Role of nanoscale materials and devices in transforming our energy system

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Industrial Revolution: Horse Power to Horsepower

300 Horsepower

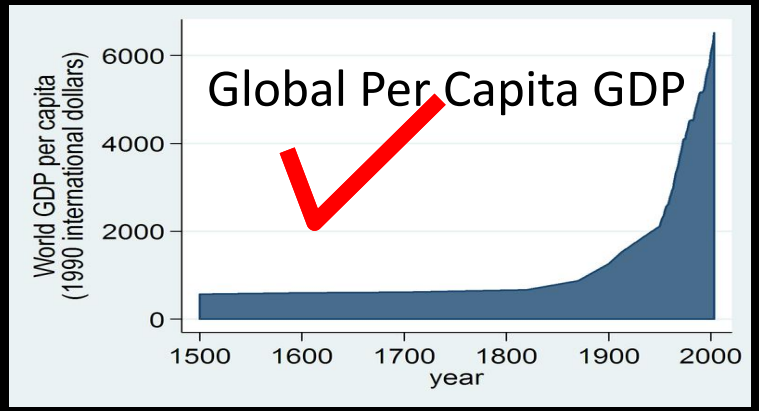
10,000 Horsepower

100,000

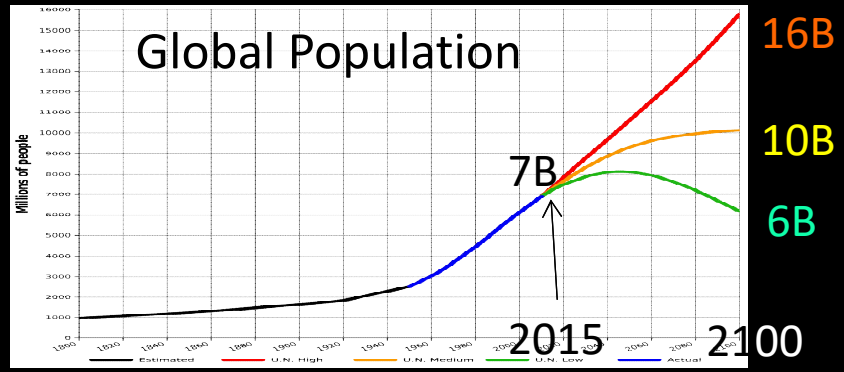
The greatest engineering achievement of the 20th century

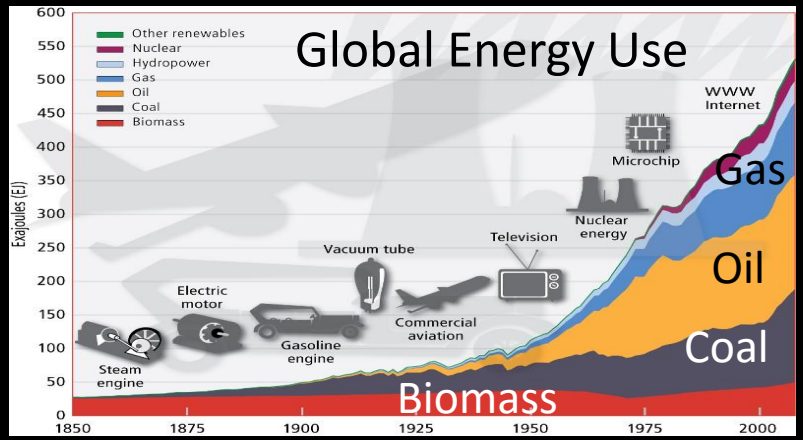
US National Academy of Engineering

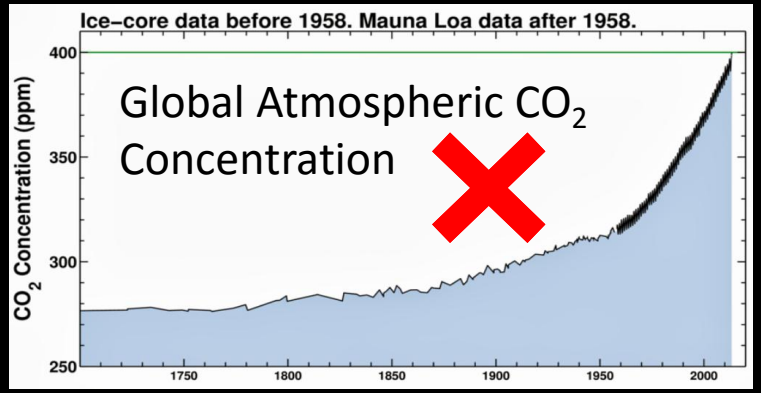
How can we decarbonize our energy system and continue economic growth?



