Role of nanoscale materials and devices in transforming our energy system

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Industrial Revolution: Horse Power to Horsepower

300 Horsepower

10,000 Horsepower

100,000

The greatest engineering achievement of the 20th century

US National Academy of Engineering
How can we decarbonize our energy system and continue economic growth?
Climate change is happening now and is accelerating

By 2100
25-55 cm - Bad
37-77 cm - Worse
51-131 cm - Ugly

How do we adapt to climate change?

Sea Level Rise is Accelerating

Kopp et al., PNAS (2016)
Mengel et al., PNAS (2016)
1.5B people don’t have access to electricity

How can we enable access to affordable energy for economic development for billions of people?
Top 10 List of Game-Changing Energy Innovations
(in no particular order)
1. Genetic engineering that reduces cost and simplifies the conversion of biomass to useful chemicals and fuels
2. Use carbon-free energy to transform CO$_2$ into liquid hydrocarbon fuels at $2/gallon
3. Internal combustion engines with >50% efficiency with multi-fuel mixtures
4. Building performance standards combined with designs, materials, sensors and control systems that significantly reduce building energy consumption
5. Ultra-high voltage transmission lines and low-cost integration of intermittent renewables at >50% penetration
6. Deep borehole geothermal energy with levelized cost <7-8 ¢/kWh
7. Modular nuclear plant construction at capital cost <$3/W (levelized cost < 7 ¢/kWh)
8. Electricity storage at capital cost <$100/kWh with >1000 cycles
9. Photovoltaic systems that are lighter and more efficient, enabling fully-installed capital cost of $0.5/W (levelized cost < 2.5 ¢/kWh)
10. Carbon capture from coal-fired power plants at cost <$30/tCO$_2$ with a carbon price >$40/tCO$_2$
Cell Efficiency

- Shockley-Queisser Limit

Balance of System Dominates Cost
- Efficiency Matters
- Weight Matters

Best Research-Cell Efficiencies

- Shockley-Queisser Limit
Carbon Capture

Current Cost = $70-80/tCO₂ post-combustion capture

Can we reduce it to < $30/tCO₂

\[ CO_2 + X \rightleftharpoons X - CO_2; \quad \Delta H < 0 \]
\[ \Delta G = \Delta H - T\Delta S; \]

X: MEA – Monoethanolamine
X: NaOH – Sodium Hydroxide

Dissociative Reaction: \( T_{\text{dis}} = \frac{\Delta H}{\Delta S} \)
Storage

Pumped Hydro
(Capital Cost = $100/kWh)
(Levelized cost of storage = 2 c/kWh)

Cost has reduced 3 times between 2008-2015

Materials and packaging innovations
400 Wh/kg; C/10
80% depth of discharge

Roughly $250/kWh
Rare Earth Free Hard Magnetic Materials for Generators & Motors

Fe$_{16}$N$_2$

“Holy Grail of Magnets”

BH$_{\text{max}}$ = 134 MGOe
Power Electronics

Switches ($\omega$)
- Integrated WBG
- SiC
- GaN
- >13kV WBG

Magnetics ($j\omega L$)
- High Flux Soft Magnets

Converters
- >10 W, >95% Single-Chip
- Single Chip AC
- High Efficiency

Capacitors ($1/j\omega C$)
- Reliable + fast + high energy density

Integrated WBG SiC GaN
8000 lbs, 60 Hz Distribution Transformer
Average Age: 42 years, 2 years beyond projected lifespan

Silicon Carbide IGBT;
15 kV, 100 A;
50 kHz from Cree Inc.

Potentially 100 lbs transformer
Low Loss High Frequency Soft Magnets

SOFT MAGNETS

![Graph showing Loss (kW/m^3) vs Frequency (kHz) for different materials like FeNC, NiZn, Kool Mu, LTCC Ferrite, etc.](image)

- **FeNC** (UI=100~150)
- **NiZn** (Ferrocube UI=80)
- **LTCC Ferrite** (UI=90)
- **CoNiFe** (UI=200)

Other materials:
- Granular film (CoZrO) (UI=400)
- Thin film (CoNiFe) (UI=600)
- Kool Mu (Magnetics UI=60)

**ΔB=40mT**

![Image of Co particles (3~5 nm) with Al₂O₃, ZrO₂ etc.](image)

![Graph showing M(T) vs Field (Oe) with Easy and Hard Axis](image)

- Easy Axis: Near-perfect lossless loop
Current refrigerants have GWP over 1000x of CO$_2$
Montreal Protocol will likely be amended

Velders et al, PNAS 106, 10949 (2009)

Up to 50% reduction in primary energy consumption
Thermoelectric Power Generation (Xternal combustion engine) & Cooling

Seebeck Coefficient, $S = \frac{V}{\Delta T}$

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

- **Engine**
  - $Q_{in}$
  - $Q_{out}$

- **Refrigerator/Heat Pump**
  - $Q_{in}$
  - $Q_{out}$
  - $T_{cold}$
  - $T_{hot}$

- **Biomass, LPG**
- **Bismuth Telluride**

- **Bi$_2$Te$_3$**

- **Percent of Carnot**
  - 0%
  - 10%
  - 20%
  - 30%
  - 40%
  - 50%

- **ZT**
  - 0
  - 1
  - 2
  - 3
Power Generation & Cooling Systems

Power Pot = $70

System level cost target = $1/W
Balance of system cost > TE device cost
Device efficiency matters
Bermuda Triangle of Thermoelectrics

