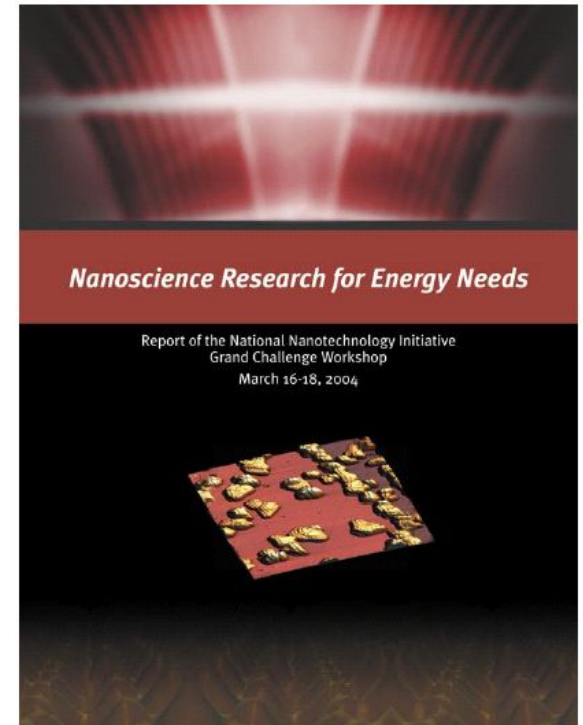
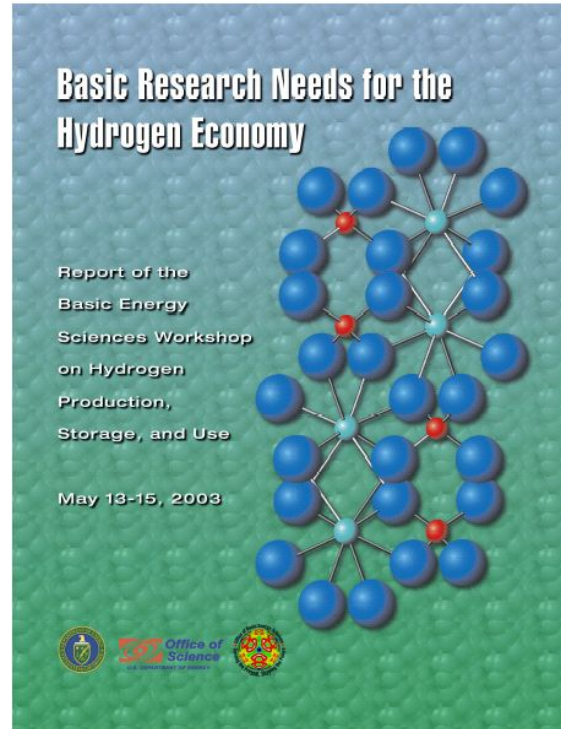