Global Exponentials







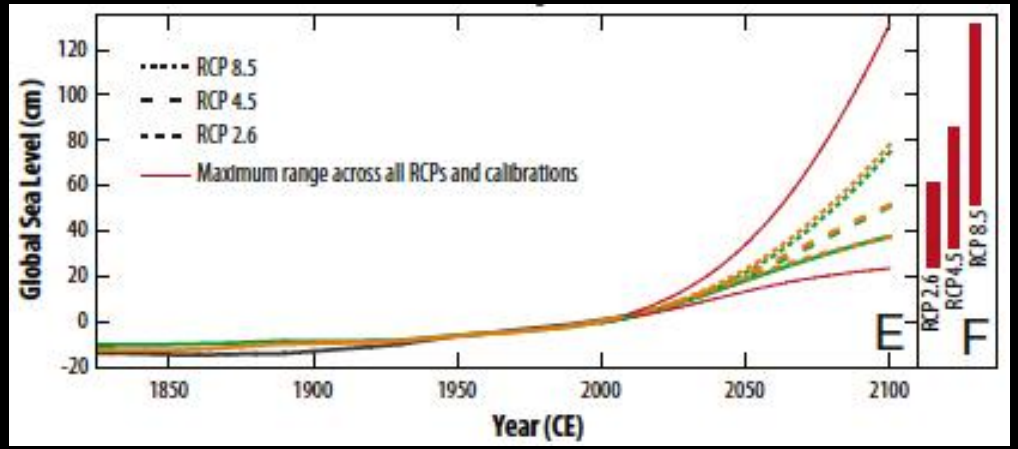
Climate change is happening now and is accelerating

By 2100

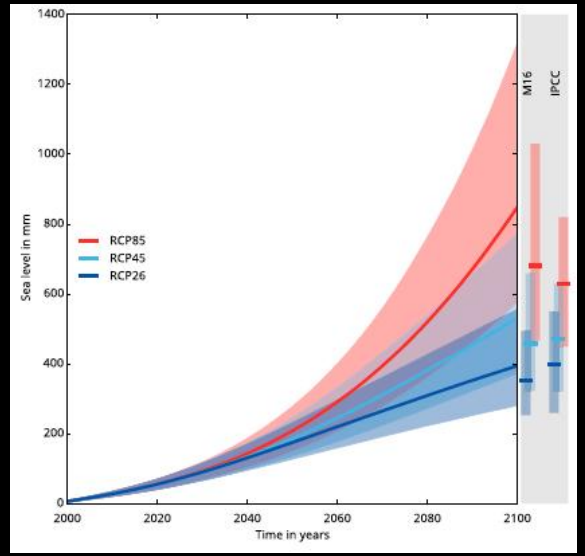
25-55 cm - Bad
37-77 cm - Worse
51-131 cm - Ugly

How do we adapt to climate change?