Semiconductors  S  Metals

Carrier concentration

\[ ZT = \frac{S^2 \sigma T}{k} \]

\[ \kappa = \kappa_{\text{Electron}} + \kappa_{\text{Lattice}} \]

\[ \kappa_E \]

\[ \kappa_L \]
III-V Semiconductors

A. Shakouri, T. Sands (Purdue), J. Bowers, A. Gossard, S. Stemmer (UCSB), R. Ram (MIT), J. Zide (Delaware)

Si Nanowires

Peidong Yang, Joel Moore (UCB, LBL)

Molecular-Hybrid Materials

Rachel Segalman, J. Urban (LBL, UCB)


Oxides

R. Ramesh (UCB, LBL)

DOE

NSF

ONR

DARPA

AFOSR
Phonon Scattering Using Nanostructures

Rayleigh scattering regime: \( \sigma \sim \frac{b^6}{\lambda^4} \)


Typical \( b \):
- Alloy — 1 Å
- Nanoparticle — 1-4 nm
Electron & Phonon Mean Free Path Differences in Si

$\lambda_{\text{electron}} < \lambda_{\text{phonon}}$


<table>
<thead>
<tr>
<th>Material</th>
<th>$\lambda_{\text{phonon}}$ (nm)</th>
<th>$k$ (W/m-K)</th>
<th>$S^2\sigma$ (W/m-K^2)</th>
<th>ZT</th>
<th>Abundance</th>
</tr>
</thead>
<tbody>
<tr>
<td>Si</td>
<td>~100-1000 nm</td>
<td>140</td>
<td>0.0047</td>
<td>0.01</td>
<td>27%</td>
</tr>
<tr>
<td>Bi₂Te₃</td>
<td>~1 nm</td>
<td>1.4</td>
<td>0.0037</td>
<td>0.8</td>
<td>Bi: 48 ppb Te: 5 ppb</td>
</tr>
</tbody>
</table>
Smooth and Rough Si Nanowires

Holey Silicon


Controlled Wire Roughness

Roughness Parameters

σ: Rms height

L: Autocorrelation length
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Thank you!
Crossover from incoherent to coherent phonon scattering in epitaxial oxide superlattices

Jayakanth Ravichandran¹²†‡, Ajay K. Yadav²³†, Ramez Cheaito⁴‡, Pim B. Rossen³, Arsen Soukiassian⁵, S. J. Suresha², John C. Duda⁴, Brian M. Foley⁴, Che-Hui Lee⁵, Ye Zhu⁶, Arthur W. Lichtenberger⁷, Joel E. Moore²⁸, David A. Muller⁶⁹, Darrell G. Schlom⁵⁹, Patrick E. Hopkins⁴, Arun Majumdar¹⁰, Ramesh¹²³⁸¹¹* and Mark A. Zurbuchen

n(CaTiO₃/CTO): m(SrTiO₃/STO)

n(BaTiO₃/BTO): m(SrTiO₃/STO)
What is our Haber-Bosch like challenge?

- CO$_2$ feedstock at $/tC
- H$_2$O
- Carbon-free energy at $/kWh

Processes:
- Electrochemical
- Photochemical
- Biochemical
- Thermochemical

Products:
- Methanol
- Ethanol
- Hydrogen
- Hydrocarbon ($/kg; $/L)
A grand challenge….

Liquid Hydrocarbon Fuel

$2/gallon

H₂: Need @<$2/kg

Today @ $5/kg

$20/MWh

CO₂ + H₂ -> CO + H₂O

Reverse Water Gas Shift Reaction
H₂ production: Steam Reforming of Natural Gas

TODAY

800-1,000°C; 14-20 atm
Nickel catalysts

CH₄ → H₂ → H₂O → CO₂

How do we produce carbon-neutral H₂ at <$2/kg at scale?
**Thermodynamic & Cost Limits**

\[ H_2O = H_2 + \frac{1}{2} O_2; \Delta H = 286 \text{ KJ/mol} = 40 \text{ kWh/kg-H}_2 \]

**Biomass**

- **Calorific Value:** 7000 BTU/lb = 15400 BTU/kg = 4.50 kWh/kg-bm
- **Cost:** $65/ton = $0.065/kg-bm
- **Energy Cost:** $15/MWh
Electrochemical Pathway

Alkaline electrolysis
40 - 90 °C

Cathode → OH
H₂ + \% O₂

H₂O + 2e⁻ → H₂ + 2OH⁻

2OH⁻ → \% O₂ + H₂O + 2e⁻

Anode → Ni/C

PEM electrolysis
20 - 100 °C

H₂O → H⁺ + \% O₂ + 2e⁻

Cathode → H₂ + \% O₂

H₂O → H₂ + \% O₂

Total reaction

ΔH = 55 kWh/kg-H₂

TODAY: $5/kg-H₂

OPTIMISTIC LIMIT: $2/kg-H₂

How can we beat the $2/kg-H₂ limit at scale with new system design?
Thermochemical Pathway

**STATE-OF-THE-ART**
Medium = 600 °C
Hot = 1,500 °C
CeO$_2$  
< 1% $\eta_{\text{Carnot}}$

**FUTURE**
Medium = 600 °C
Hot = 800 °C
Fluidized bed reactor?
- Matching heat input to chemistry
- Heat recuperation

**PEROVSKITE**

Material
Reactor

$\text{H}_2\text{O}$  
$\text{H}_2$

Medium
MeO$_{x-d}$  
MeO$_x$

O$_2$

A-site (La/Sr)
B-site (Co/Cr)

Oxygen
(In)Famous Predictions from the Past

“Radio has no future”

“X-rays will prove to be a hoax.”

“Heavier-than-air flying machines are impossible”

Lord Kelvin in 1890s
(In)Famous Predictions from the Past

“Man will not fly for 50 years.”

Wilbur Wright in 1901
Any sufficiently advanced technology is indistinguishable from magic.

Arthur C. Clarke