA**

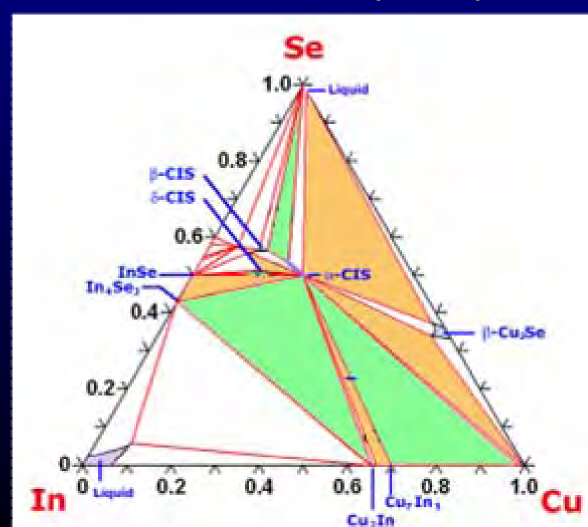
Bulk & Point Defects ↔ **Equilibrium Phase Diagrams**

Solid State Coulometric Titration

W/Cu,Cu_2O//YSZ//$Cu_{2-x}Se$, Cu_2O/C/W



Isothermal Section (500 °C)

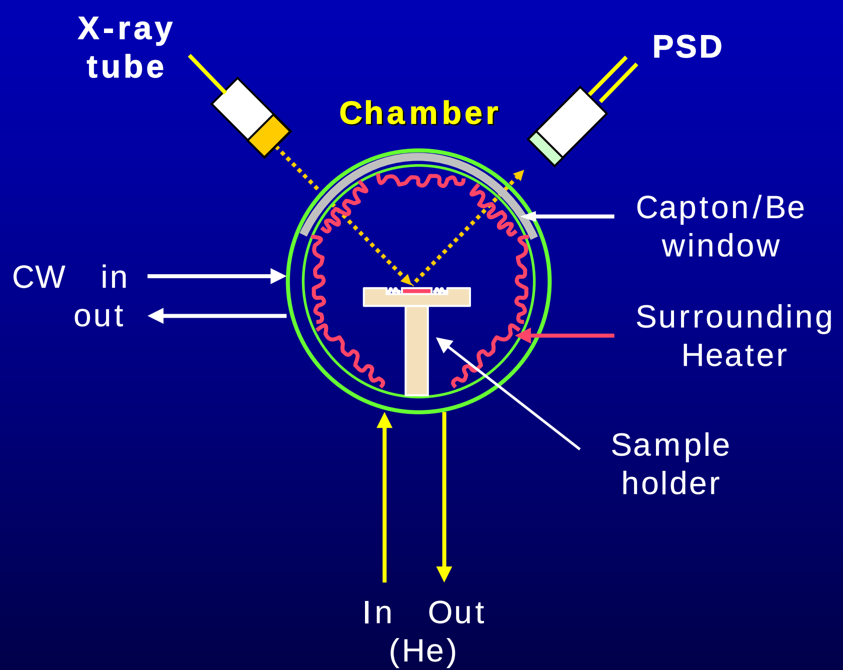


- Solution modeling
- First principles calculations
- EXFAS measurements

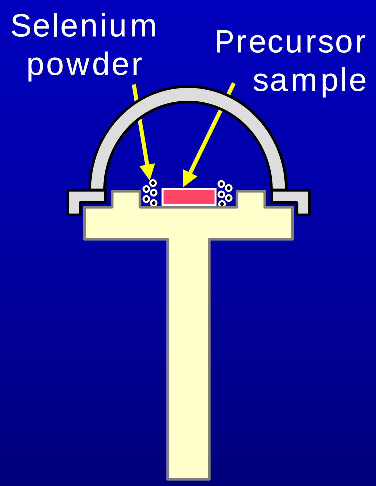
Phase	Model
Liquid	Ionic two sub-lattice model (Cu+1,Cu+2)p(Se-2,Va,Se)q
α-$Cu_{2-x}Se$	Sub-lattice model (3 sub-lattices) $(Cu,Va)_1(Se,Va)_1(Cu)_1$
β-$Cu_{2-x}Se$	Sub-lattice model (3 sub-lattices) $(Cu,Va)_1(Se,Va)_1(Cu)_1$
Fcc (Cu)	Regular solution model

