An Overview of Materials Science and Engineering at Michigan

October 28, 2011

Peter F. Green, Chair

Department of Materials Science and Engineering

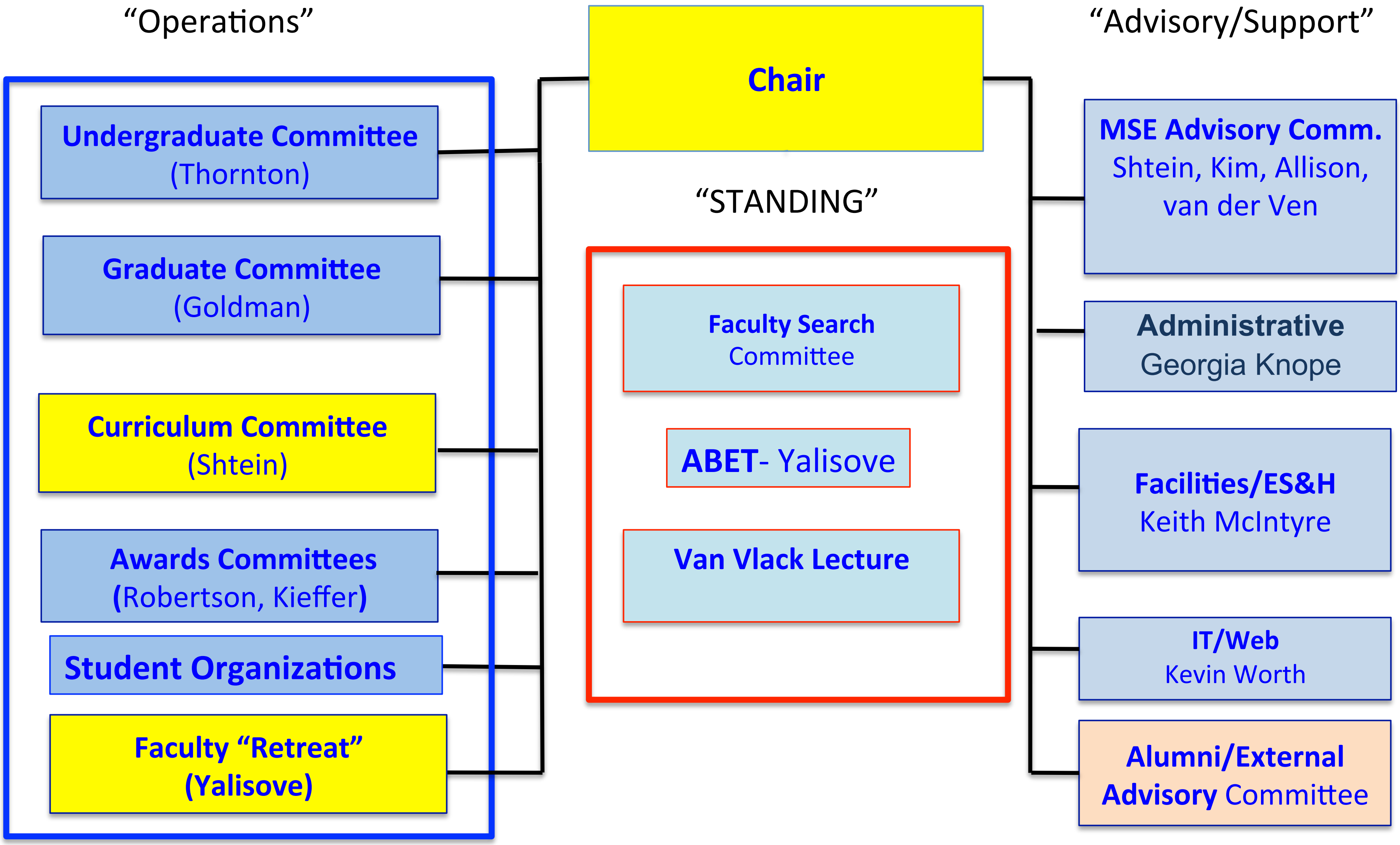
OUTLINE

- The Department: mission, organization, faculty
- Educational and Research Programs
- Energy Center: DOE EFRC
- Outreach
- Challenges

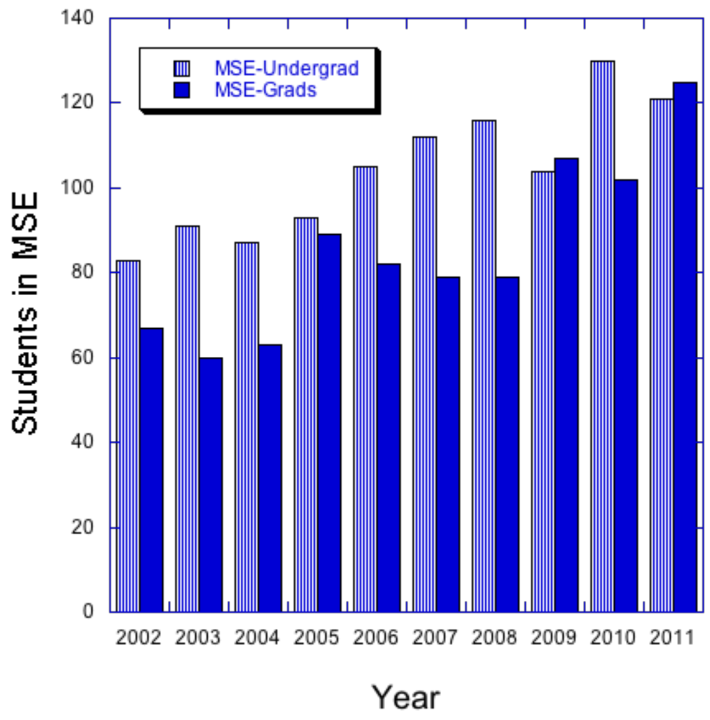
Mission Statement

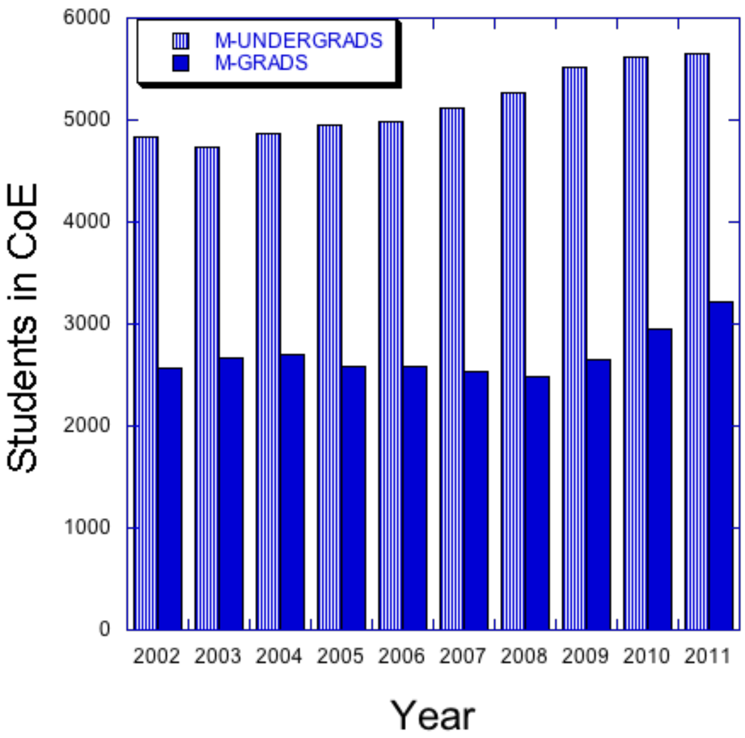
- Our *Mission* is:
  - to educate creative and productive scientists and engineers in the fundamental principles of the science and engineering of materials, who will provide future leadership in industry, academia and government laboratories;
  - to produce new advances in the science and technology of materials;
  - to serve as a bridge between various materials research efforts throughout the University via various scientific and technical centers;
  - to collaborate with industrial and government researchers on problems of technological significance.