# Energy and Nanotechnology

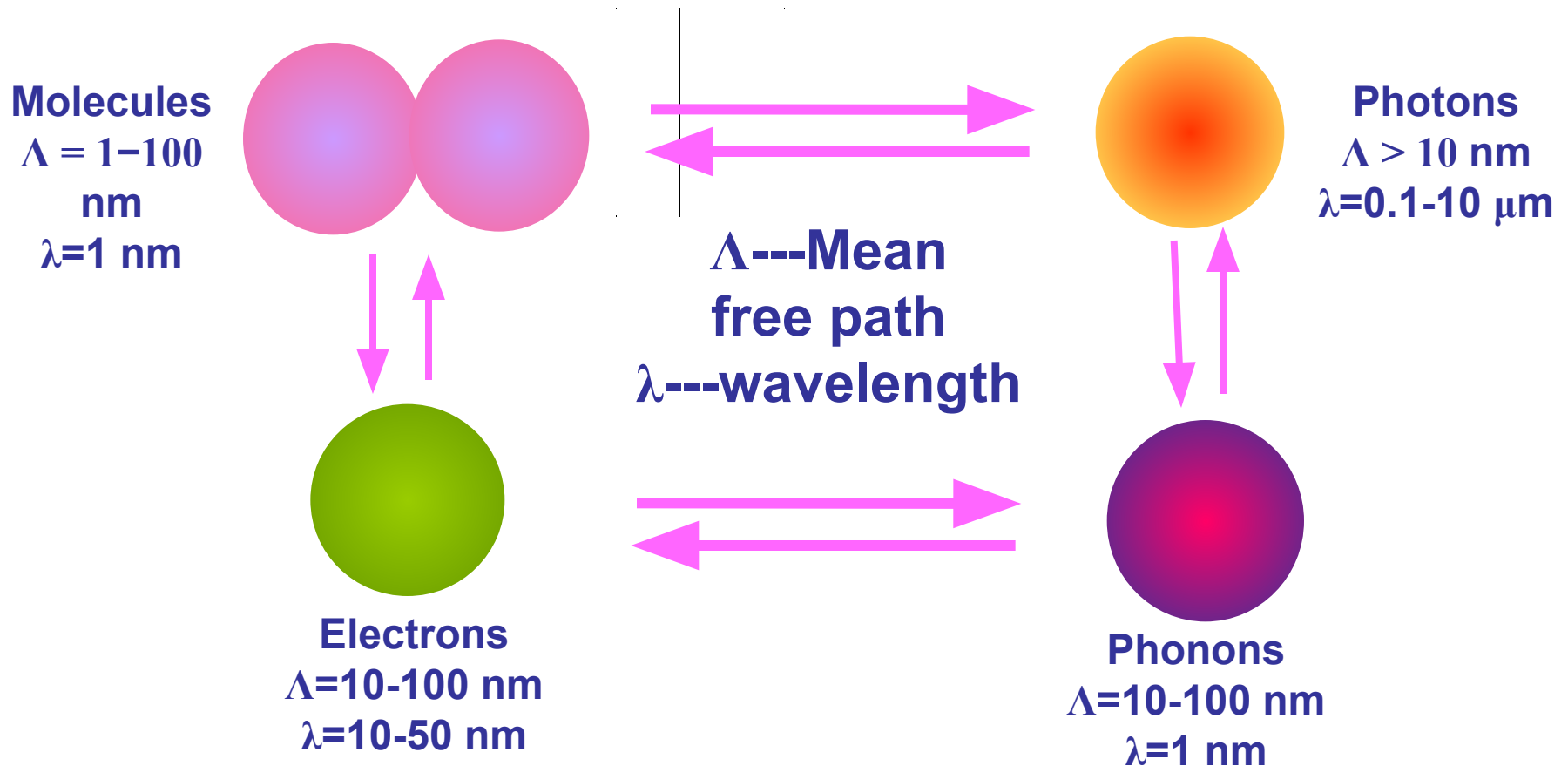
# Sources



<http://www.sc.doe.gov>

# Nano for Energy

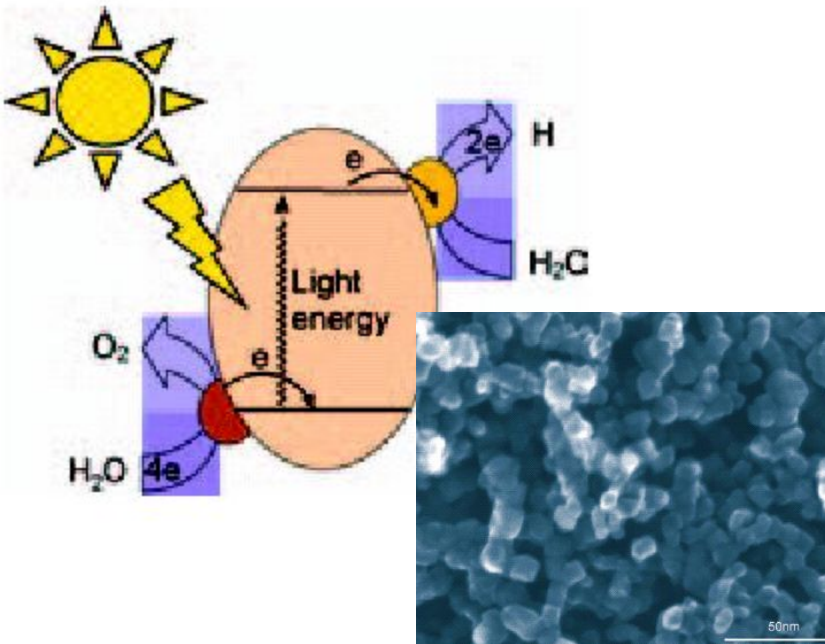
- Increased surface area
- Interface and size effects



# Nanoscience Research for Energy Needs

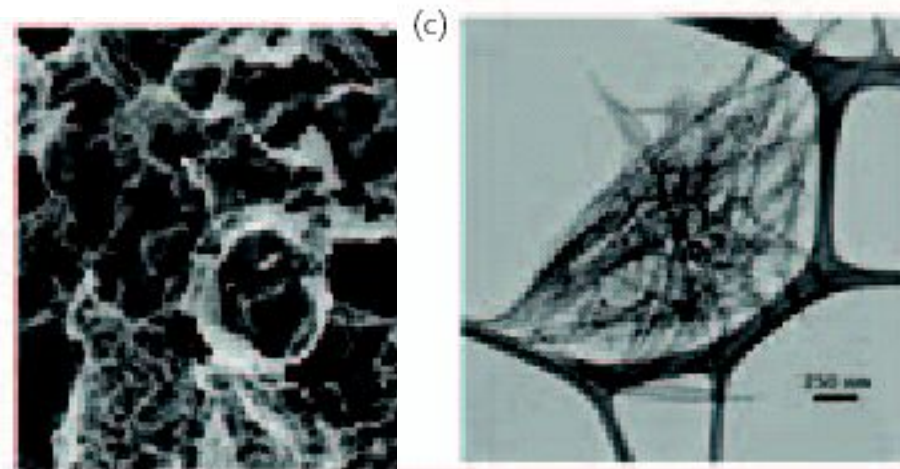
- Catalysis by nanoscale materials
- Using interfaces to manipulate energy carriers