HT-XRD System

Panalytical Philips X'pert System

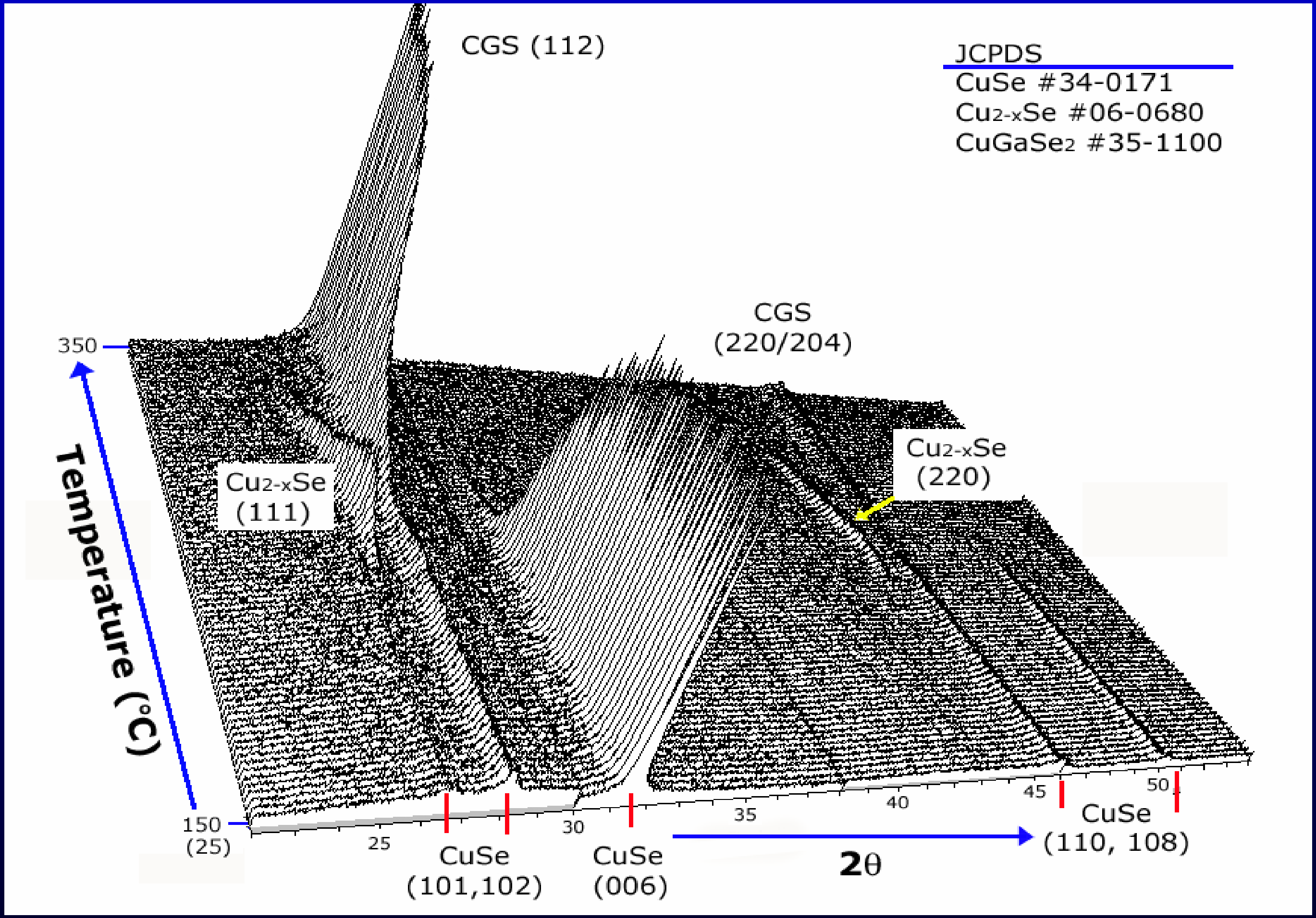


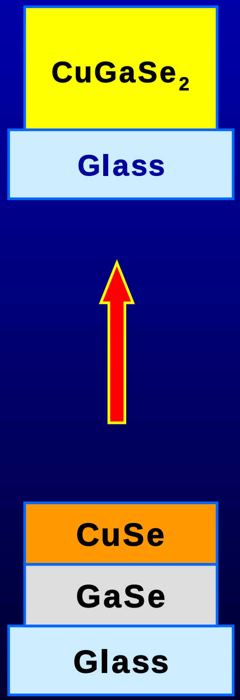