Sea Level Rise is Accelerating



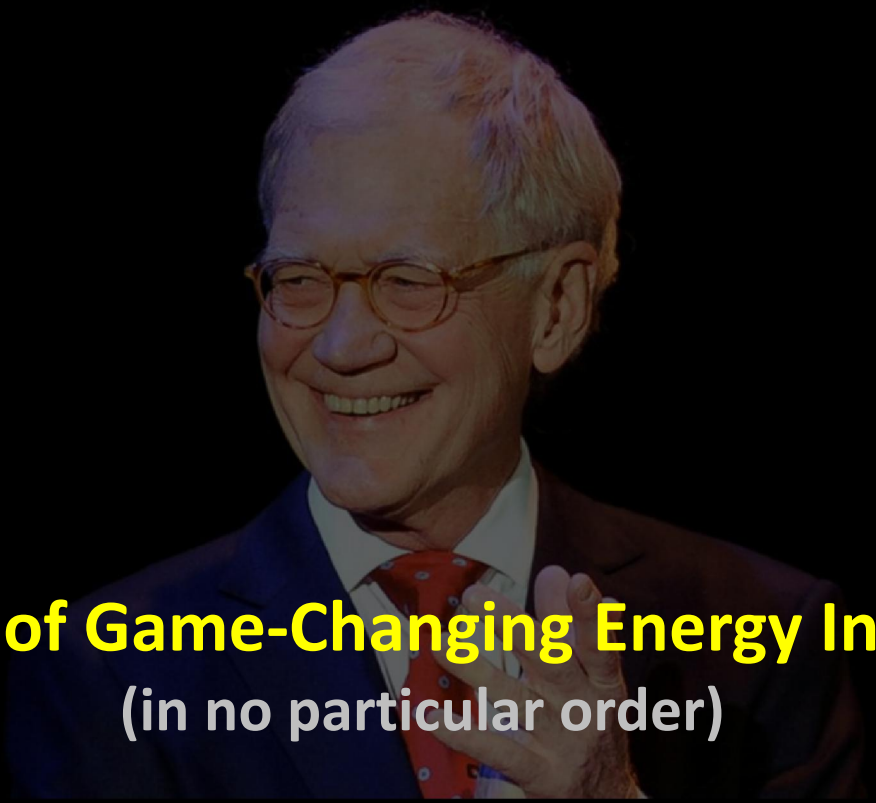
Kopp et al., PNAS (2016)



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?