- Linking structures and function at the nanoscale
- Assembly and architecture of nanoscale structures
- Theory, modeling, and simulation for energy nanosciences
- Scalable synthesis methods

# Examples



## Grätzel cell for photovoltaic generation and water splitting

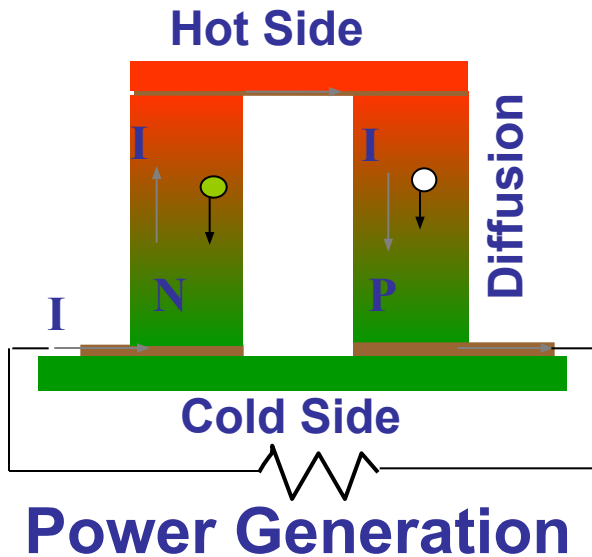
- Radiation transport to maximize absorption
- Two phase flow
- Electrochemical transport
- Multiscale, multiphysics transport