Graphite Dome



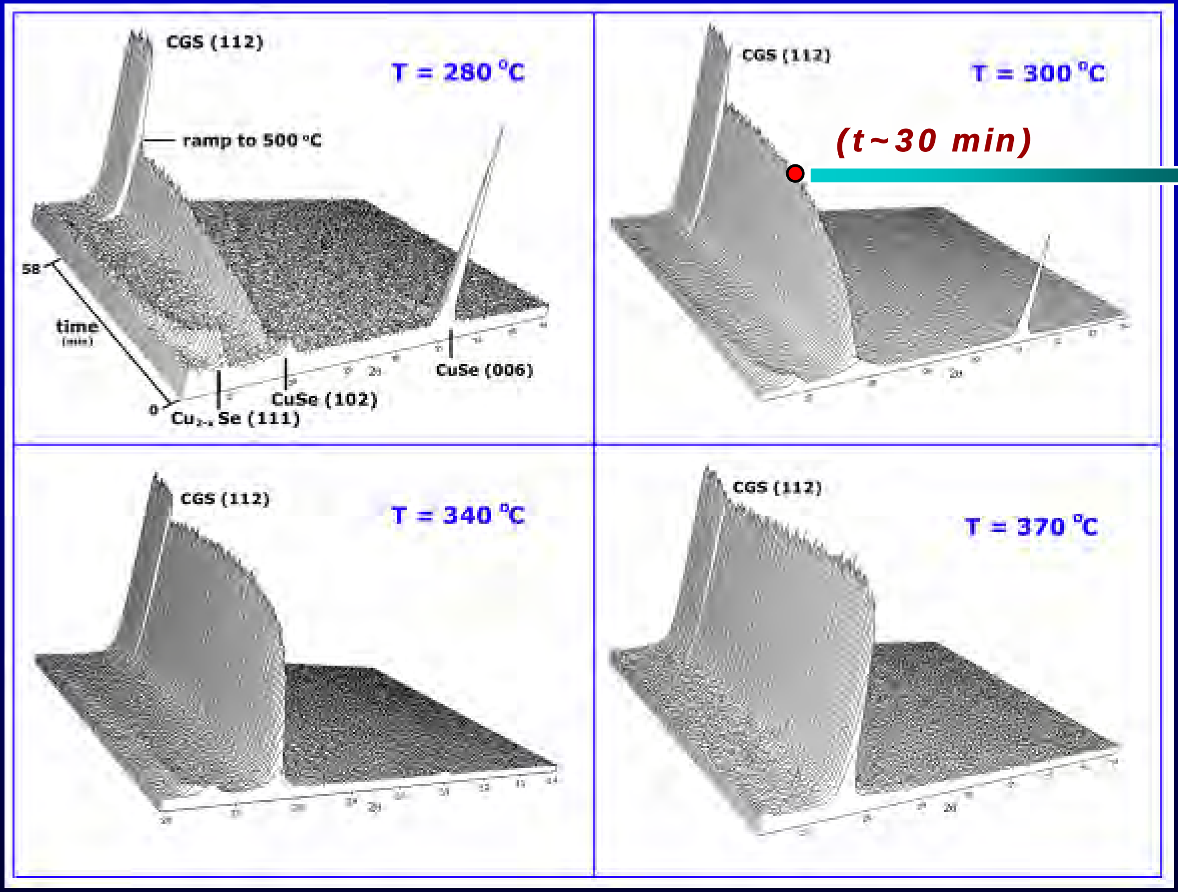
➔ **High Temperature Materials Laboratory (ORNL)**