A “Snapshot” of the MSE Organization:
Operations, Standing and Support/Advisory functions

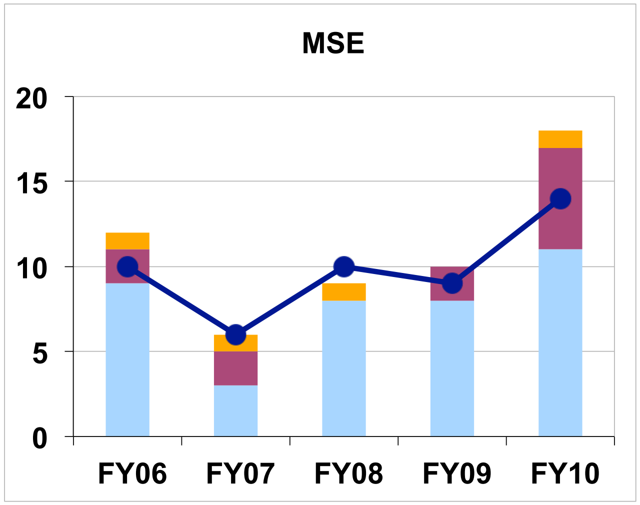


Enrollment Trends in MSE and the CoE

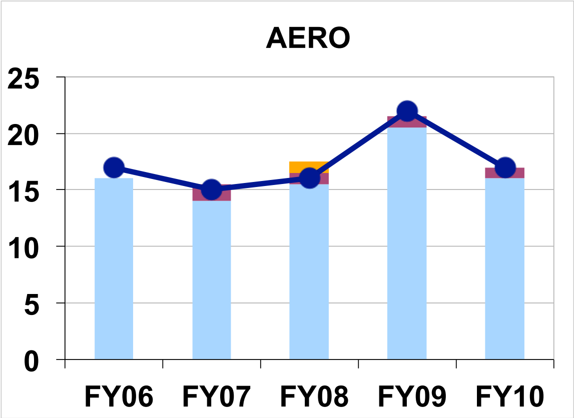


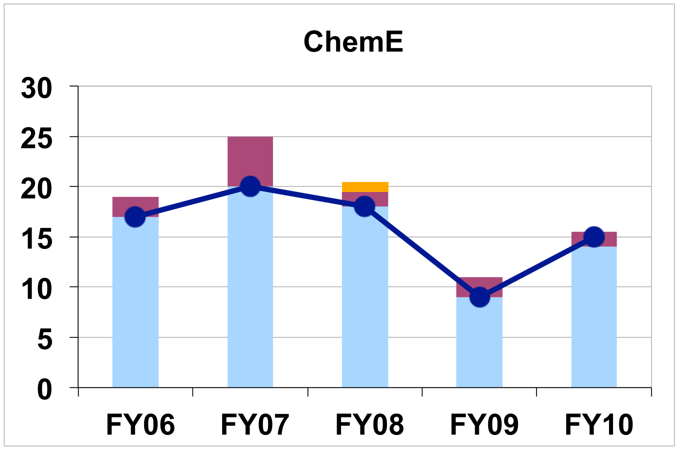


Doctoral Degrees Granted



Aerospace Engineering and Chemical Engineering have ~3 time as many undergraduates as MSE. Their graduate programs are comparable in size to MSE.





Multi-investigator programs with which MSE faculty are involved

This is an important role of the department within the University

Multi-investigator Programs

- **MURI: Three-Dimensional Approaches to Assembling Negative Index Metamedia; [PI – R. Merlin (Physics)** Tailoring metal-semiconductor nanocomposites to achieve negative index of refraction in the infrared range. **$5 million (AFOSR) ending**

- **MURI: Dynamics of Thermal Transport at Interfaces Between Dissimilar Materials; [PI – K. Pipe (ME)-all other faculty are MSE]** Fundamental mechanisms governing thermal transport across interfaces between dissimilar materials**. $5 Million (AFOSR)**

- **MURI: Hyperspectral and Extreme Light Diagnostics for Defense-Critical Advanced Materials and Processes (PI- Pollock)** The objective of this MURI program is to develop the scientific basis for use of ultrafast lasers as materials diagnostics and microfabrication tools for advanced materials and components in Air Force systems. **$5 million- ending**

- **MURI: Bio-Integrating Structural and Neural Prosthetic Materials (PI- Cederna (Med School), MSE CoPI- Kim and Martin)** Collaboration with the Med school. **$5 million**

- **Energy Frontier Research Center: Center for Solar and Thermal Energy Conversion in Complex Materials (PI- Green (and 28 Michigan faculty including 11 MSE faculty). $19.5million (DOE)**

Educational Programs

- **GAANN: Integrating Computational and Experimental Research in Materials Science: An Area of National Need (PI- Kieffer, Other MSE personnel- Falk, Glotzer, Green, and Millunchick)** This is a training grant from the US department of education designed to prepare Ph.D. students in MSE for careers as educators and academicians. GAANN fellows are required to combine computational and experimental techniques of investigation in a substantive way for their thesis research and partake in the development, deployment, and evaluation of novel instructional technologies. This grant supports 9 graduate students and facilitates collaborative research involving the Forrest, Goldman, Kieffer, Love, Millunchick, Pan, Thornton, and van der Ven groups.

- **IGERT: Full Proposal: Open Data: Graduate Training for Data Sharing and Reuse in E-Science (PI – Hedstrom (School of Information), MSE CoPI- Millunchick, Other MSE personnel- Kieffer and Glotzer)** The Open Data IGERT graduate training program focuses on the methods, practices, and norms for data sharing and data reuse in e-science, and involves researchers from the School of Information, Computer Science, Bioinformatics, Chemical Engineering and Materials Science and Engineering.

- **Modern Optics in the City of Light: an international REU site in Paris (PI- Yalisove, other MSE personnel- Pollock, Jones, and Martin)** Optics in the City of Light is an NSF international Research Experience for Undergraduates (iREU) that offers up to 8 undergraduate junior level students the opportunity to spend 9 weeks in a variety of laboratories in Paris performing research with a wide range of ultrafast lasers. Students in this program will experience strong collaborative science that is currently taking place between University of Michigan (UM) Center for Ultrafast Optical Science (CUOS), the Materials Science and Engineering Department at UM, Ecole Polytechnique, Ecole Nationale de Techniques Avancées (ENSTA), the Louvre, and l'Institut d' Optique Graduate School

Energy Programs at Michigan

- **Center for Solar and Thermal Energy Conversion**
- **U.S.-China Clean Energy Research Center – Clean Vehicle Consortium**

  Development/ improvement of technologies with potential to reduce the dependence of vehicles on oil and improve vehicle fuel efficiency.

- **Lake Michigan Offshore Wind Feasability Assessment**
- **U-M Fraunhofer Alternative Energy Technologies for Transportation Program**

  more efficient and sustainable technologies for transportation.

- **The Consortium for Advanced Simulation of Light Water Reactors** (CASL): modeling and simulation capabilities to create a usable environment for predictive simulation of light water reactors.

Other Energy Programs

- EFRC on Batteries: (State University of New York, Stony Brook) van der Ven and Thornton
- Nuclear Hub: research in nuclear energy…simulations/modeling led by Oak Ridge (Thornton and van der Ven)
- DOE-Nuclear Engineering University Program(NEUP)
- DOE-NEUP grant on irradiated steels: led by Gary Was
- DOD ICME grant led by Allison (Thornton, Marquis and van der Ven)
- NSF MRSEC
- NSF FRG

MSE undergraduate program

All MSE undergrads take the following 10 MSE courses

- Principles of Engineering Materials
- Physics of Materials
- Thermodynamics of Materials
- Kinetics and Transport in Materials Engineering
- Structures of Materials
- Materials Laboratory I
- Materials Laboratory II
- Mechanical Behavior of Materials
- Materials and Engineering Design
- Materials Processing Design

Materials concentration courses

MSE undergraduate students choose three of the following seven courses:

- Physical Metallurgy
- Ceramic Materials
- Polymeric Materials
- Composite Materials
- Biomaterials, Design and Application of
- Electronic, Magnetic and Optical Materials, for Modern Device Technology
- Characterization of Materials,
- Structural and Chemical

MSE the Discipline

MSE faculty (22 faculty)-20 FTE

- Associate Research Scientists: 2
- Research Professor: 1
- Lecturer: 1

- 5 Assistant Professors
  - Emmanouil Kiopakis (Theoretical Condensed Matter Physics)
  - Pierre Ferdinand Poudeu (Solid State Chemistry)
  - Emmanuelle Marqius (Metallurgy)
  - *Boukai (Thermoelectrics)*
  - *Tuteja (soft materials)*

- 4 Associate Professors (4): Thornton, Shtein, Lahann(0.25); Kim (0.75), van der Ven (Newly Promoted)

- Professors: 11.25

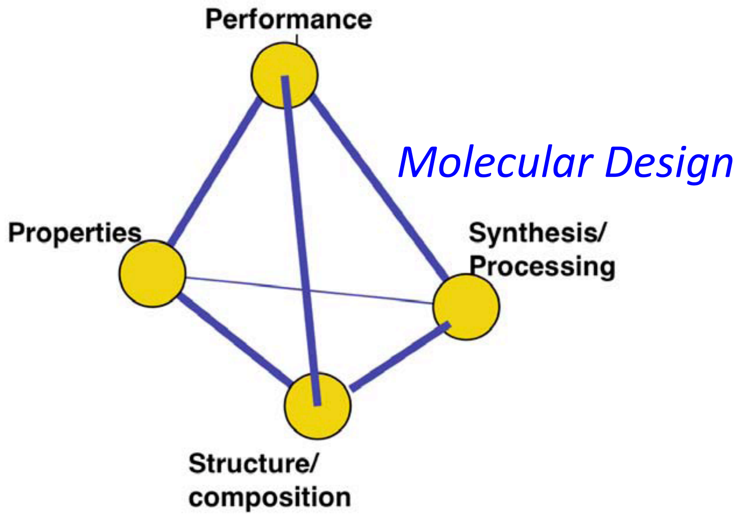
~14 Courtesy Appointments from around the college

MSE: Interdisciplinary Projects and Programs

- Natural bridge between areas of engineering, medicine and the sciences.