## Catalytic nanostructured hydrogen storage materials

- Mass transport
- Heat transfer (intake and release)
- Small scale thermodynamics
- Two phase flow
- Multiscale and multiphysics

# Thermoelectrics Devices



**Figure of Merit:**

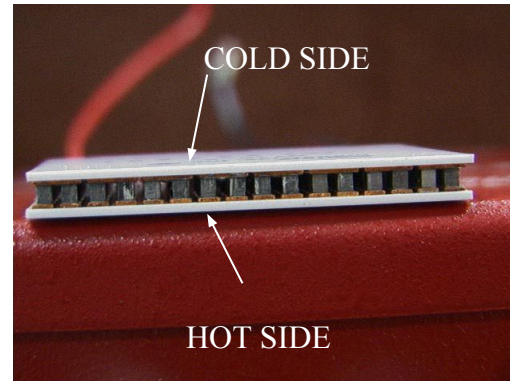
Electrical Conductivity

Seebeck Coefficient

$$ZT = \frac{\sigma S^2 T}{k_e + k_p}$$

Electron Thermal Conductivity

Phonon Thermal Conductivity



Media Clip

- Refrigeration
- Power Generation:

$T(\text{hot})=500\text{ C}$ ,  $T(\text{cold})=50\text{ C}$

$ZT=1$ , Efficiency = 8 %

$ZT=3$ , Efficiency =17 %

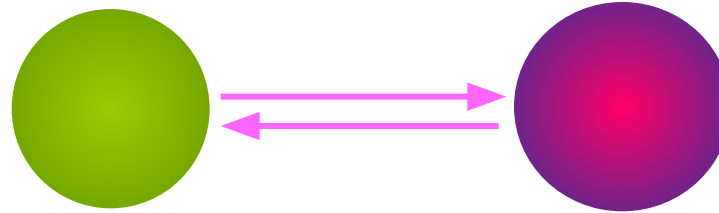
$ZT=5$ , Efficiency =22 %

- Critical Challenges:

Reduce phonon heat conduction while maintaining or enhancing electron transport

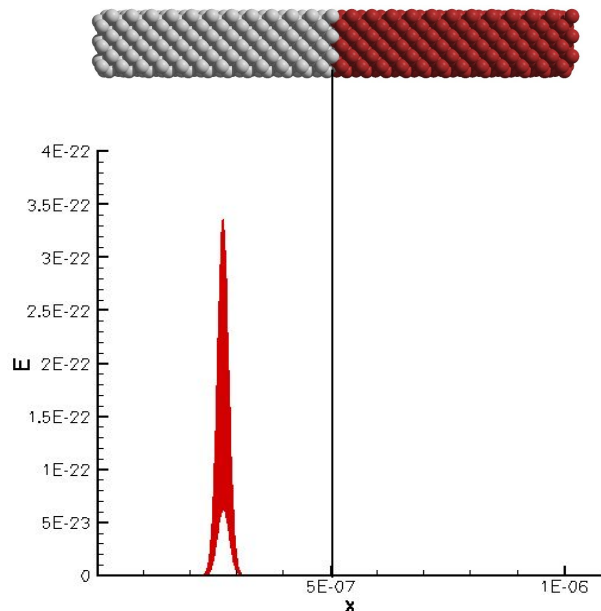
# Nanoscale Effects for Thermoelectrics

Interfaces that Scatter Phonons but not Electrons

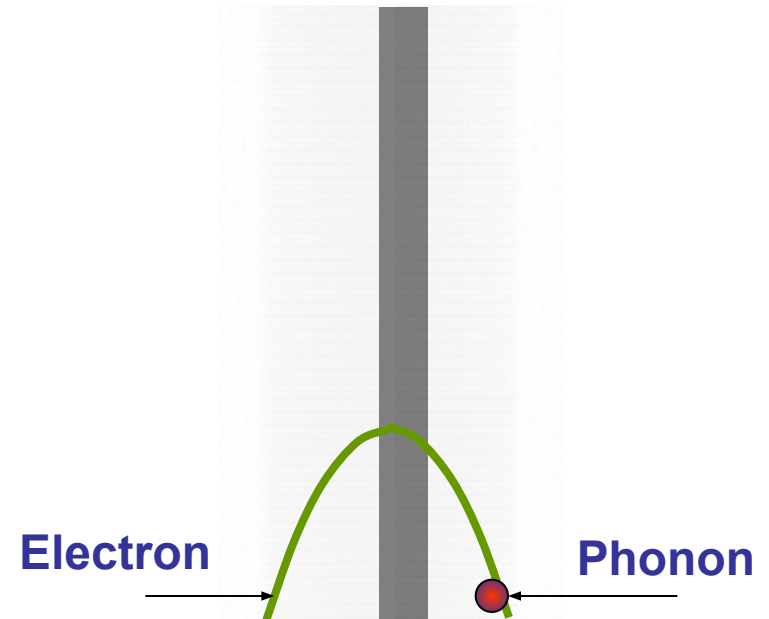


**Electrons**  
 $\Lambda=10-100$  nm  
 $\lambda=10-50$  nm

**Phonons**  
 $\Lambda=10-100$  nm  