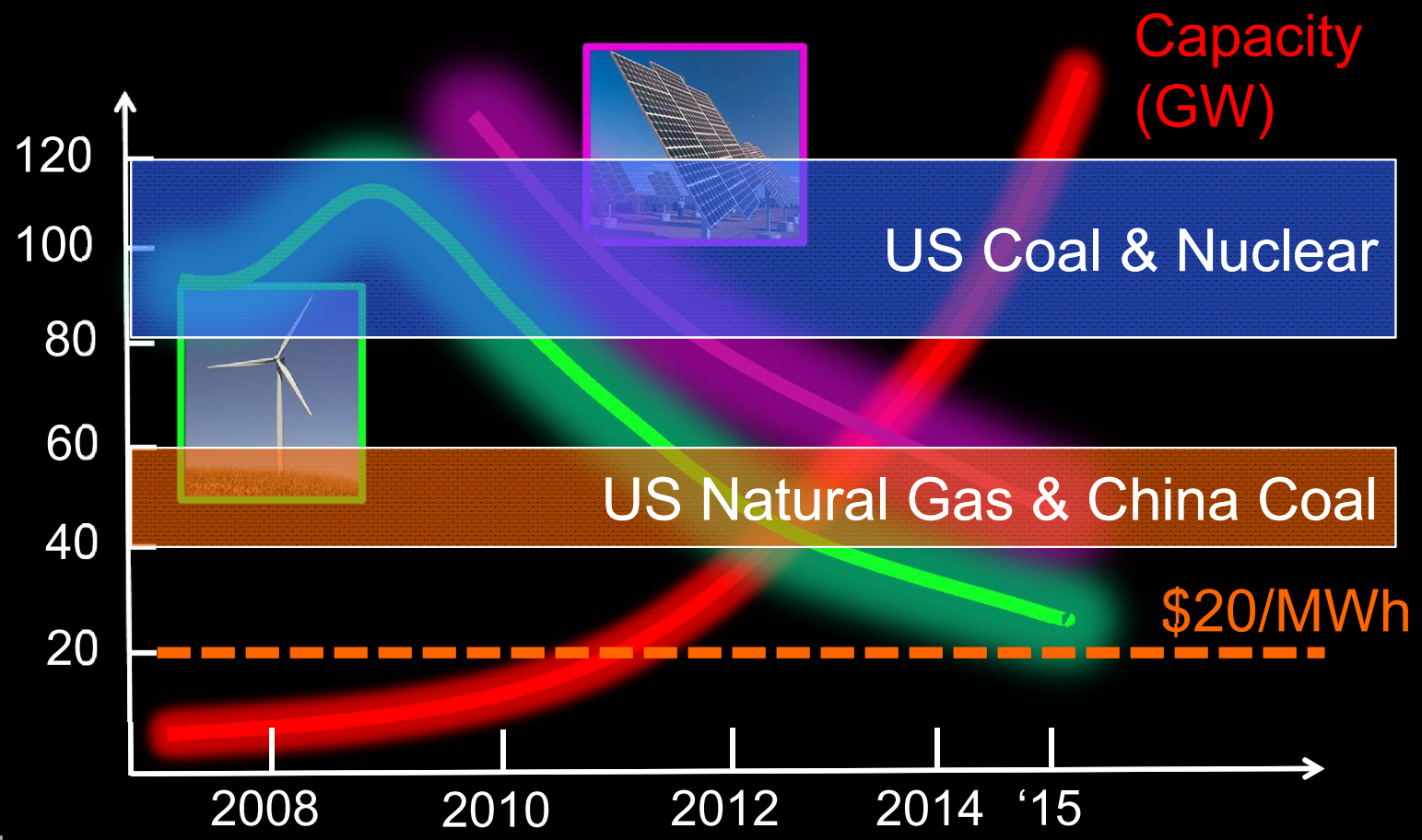


Top 10 List of Game-Changing Energy Innovations

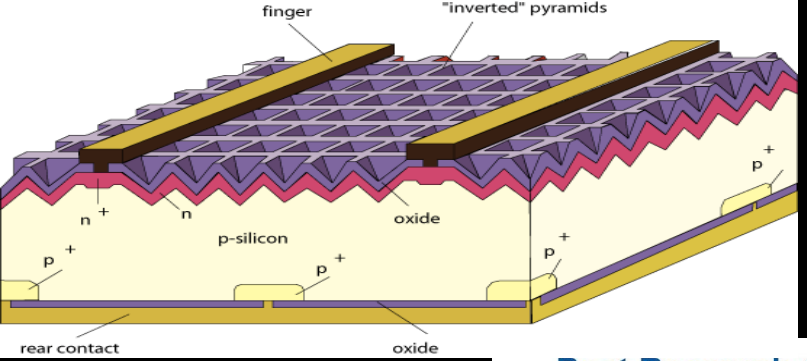
(in no particular order)

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 <$30/t$CO_2$ with a carbon price >$40/t$CO_2$