Nanoscience and nanotechnology are cross-cutting areas of emphasis

- **IDEAS from**: Thermodynamics, kinetics/transport properties, Quantum mechanics, statistical mechanics,
- **Develop** rules and methods/ strategies for the synthesis/ processing of materials with specific properties “tailored” for specific applications
- **Measure, calculate, or compute**, the structure and properties of materials of varying compositions and structures.



The Materials Science Tetrahedron

Areas of Emphasis in MSE

Material Systems

- Metals
- Ceramics
- "Hard" Semiconductors
- Soft Matter

Design - processing/ synthesis - measurement

- Quantum, Stat. Mech., Thermo, Kinetics
- Molecular design and synthesis
- Computational Materials Science
- Measurement of properties: Macroscopic, nanoscale
- "Tailoring" of morphology: control of structure from macro- to nano-scale

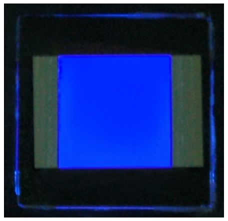
Material Functionality

- Thermoelectrics
- Structural materials
- Piezoelectric/Ferroelectric
- Sensors
- Superconductors
- Electronic materials
- Solar Cells

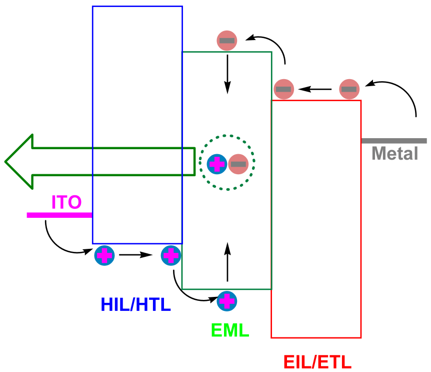
Organic phosphorescence-Worlds first Kim and coworkers

- Organic compounds rarely exhibit phosphorescence, a property more commonly associated with inorganic or organometallic species.
- crystal-design strategy that relies on halogen bonding to combine the heavy-atom effect with triplet-state emission from aromatic carbonyls to produce high-quantum-yield phosphorescence from purely organic materials.
- emission of green light is activated as the crystals forms.

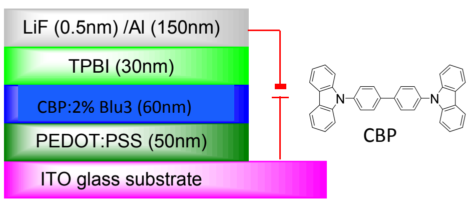
- C&EN News of the Week, RSC Chemistry world News:

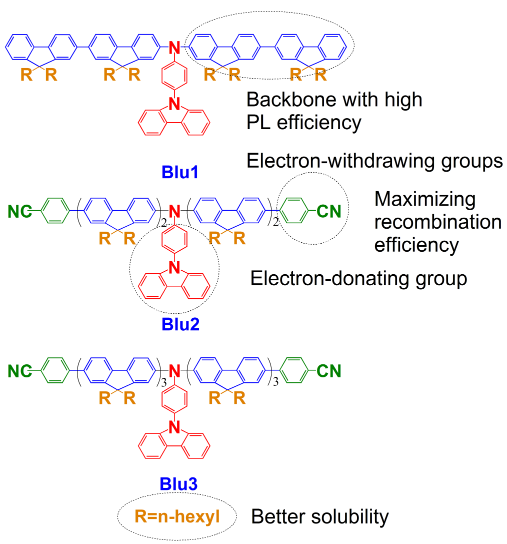


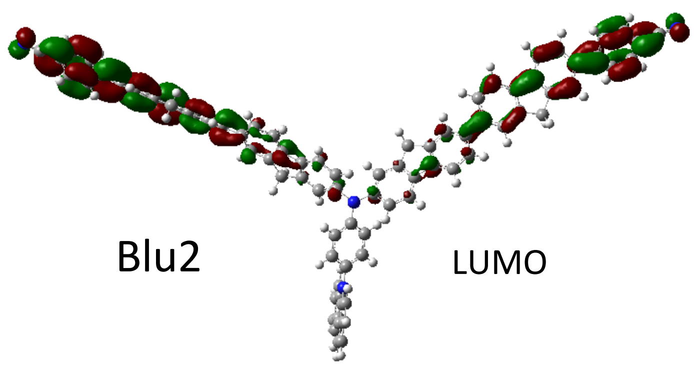
Record Efficiency in Fluorescent OLED

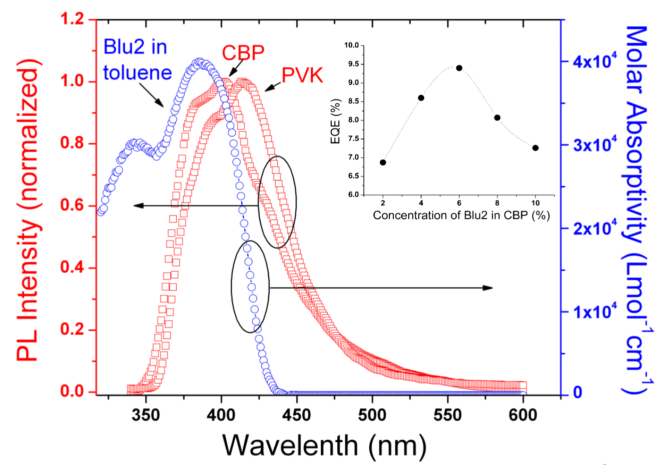


- Systematic variation of molecular architectures, i.e., addition of electron withdrawing groups at specific spacing from donating groups
- Predict stability and intrinsic electronic properties (e.g., HOMO-LUMO gaps, recombination efficiencies, etc.) based on DFT and TD-DFT calculations
- Experimental realization: Our collaborators achieved 9.40% external quantum efficiency for blue OELD device (CIE coordinates: [0.147, 0.139]) based on our prediction (Zhen *et al*., Adv. Funct. Mater. **21**, 699 (2011)