Temperature Ramp Anneal





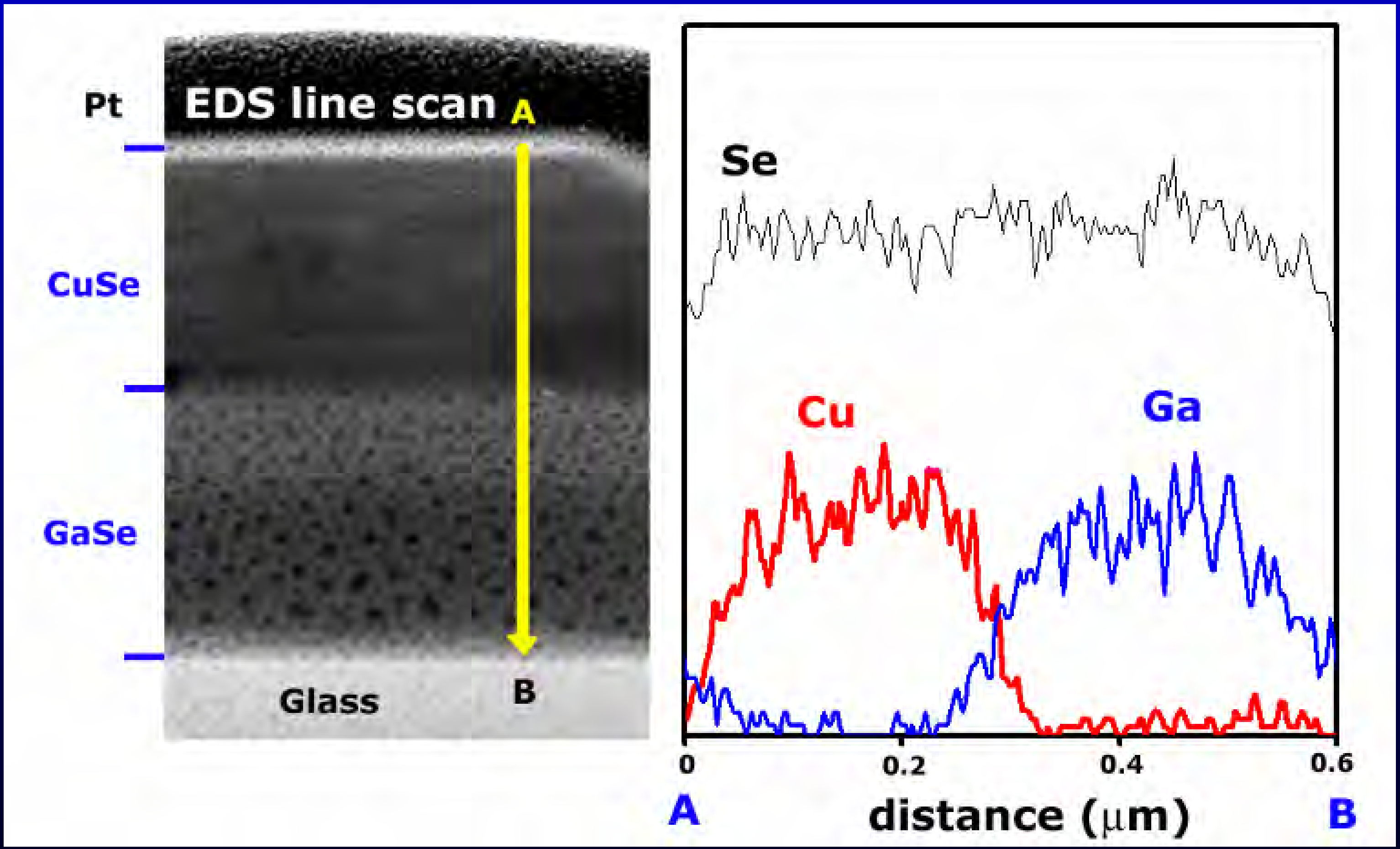
Isothermal annealing



TEM-EDS

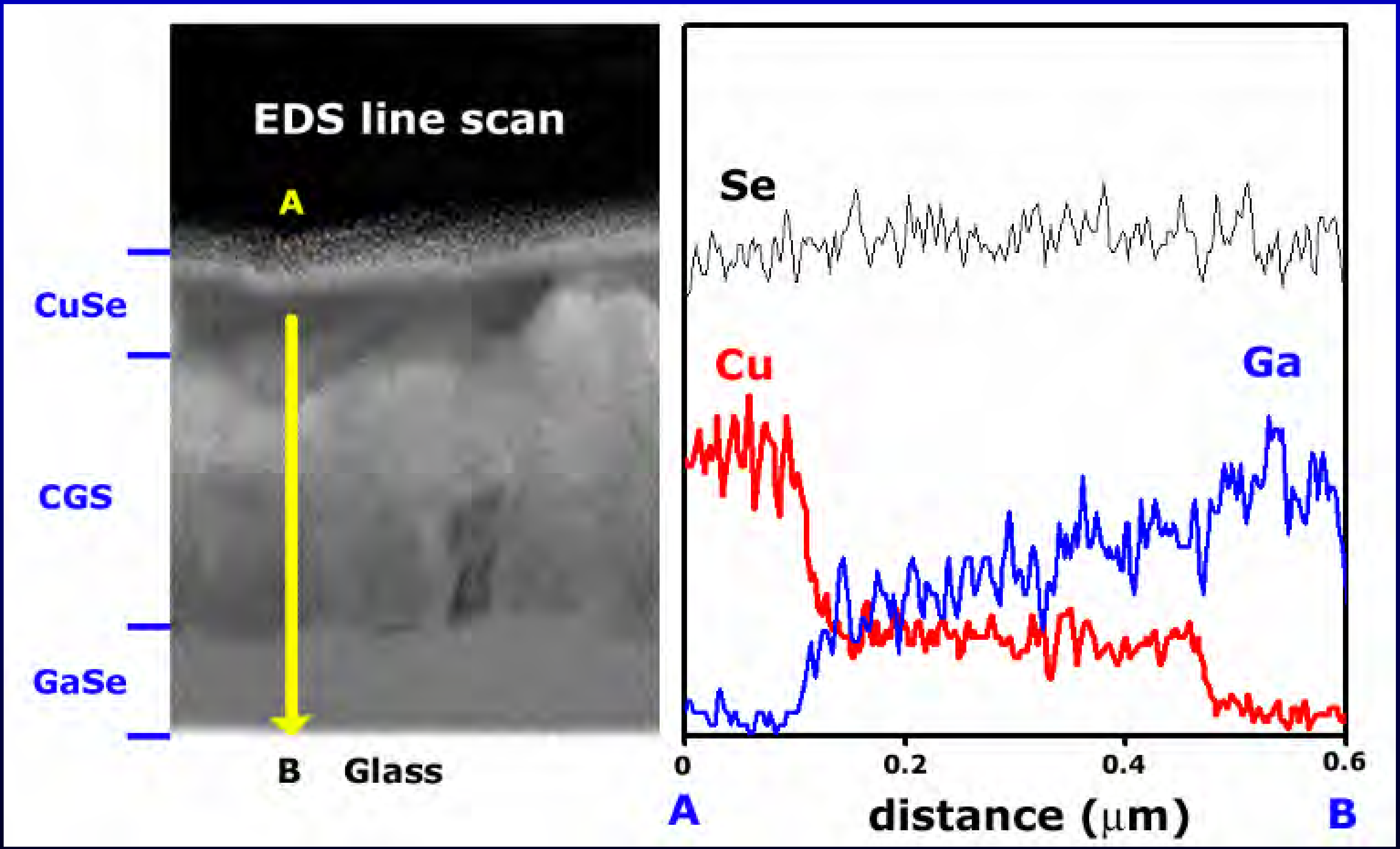
TEM-EDS Analysis

Glass / GaSe / CuSe Precursor



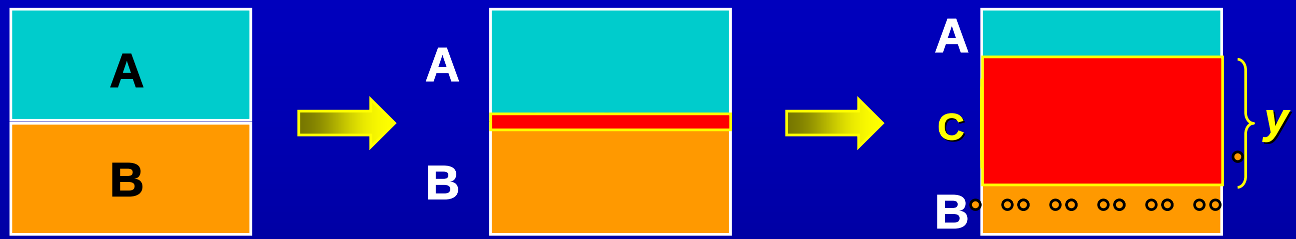
TEM-EDS Analysis