 $\lambda=1$  nm

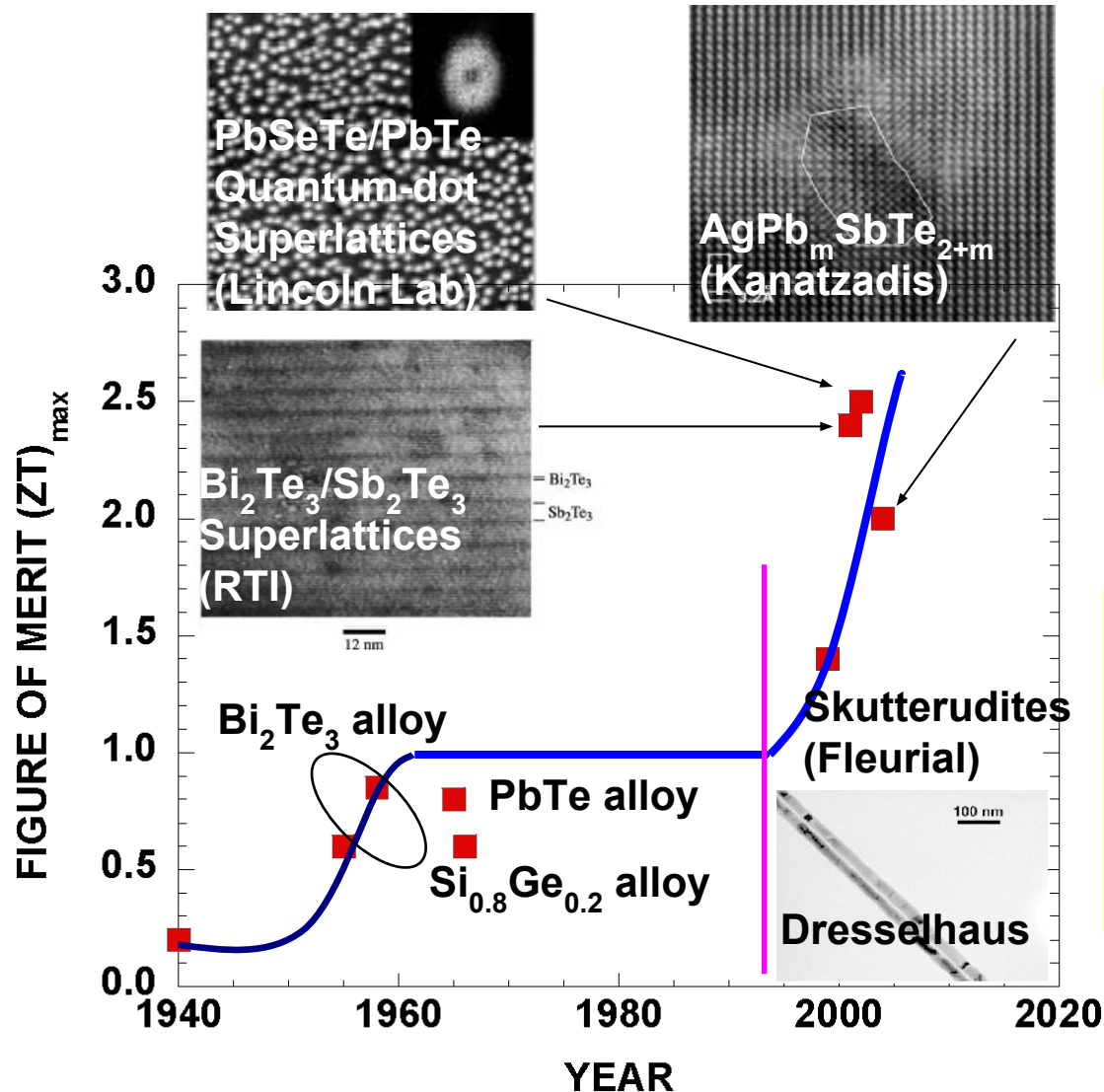


**Molecular Dynamics (Freund)**





# State-of-the-Art in Thermoelectrics



PbTe/PbSeTe	Nano	Bulk
$S^2\sigma$ ( $\mu\text{W}/\text{cmK}^2$ )	32	28
$k$ (W/mK)	0.6	2.5
$ZT$ (T=300K)	1.6	0.3

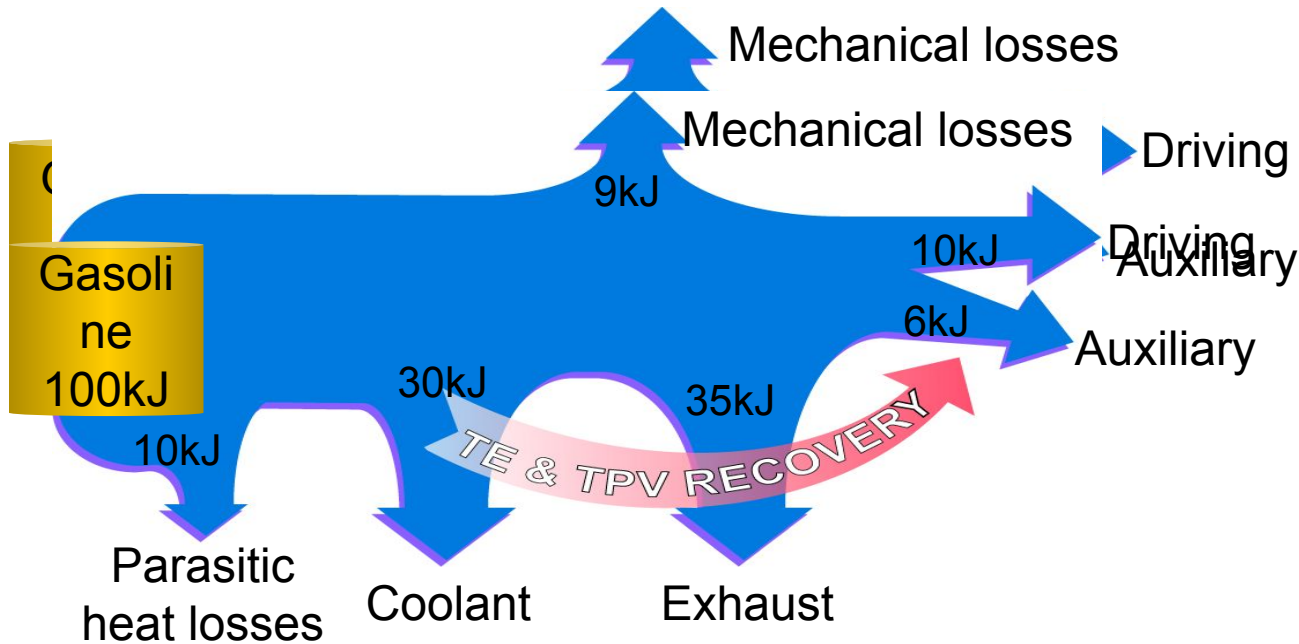
Harman et al., Science (2003)