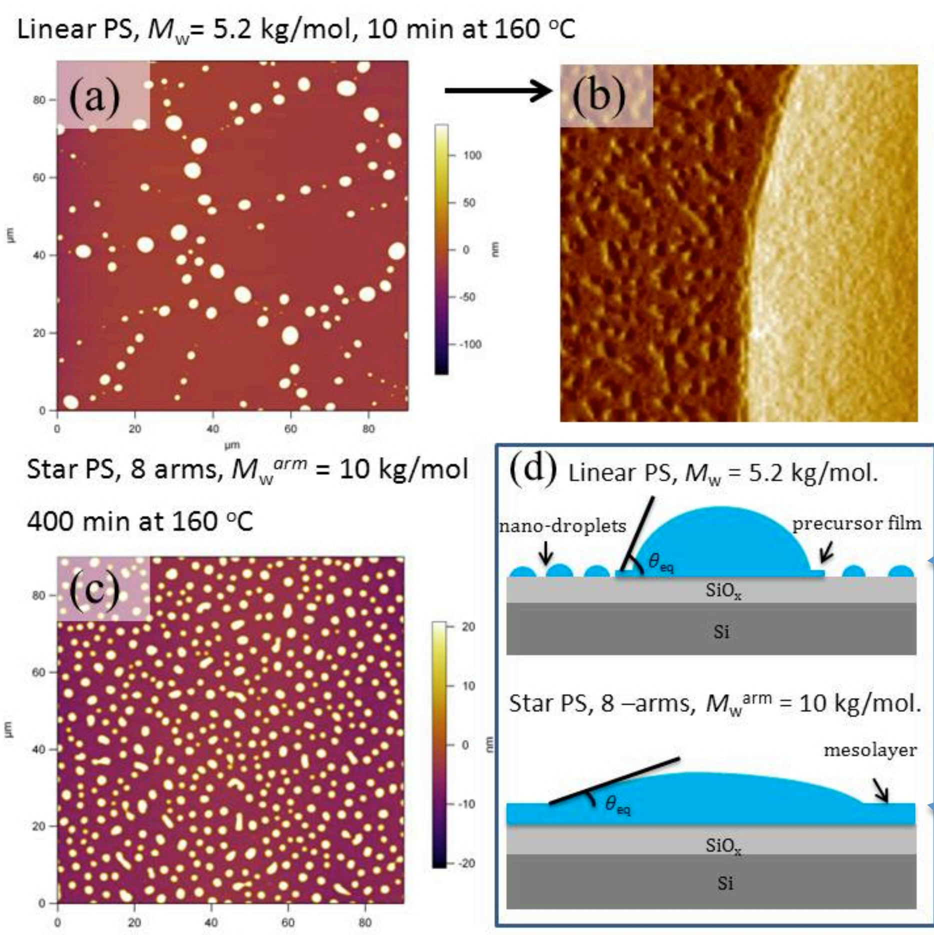






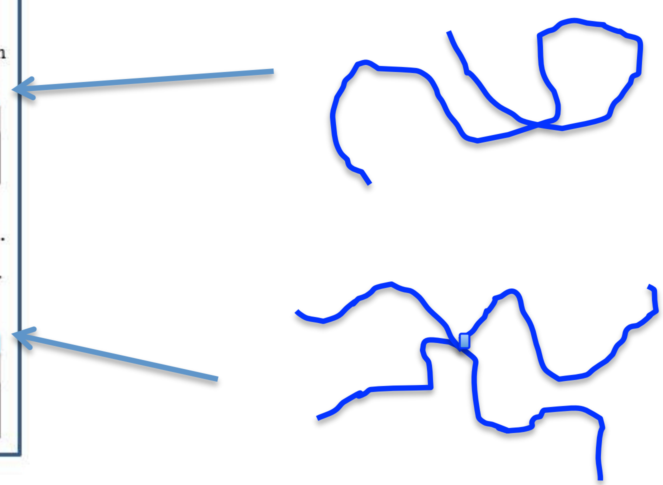
Wetting of Macromolecules

Glynos et al. Physical review Letters, 2011



The wetting characteristics of Star and Linear Chains of the of the same chemical structure are significantly different at the NANOSCALE

Entropic Effects become very important



Design, Synthesis and Evaluation of solid-state inorganic materials

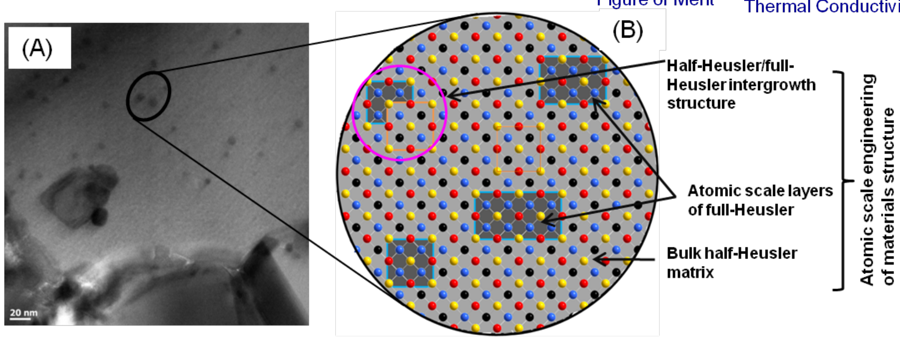
Assistant Professor: Poudeu

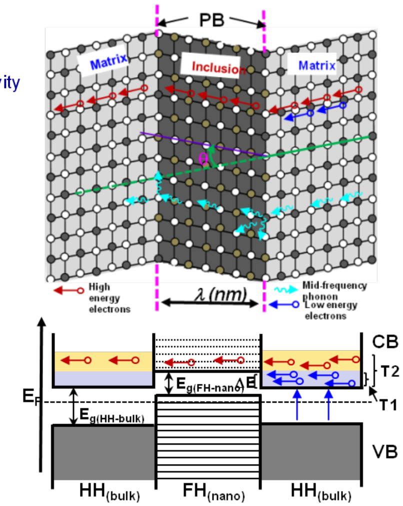
❑Thermoelectrics

Thermopower Electrical Conductivity

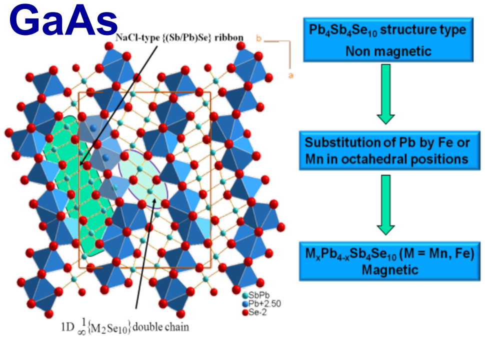
$$ZT = \frac{S^2\sigma}{\kappa}T$$

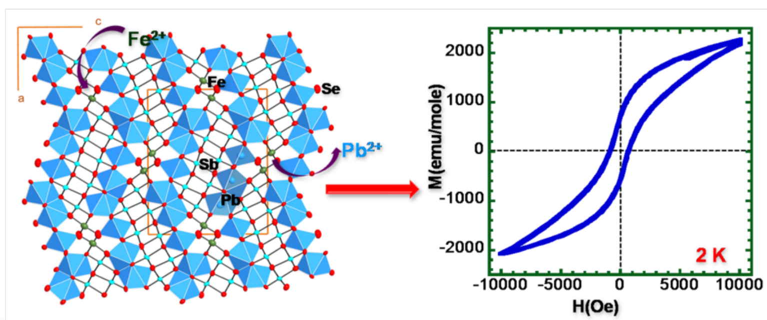
Figure of Merit Thermal Conductivity





❑ LDFS: Beyond GaAs





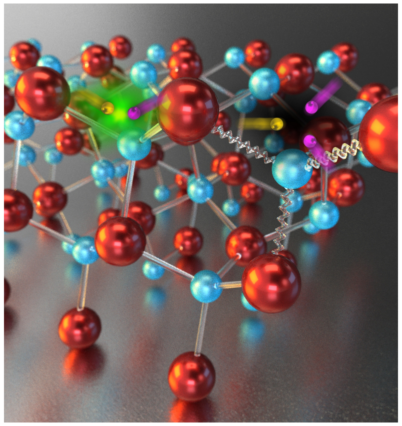
Goal: High Curie temperatures (Tc >300K) ferromagnetic semiconductors through enhanced coupling of localized magnetic centers by charge carriers

Integration of ferromagnetism in LD Semiconducting Chalcogenides

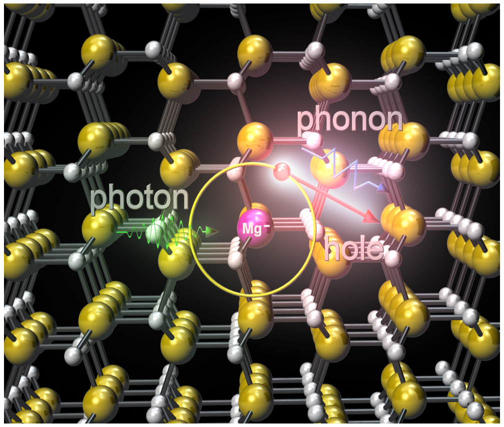
Computational Materials Physics
Electronic, Optoelectronic, Photovoltaic, and Thermoelectric Materials

Manos Kioupakis

Assistant Professor, Materials Science and Engineering



Efficiency of LED light bulbs



Absorption in lasers and transparent conductors

Absorption in Si solar cells

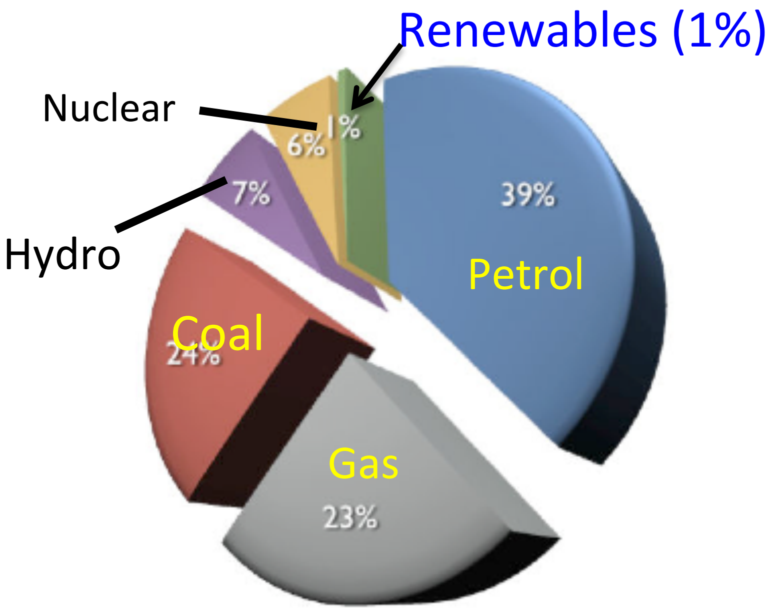
Future Work: Photovoltaic and Thermoelectric Materials for Energy

RESEARCH IN THE CENTER FOR SOLAR AND THERMAL ENERGY CONVERSION (CSTEC)