Glass / GaSe / CGS / CuSe annealed for 30 min, at 300 °C



Solid-state Growth Models

- **Parabolic growth model**

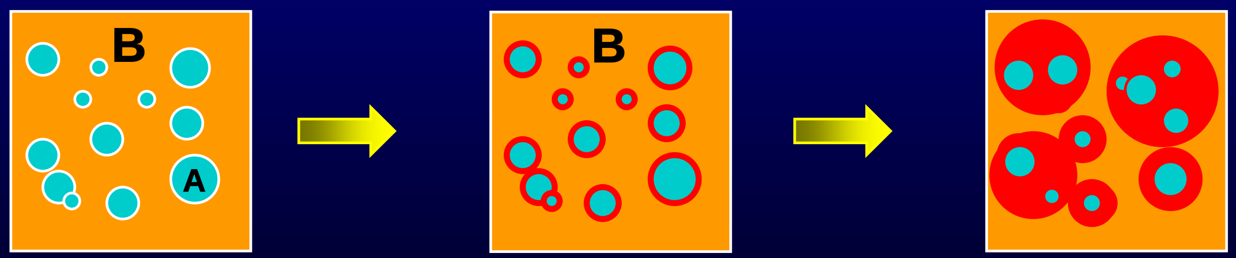


Before reaction — Nucleation at A-B interface — Diffusion thru product & reaction (ex. $D_{BC} > D_{AC}$)