Carbon-Free Electricity

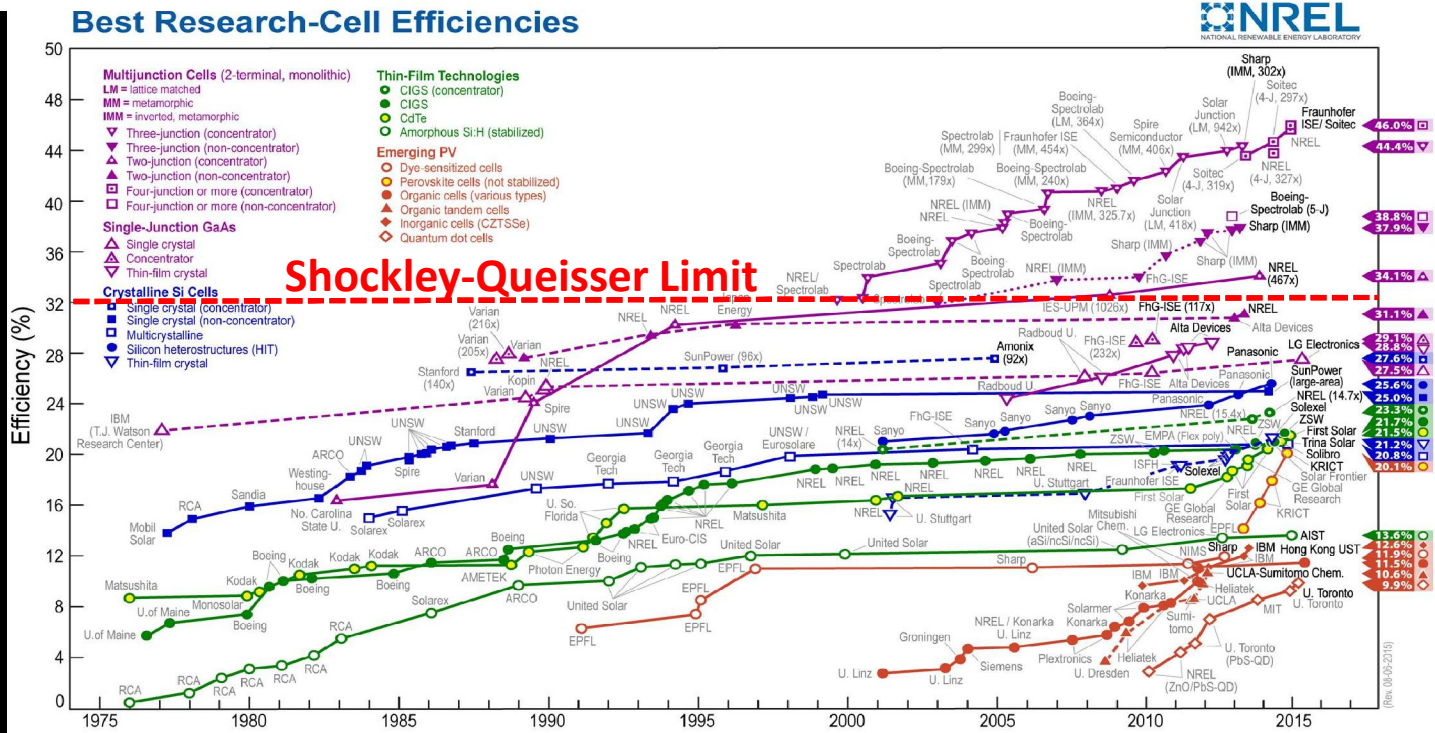


Source
1. DOE EERE Sunshot Q1'15 Report
2. DOE EERE Wind



Balance of System Dominates Cost

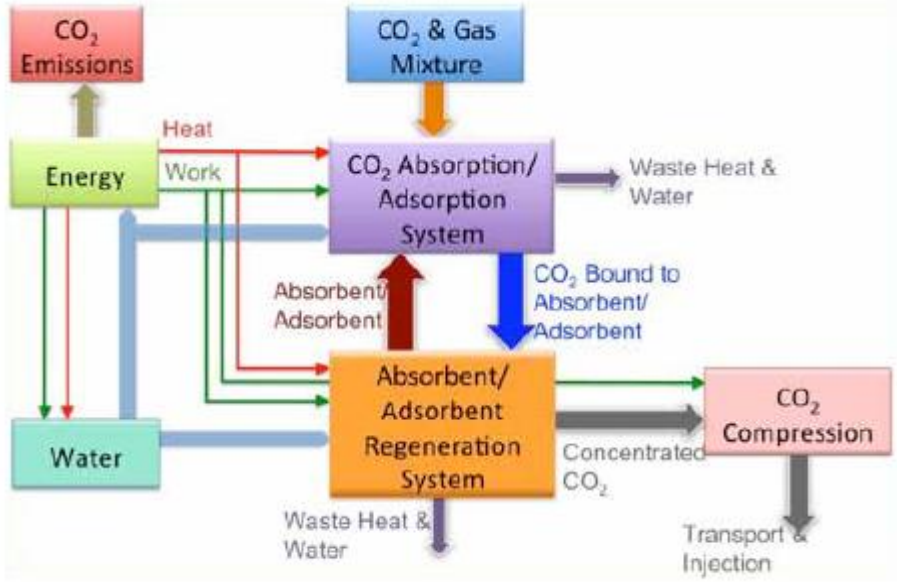
- Efficiency Matters
- Weight Matters

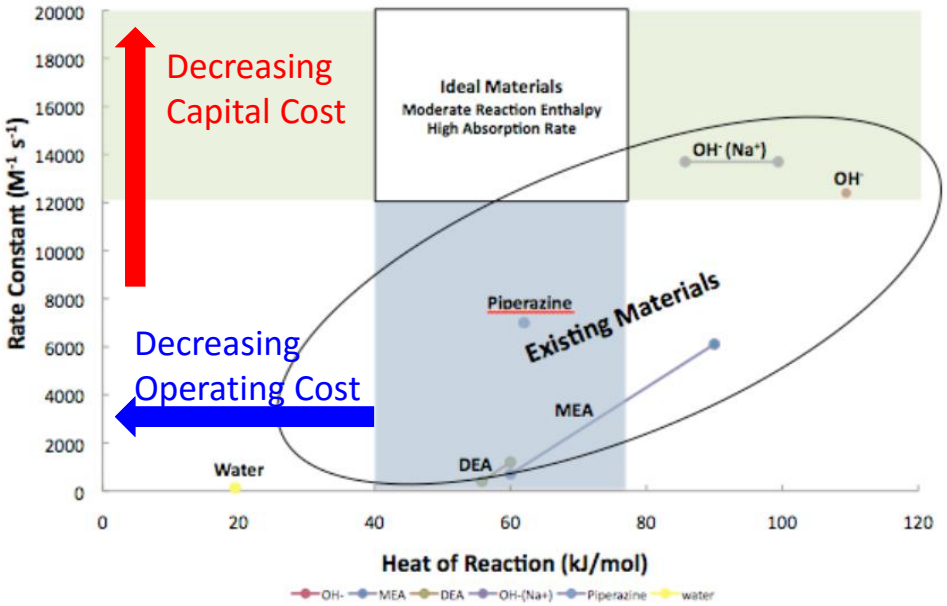


Carbon Capture

Current Cost = \$70-80/tCO_2 post-combustion capture

Can we reduce it to < \$30/tCO_2