MSE in Action…the cutting edge

The Challenge: Energy Consumption and Availability

Consumption Portfolio

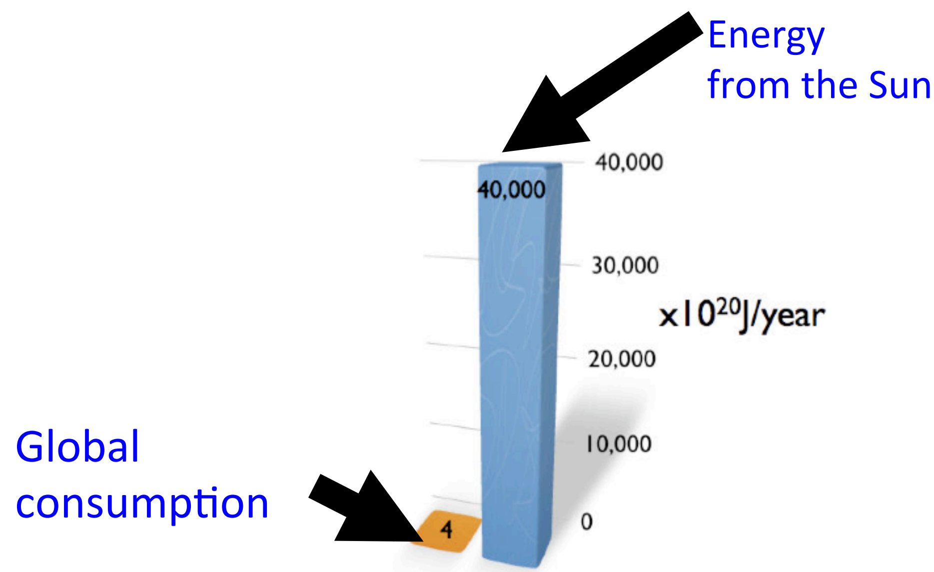


World Usage predicted to double (~28 TW) by 2050

More energy comes from the sun in 1 hr than we use in 1 year

US usage : 3.3 TW
World usage : 15 TW

~ 0.1% electricity comes from sunlight



IEA Report 2005

Tailoring absorption as well as carrier and phonon transport in order to develop high efficiency Photovoltaics and Thermoelectrics

SOLAR

Absorption
Carrier (e^-, h^+) pair creation, thermalization (phonons)

Exciton transport

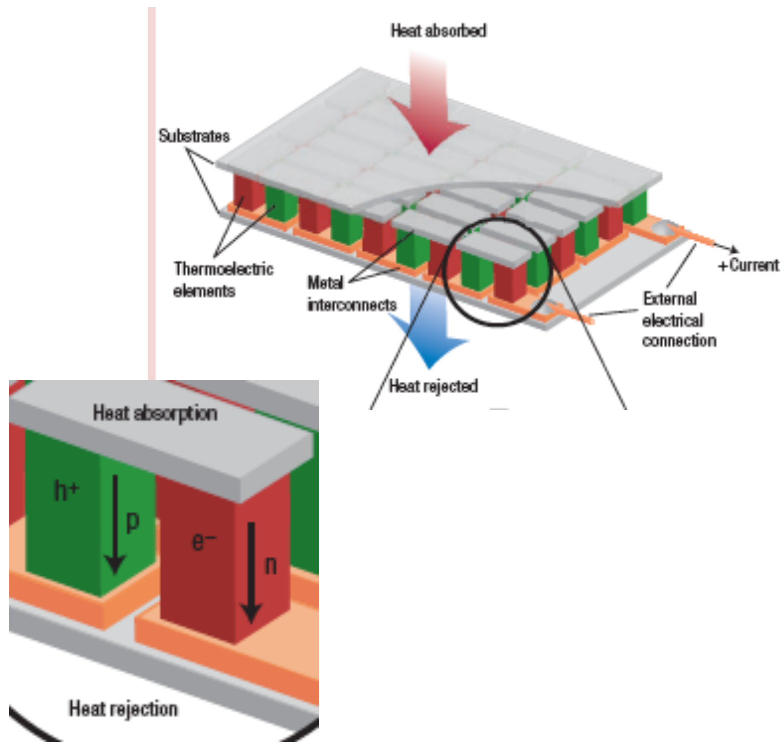
Organics

Charge dissociation and Separation

Carrier Transport

(h^+, e^-) harvesting

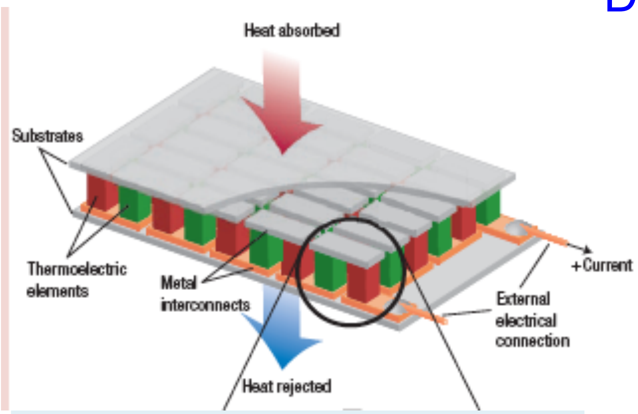
Thermal: TE



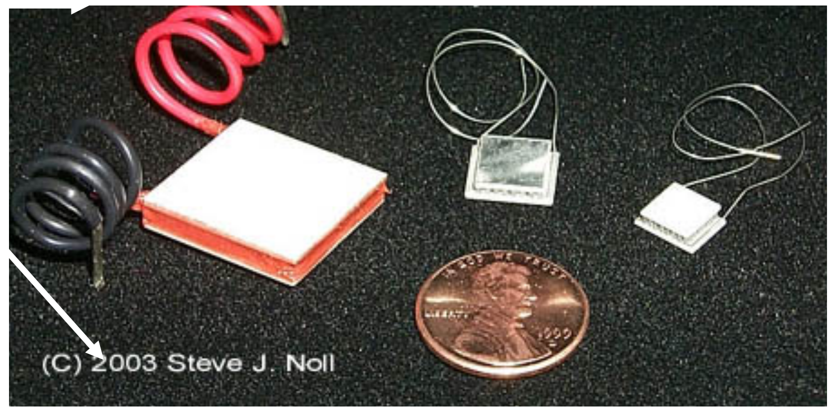
Snyder et al. Nature Mat, 7, 107

Thermoelectrics: Improvements in efficiency will result in significant energy savings

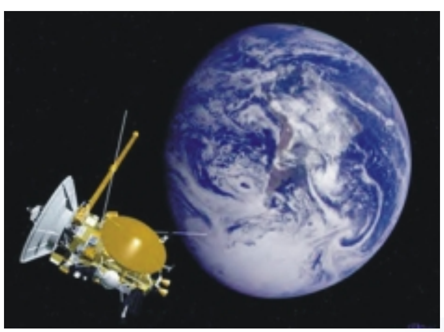
DEVICES



Snyder et al. Nature Mat, 7, 107



Power Generation



Refrigeration

Waste Heat Recovery

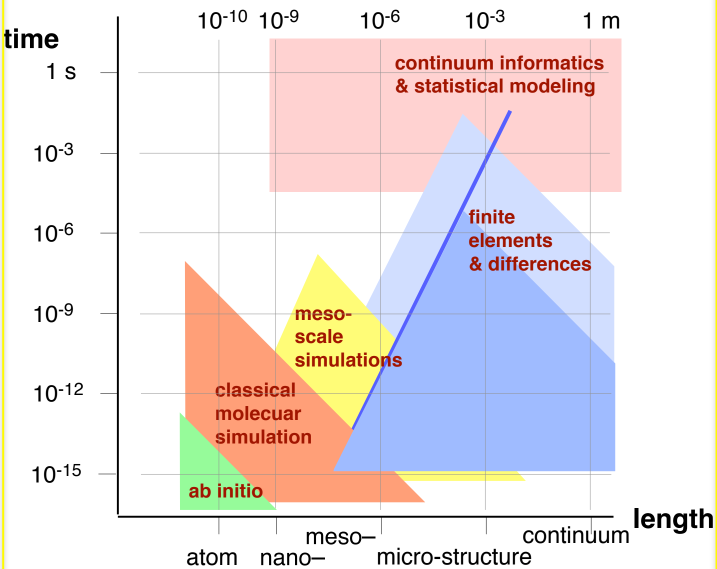
- **Vehicles**
- **Buildings**

Night vision detectors

Research Strategy

Integrated theoretical/computation/experimental efforts

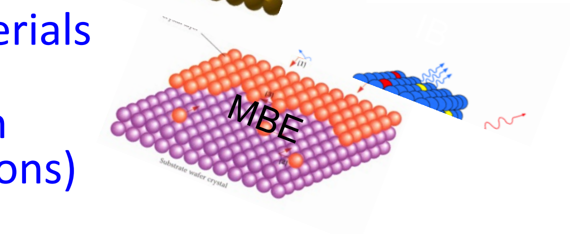
Simulations/Theory:

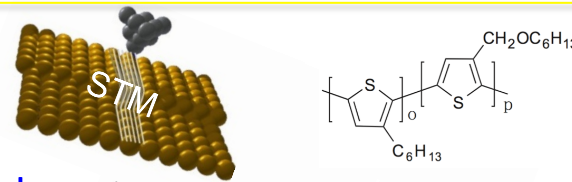


Synthesis

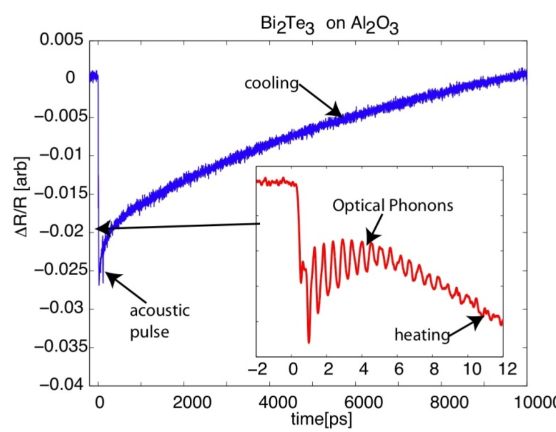
nanostructures/
nanostructured materials

Imaging tools (length scales / < nm to microns)





Measurement of dynamics of carriers and phonons (ultra fast spectroscopies)



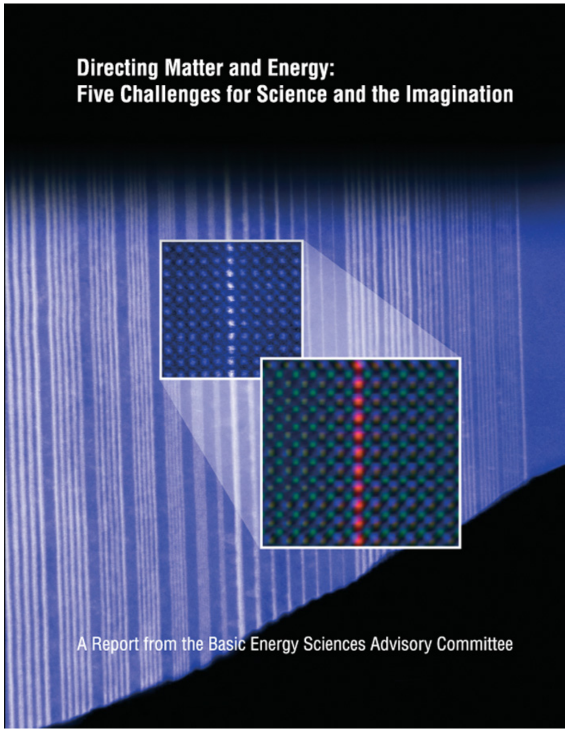
Four DOE Science Grand Challenges will be Addressed by Researchers in the Center

1. How do we control materials processes at the level of electrons?

2. How do we design and perfect atom- and energy-efficient syntheses of revolutionary new forms of matter with tailored properties?

3. How do remarkable properties of matter emerge from the complex correlations of atomic or electronic constituents and how can we control these properties?

4. How do we characterize and control matter away—especially very far away—from equilibrium?



Solar and Thermal Energy Conversion

fundamental concepts and material systems for high efficiency energy conversion

- **OBJECTIVES**: Investigate and elucidate fundamental processes that govern the efficiency of solar and thermal energy conversion in nanostructured, complex, and low-dimensional inorganic, hybrid, and organic materials.

- The efforts of the center are divided into 3 areas:
  - **CSTEC THRUST 1**: ***Inorganic PV***
    site-controlled nanostructures, type-II band-offset materials, highly mismatched alloys

  - **CSTEC THRUST 2: *Thermoelectrics***
    single-molecular junctions, nanowires, quantum-dot structures, thin films, and bulk nanocomposites

  - **CSTEC THRUST 3: *Organic and Hybrid PV Materials***
    - **Thrust 3a**: absorption phenomena in organic and hybrid systems
    - **Thrust 3b**: molecular design, synthesis, carrier transport and device performance.

MSE OUTREACH

- ASM Teachers Camp

- High School Research Experience (Pioneer, Greenhills, Ypsilanti)

- REU Program in Paris
- **Cass Technical High School, Detroit**

- Computational Materials Science for High School Kids

- Pod cast lectures

ASM Materials Camp, 2006-

Materials Science and Engineering,
class room and hands-on training, for
high school teachers

-Approximately 30 high school teachers
from around the country spend one
week in the department for training

MATERIALS CAMP
ASM Materials Education Foundation

Outreach Programs in MSE: Cass Technical High School in downtown Detroit (Akram Boukai)

Cass Tech (2142) students: 95% are African-American and 2% are Hispanic.
- hands-on battery demonstrations.
- Students built a batteries using vinegar and several different metals.
- powered a handheld
calculator with the battery.

Detroit Are Pre-College Engineering Program: **5 week Saturday series** of materials science demonstrations



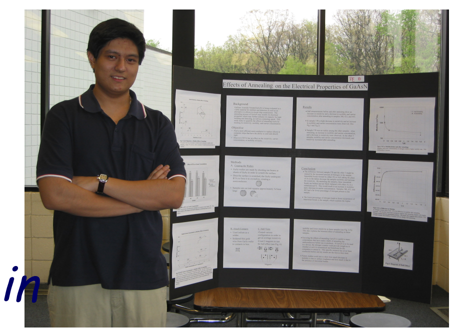
Pictures from the various outreach activities at Cass Tech and DAPCEP organized by Professor Akram Boukai. Left and center pictures are from Boukai's visit to Cass Tech High School. Right picture is from Boukai's participation in DAPCEP.

Research Partnership with Local High Schools

Hands-on research opportunities for students from local high schools Greenhills (2005-); Ypsilanti (2008-); Ann Arbor Skyline (2009-):

<u>Summer:</u> projects are kick-started in UM faculty (MSE + CoE) labs

Ms. Jayne Choi (2006): 1st place in Physics & Engineering Category of SE Michigan Science Fair, placing 7th overall



Mr. Andrew Lee (2007): National Nanotechnology Infrastructure Network Award, SE Michigan Science Failr

- *Major step forward from "science fair" classes in public high schools*
- *Science fair publicity to increase public awareness & interest in STEM in the region, state, & nation*

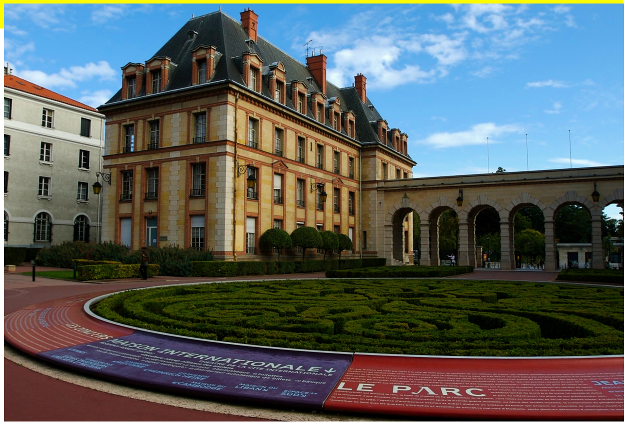
Research Experience in Paris

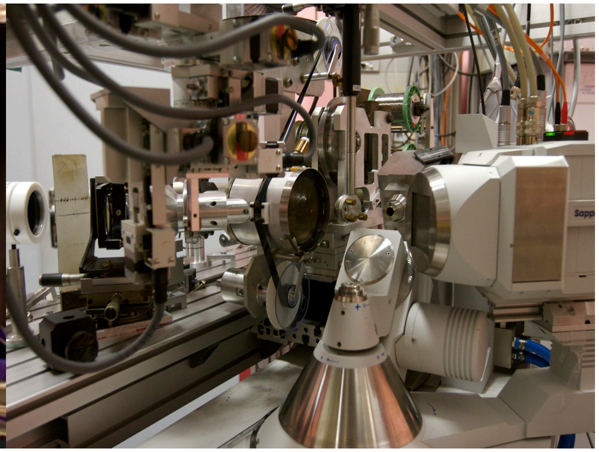
Ecole Polytechnique
Ecole Nationale de Techniques Avancées (ENSTA)
The Louvre l'Institut d' Optique Graduate School