Bi <sub>2</sub> Te <sub>3</sub> /Sb <sub>2</sub> Te <sub>3</sub>	Nano	Bulk
$S^2\sigma$ ( $\mu\text{W}/\text{cmK}^2$ )	40	50.9
$k$ (W/mK)	0.6	1.45
$ZT$ (T=300K)	2.4	1.0

Venkatasubramanian et al.,  
Nature, 2002.



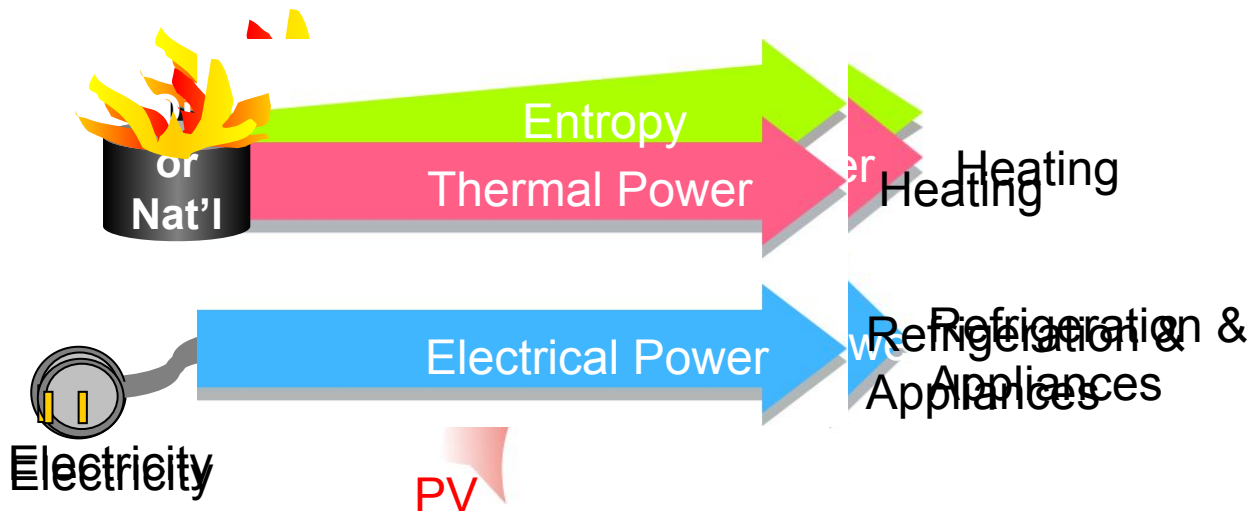
# Potential Applications



## Transportation

In US, transportation uses ~26% of total energy.

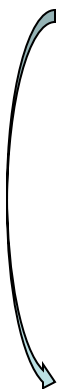
10% energy conversion efficiency = 26% increase in useful energy



## Residential

In US, residential and commercial buildings consume ~35% energy supply

# Challenges and Opportunities

- 
- Mass production of nanomaterials
  - Energy systems: high heat flux
  - Nanomaterials are trans-boundary
  - Basic energy research leads to breakthroughs
  - Transports (molecular, continuum) are crucial
  - Inter-departmental collaborations