$CO_2 + X \leftrightarrow X\text{-}CO_2$; $\Delta H < 0$

X: MEA – Monoethanolamine

X: NaOH – Sodium Hydroxide

$\Delta G = \Delta H - T\Delta S$;

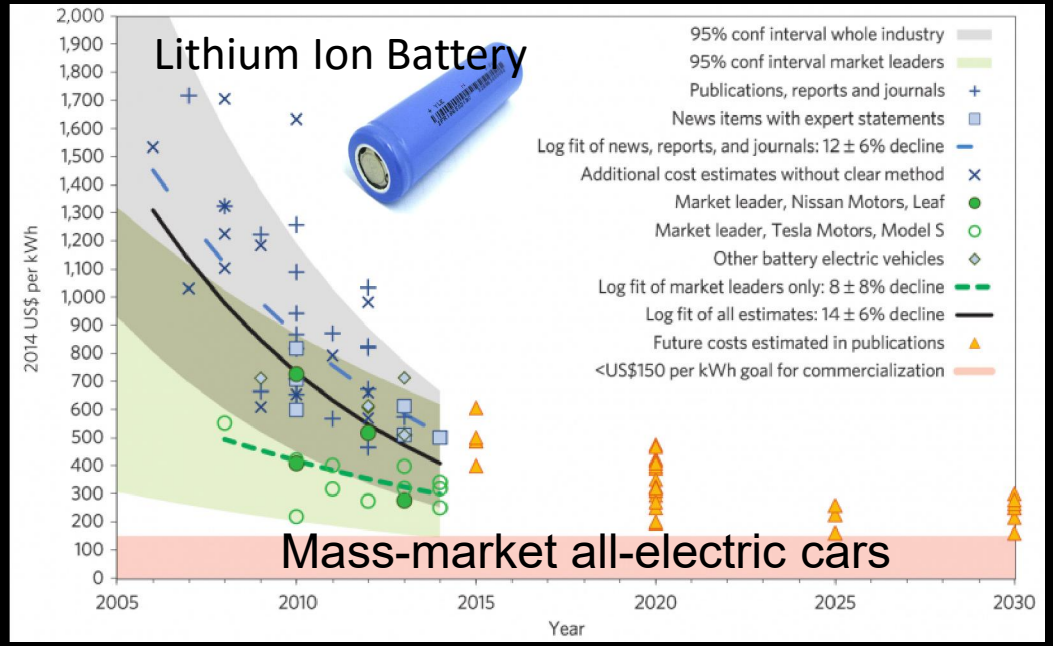
Dissociative Reaction: $T_{dis} = \Delta H/\Delta S$

Storage

Pumped Hydro

(Capital Cost = $100/kWh)

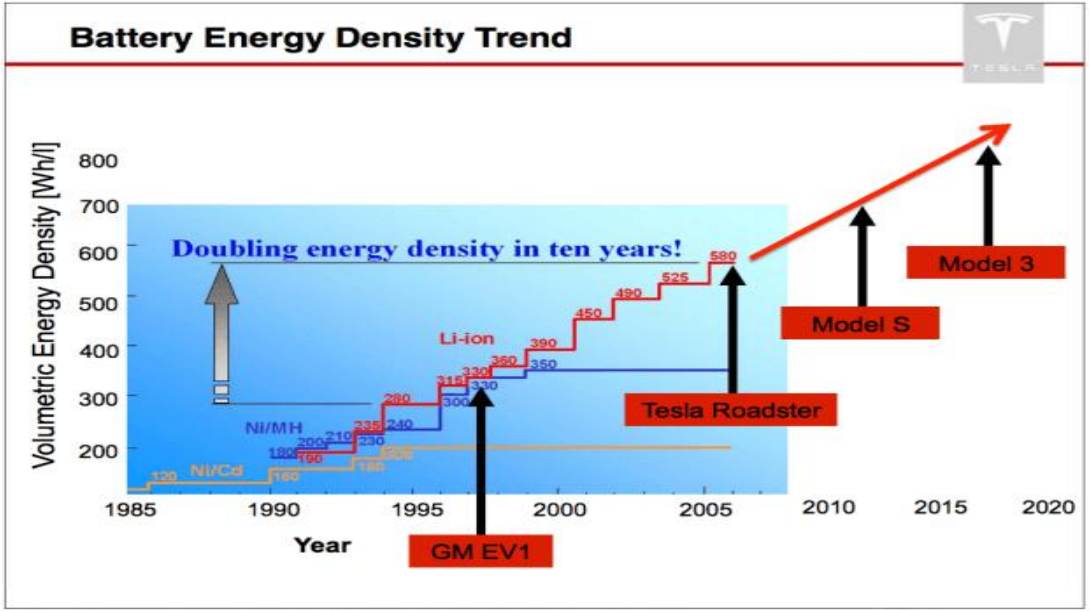
(Levelized cost of storage = 2 c/kWh)