(Yalisove) CoE/CUOS/MSE

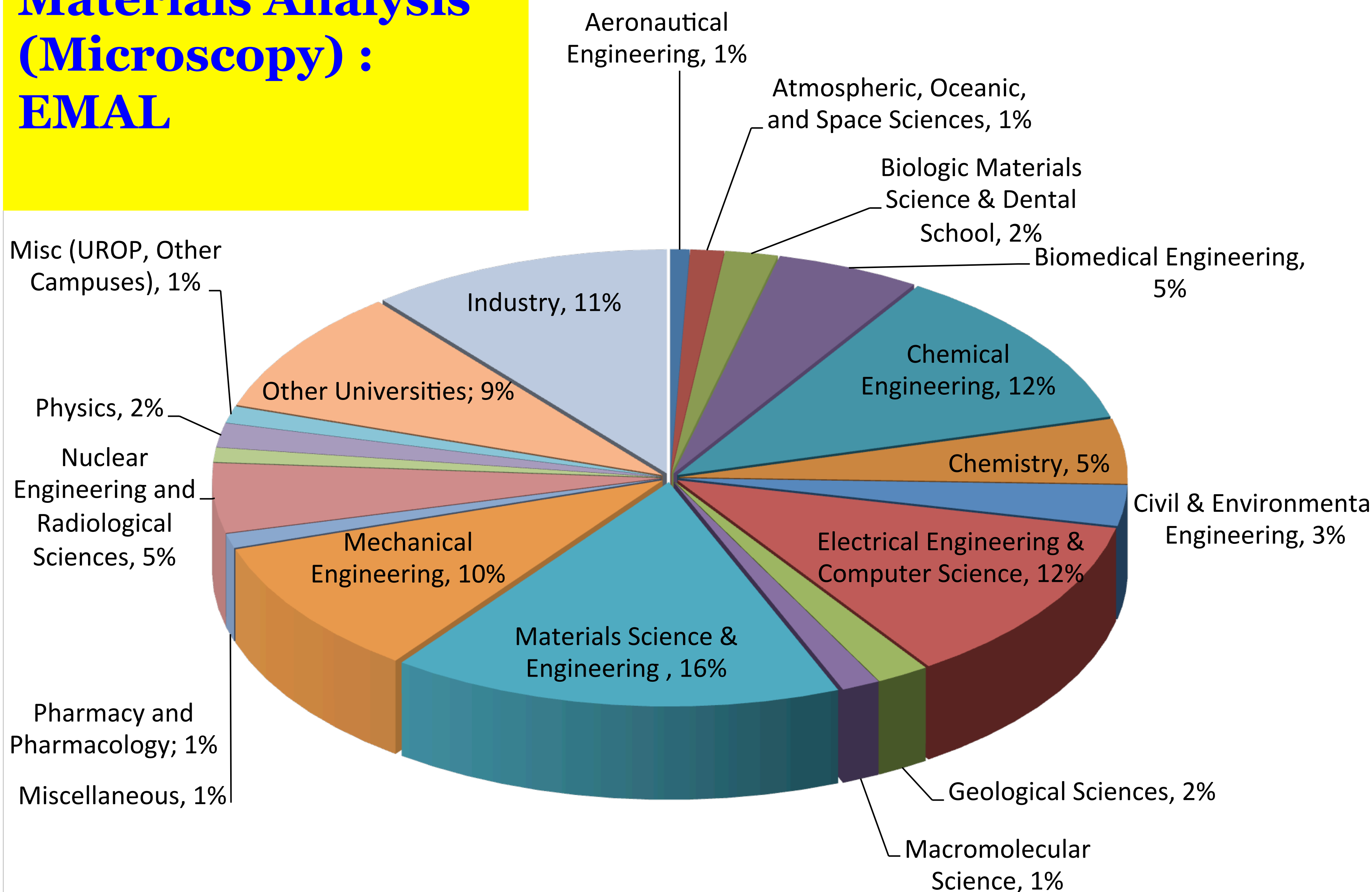
8 students this summer
60% Women/URM
Average GPA=3.91

Students stay at Cite Universitaire in downtown Paris





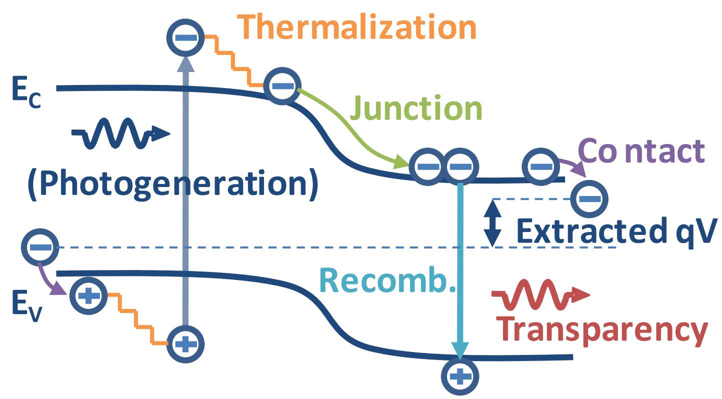
Materials Analysis (Microscopy) : EMAL

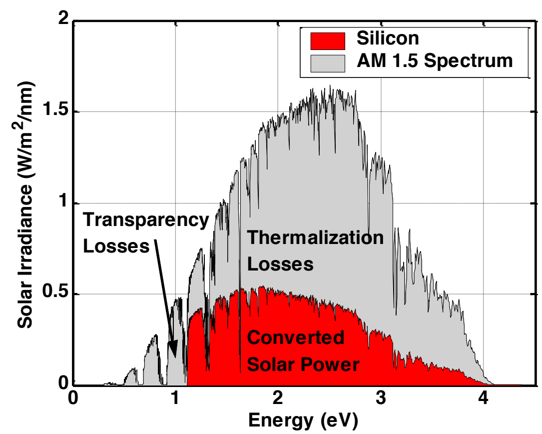


Thank You

Inorganic Photovoltaics: Challenges

Loss Mechanisms in Photovoltaics



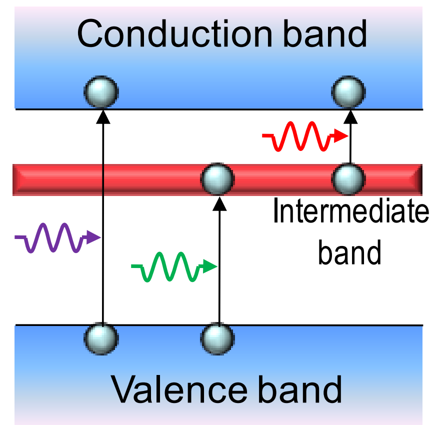


- **CHALLENGE**: Mitigate intrinsic loss mechanisms/processes
  - Thermalization and transparency losses; Control recombination, defects, role of interfaces
  - Synthesize/fabricate materials/nanostructures with *outstanding* electronic transport properties that can also absorb more of the solar spectrum

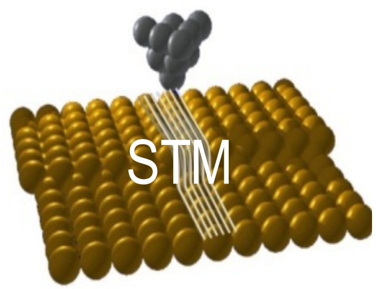
Inorganic PV (CSTEC Thrust 1): explore absorption & transport processes limiting PV conversion efficiency

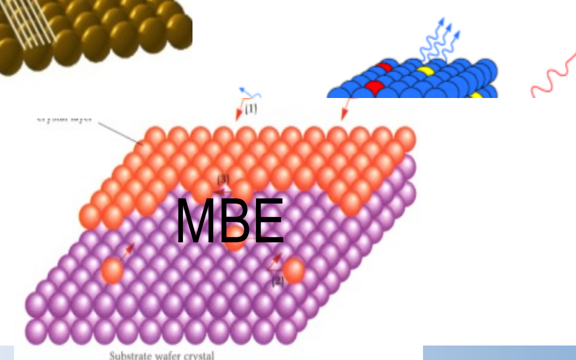
- **Nanostructuring and alloying promise:**
  - Enhanced optical absorption
  - Tailored electron transport
  - Reduced energy losses

- Systems
  - Intermediate Band
  - Type-I , Type-II nanostructures
  - Mismatched alloys
  - Superlattices



- **Convert more photons, increase J_{SC}, maintain large V_{OC}**
- **Quantum Dots**