$$\frac{dy}{dt} = \frac{D \cdot k}{y}$$

$$y^2 = k_p \cdot t$$

- **Avrami growth model**



Phase A in matrix B — Nucleation — Diffusion & growth

$$x = 1 - \exp[-(kt)^n]$$

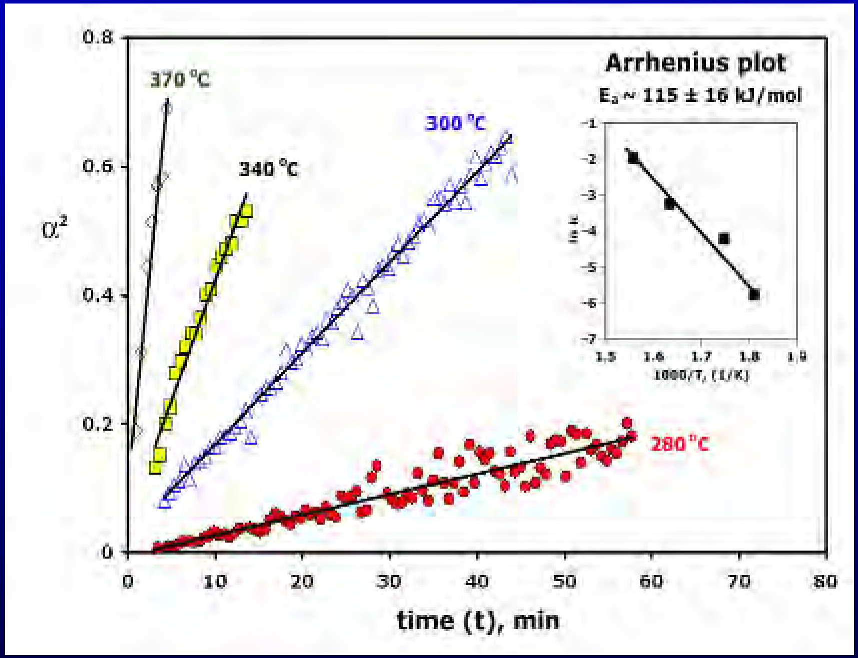
$$\ln[-\ln(1-x)] = n\ln t + n\ln k$$

$0.5 < n < 1.5$

(1-D diffusion)