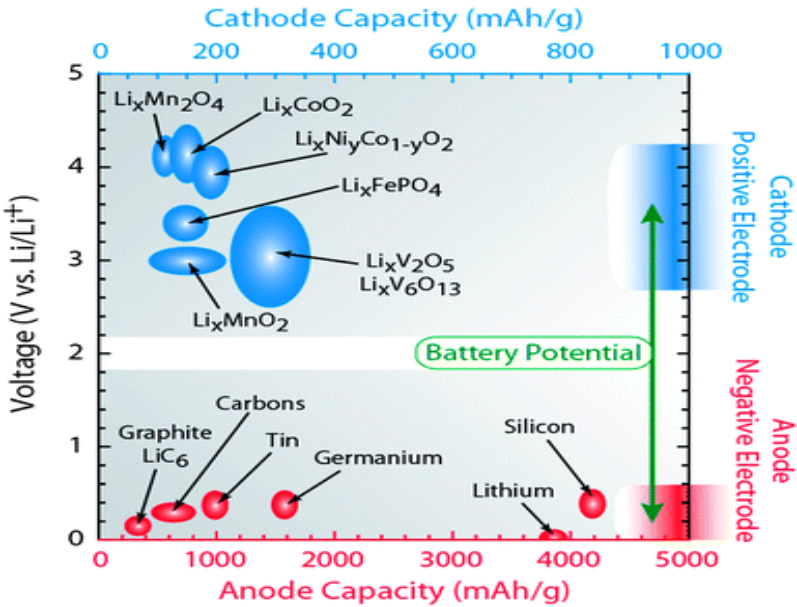


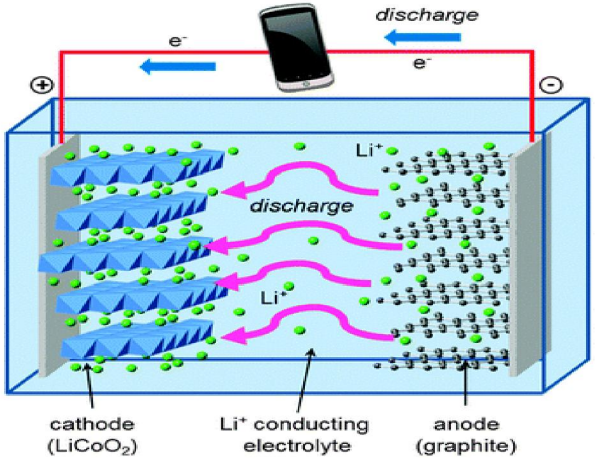
Nykvist & Nilsson, *Nature Climate Change* (2015)

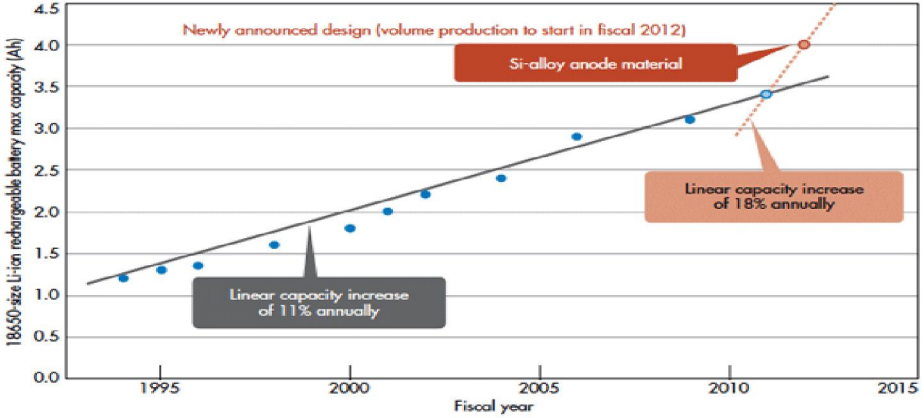
Cost has reduced 3 times between 2008-2015