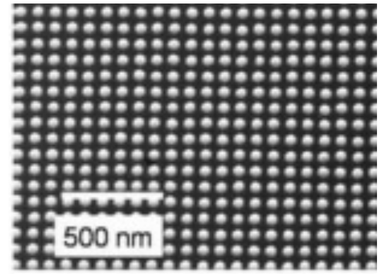
Site Control of III-Nitride QDs

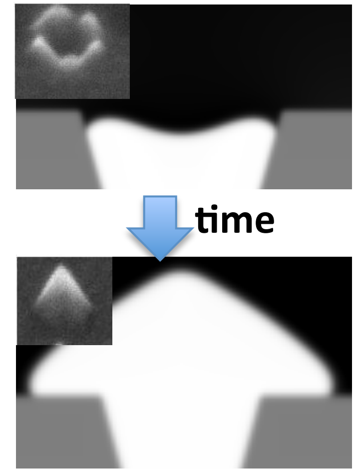
Nanowires

And

Quantum Dots

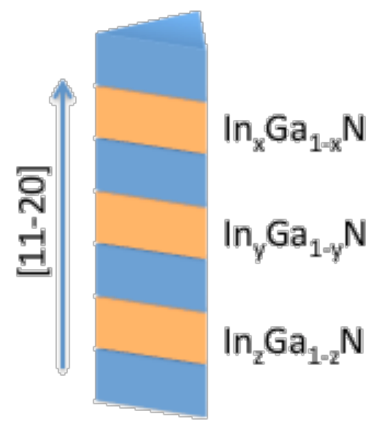
Theory/experiment on QD growth

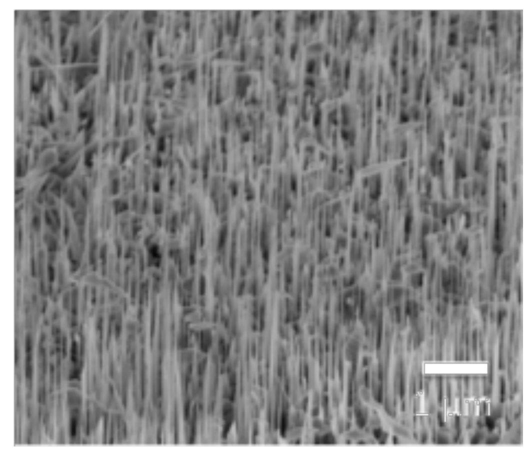




L. Aagesen, K. Thornton, L. K. Lee, and P.-C. Ku, in preparation (2011).

Tailored Nanowire growth





L. K. Lee and P.-C. Ku, in preparation (2011)

CSTEC Thrust 2: Thermoelectrics

Focus: Explore strategies that enable control of carrier and phonon processes that limit TE conversion.

Goal is to Maximize the Figure of Merit

$$\boxed{ZT = \frac{S^2 \sigma T}{\kappa}}$$

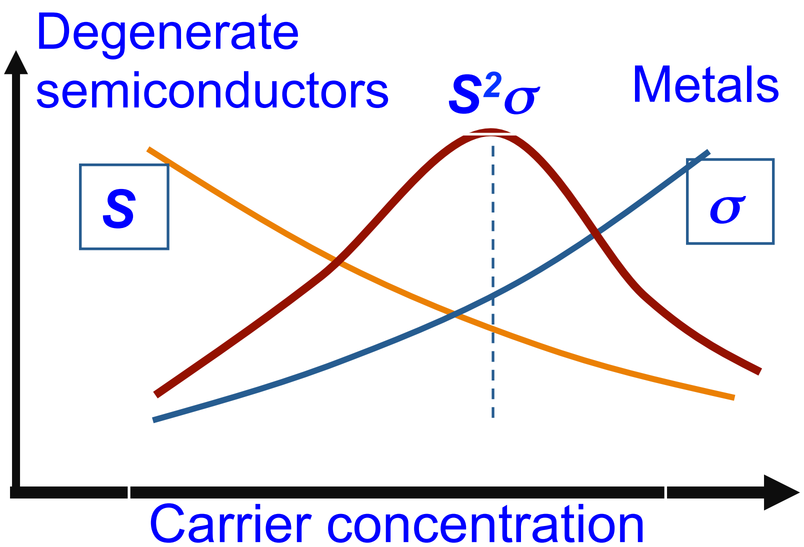
Challenge: Transport parameters are interrelated

Eg,: Metals, degenerate semiconductors:

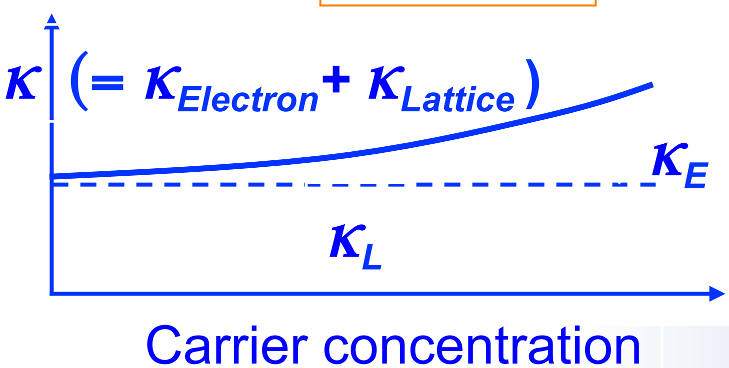
$$S \propto \frac{m^* T}{n^{2/3}} \qquad \sigma = ne\mu \qquad \kappa_e \propto \sigma T$$

Wiedemann-Franz law

Manipulating connections between σ, S and κ

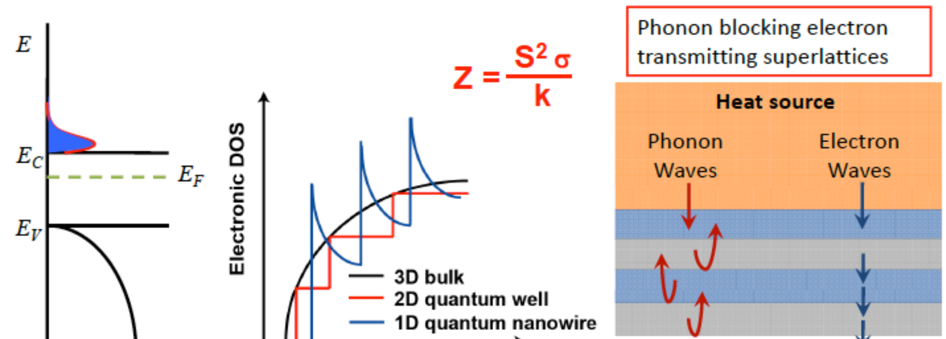


$$ZT = \frac{S^2\sigma T}{\kappa}$$



Goals of nanostructuring

- Increase $S^2\sigma$ by using materials that have increased DOS near the band edge; this means that you don't have to bring E_F as close to E_C (leading to high S) in order to get high σ.
- Decrease k by adding interfaces and phonon scattering centers (this method has proven most practical so far).



Venkatasubramanian et. al, *Nature* **413**, 597 (2001)

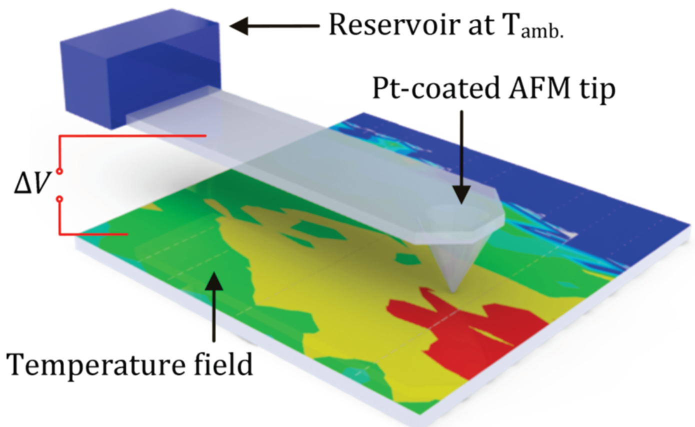
$$\sigma(E)dE \sim n(E)\left(-\frac{\partial f}{\partial E}\right)dE$$

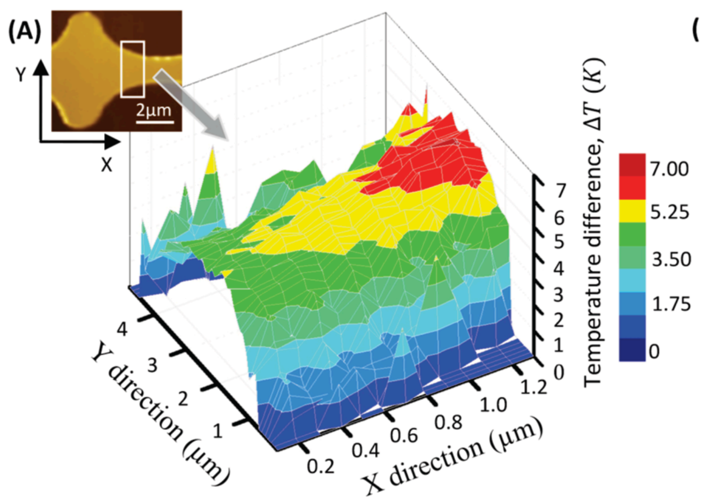
$$S = \frac{1}{eT}\frac{\int \sigma(E)(E - E_f)dE}{\int \sigma(E)dE}$$

Nanoscale thermometry

Profs. Reddy, Dunietz, Kaviany

Mapping of thermal fields with 100 nm spatial resolution and less that 10 mK thermal resolution[Nano Letters 10, 2613 (2010)].





3D temperature field of a cross section of a test object

Akram Boukai: All-Inorganic Eutectic Solar Cell

Lamellar $Mg_2SI–Si$ Heterojunctions for
Efficient Charge Carrier Collection in Metallurgical Grade Materials