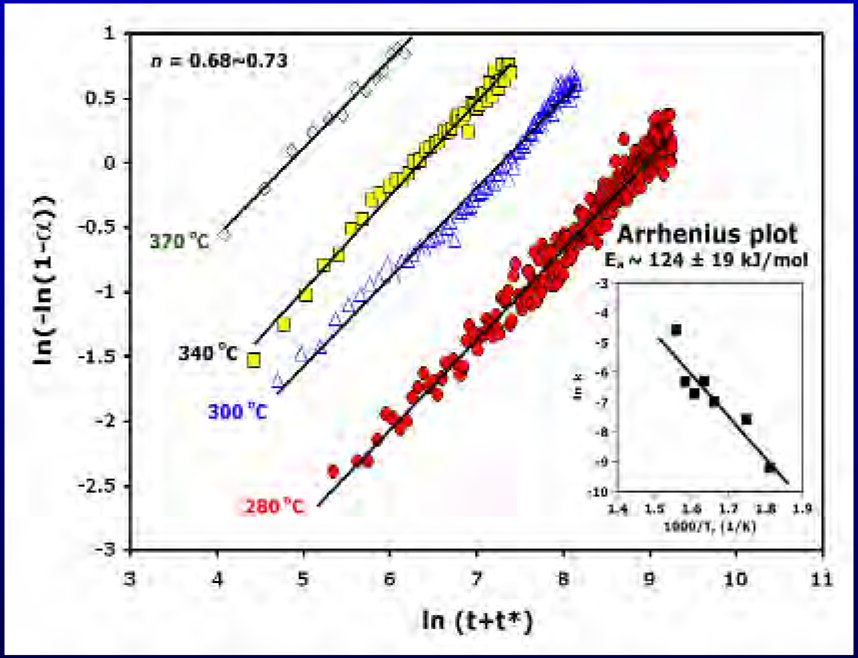
Kinetic Analysis

Parabolic model



$\alpha^2 \sim k \cdot t$

Avrami model

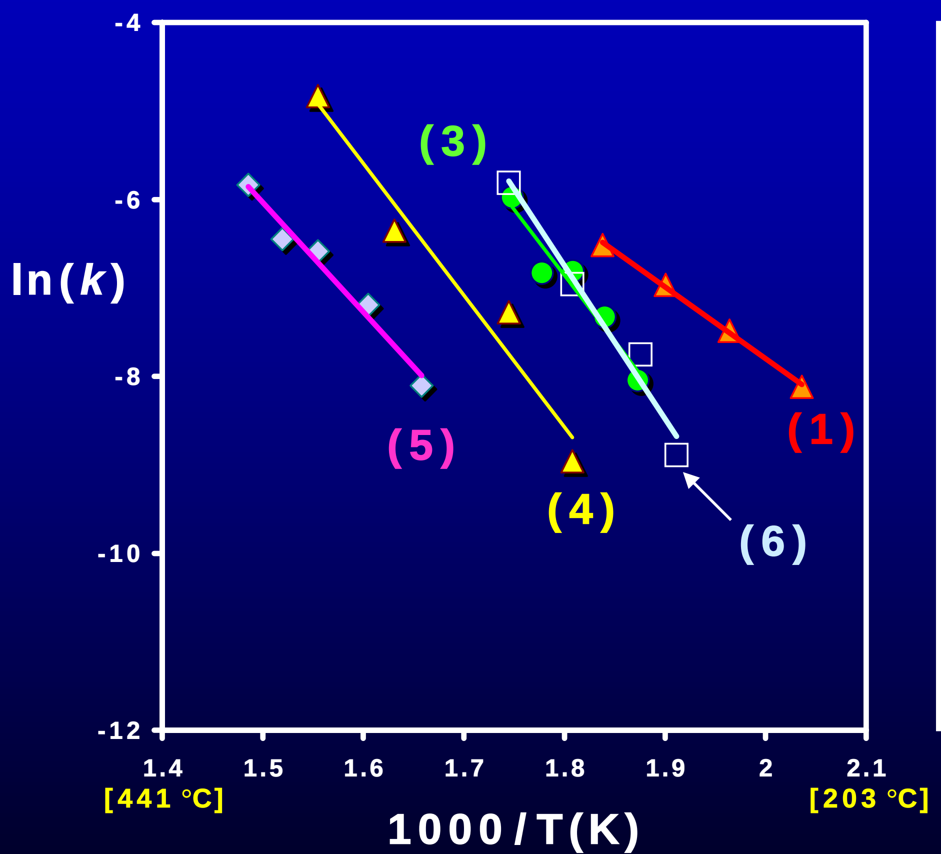


$\ln[-\ln(1-\alpha)] = n\ln(t+t^*) + n\ln k$

➔ Analysis suggests one-dimensional diffusion controlled reaction

Reaction rate

- **Avrami model**



	Precursors	Activation energy (kJ/mol)	
		Avrami	Parabolic
1	InSe/CuSe	66	65
2	$CuSe/In_2Se_3$	N/A	162 (±5)
3	Cu-In + Se(vapor)	124 (±19)	100 (±14)
4	GaSe/CuSe	118 (±22)	107 (±15)
5	Cu-Ga + Se(vapor)	108	N/A
6	Cu/In/Ga + Se(vapor)	144	N/A

Role of Universities

- ***Consulting activities***
  - *Experiences positions Universities to offer guidance to industry*
- ***Supply industry with qualified scientists and engineers***

Where will all the new ideas and people come from?

http://www1.eere.energy.gov/solar/solar_america/pdfs/d_horwitz_os_bes.pdf

Acknowledgements

What Determines University Research Areas?

Why do you rob banks, Willy?
"Cause that's where the money is"
Willy Sutton
Bank Robber

Sutton's law states that in attempting to diagnose a problem, one should first do the experiment that can confirm the most likely diagnosis. "When you hear hoof beats in Texas, think horses, not zebras."

Basic Research Recommendations

- ***Novel nanoscale and self-assembled materials***
  - Studies of nucleation and growth of novel materials involving kinetically or thermodynamically driven self-assembly of tailored building blocks.
  - Construction of the active layers and devices using carefully controlled vapor or solution-based.

Basic Research Recommendations

- ***Theory, modeling, and simulation***
  - New theoretical, modeling, and computational tools are needed which span many decades in space, time and structure are required to guide and interpret experiment and assist in the design of molecules, materials and systems.
  - Improved theory and methods are needed to understand electron transfer and charge separation, excited-states, their properties and their potential energy surfaces.
  - Enhanced capabilities to accurately predicted band-gaps, lifetimes and band offsets in materials that are realistic candidates for solar energy systems.

Basic Research Recommendations

- ***New concepts in solar electric conversion***
  - Nano-structured architectures that can efficiently absorb the full spectrum of wavelengths in solar radiation
  - Multiple exciton generation
  - Structures that are defect tolerant and self repairing.
  - The use of these materials in multiple junction cells
  - Advances in nanoscale characterization using electron, neutron, and x-ray scattering and spectroscopy and integration of these probes with studies of photoinduced charge separation and transport will be essential to understand the structure/property relationships in these materials.

- ***Photoelectrochemical solar cell research:***
- – Need to extend photoelectrode lifetimes and find low-cost solids and electrolytes.
- – Search for new combinations of sensitizers and redox couples for higher solar conversion efficiencies.
- – Enhance absorption in the infra-red spectrum by sensitizing dyes and quantum dots.
- – Develop novel mesoscopic electrode designs, derived from nanostructured and nanoporous solids.

References

- http://www1.eere.energy.gov/solar/solar_america/pdfs/d_horwitz_os_bes.pdf