Materials and packaging innovations


Battery Energy Density Trend
Volumetric Energy Density [Wh/l]
Doubling energy density in ten years!
Li-ion
Ni/MH
Ni/Cd
Year
GM EV1
Tesla Roadster
Model S
Model 3


Cathode Capacity (mAh/g)
Voltage (V vs. Li/Li+)
Anode Capacity (mAh/g)
Battery Potential
Cathode
Positive Electrode
Anode
Negative Electrode
Carbons
Graphite
Tin
Germanium
Silicon
Lithium

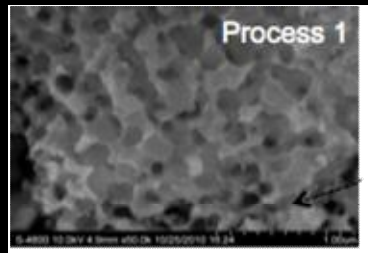

discharge
e⁻
Li⁺
cathode (LiCoO2)
Li⁺ conducting electrolyte
anode (graphite)


Newly announced design (volume production to start in fiscal 2012)
Si-alloy anode material
Linear capacity increase of 18% annually
Linear capacity increase of 11% annually
18650-size Li-ion rechargeable battery max capacity (Ah)
Fiscal year

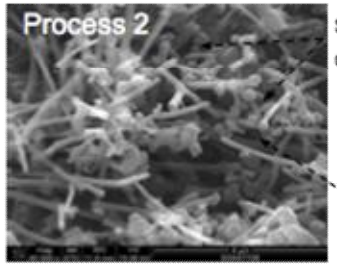
400 Wh/kg; C/10
80% depth of discharge

Roughly $250/kWh

POROUS Si ANODE



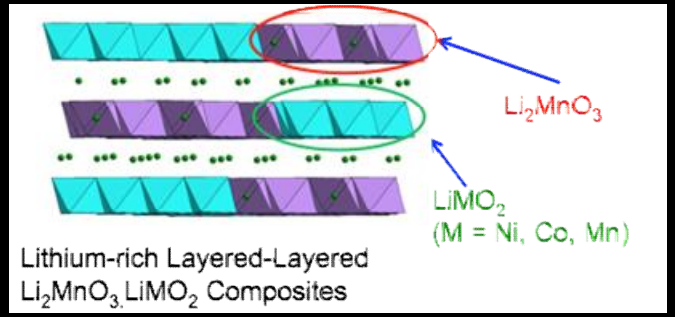
Porous-Si



silicon-fiber composite

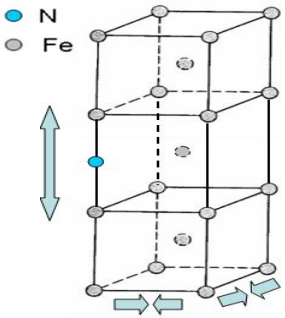
Carbon fibers

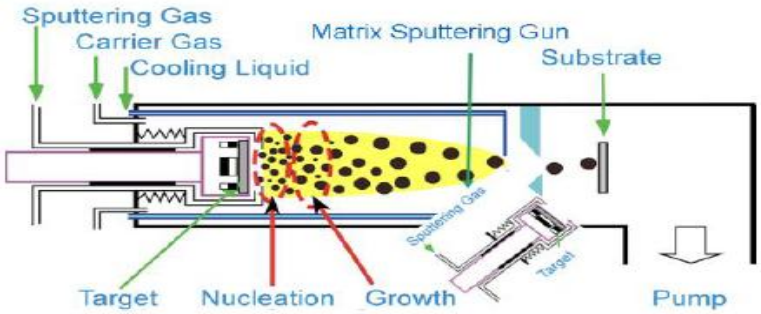
Mn-BASED CATHODE



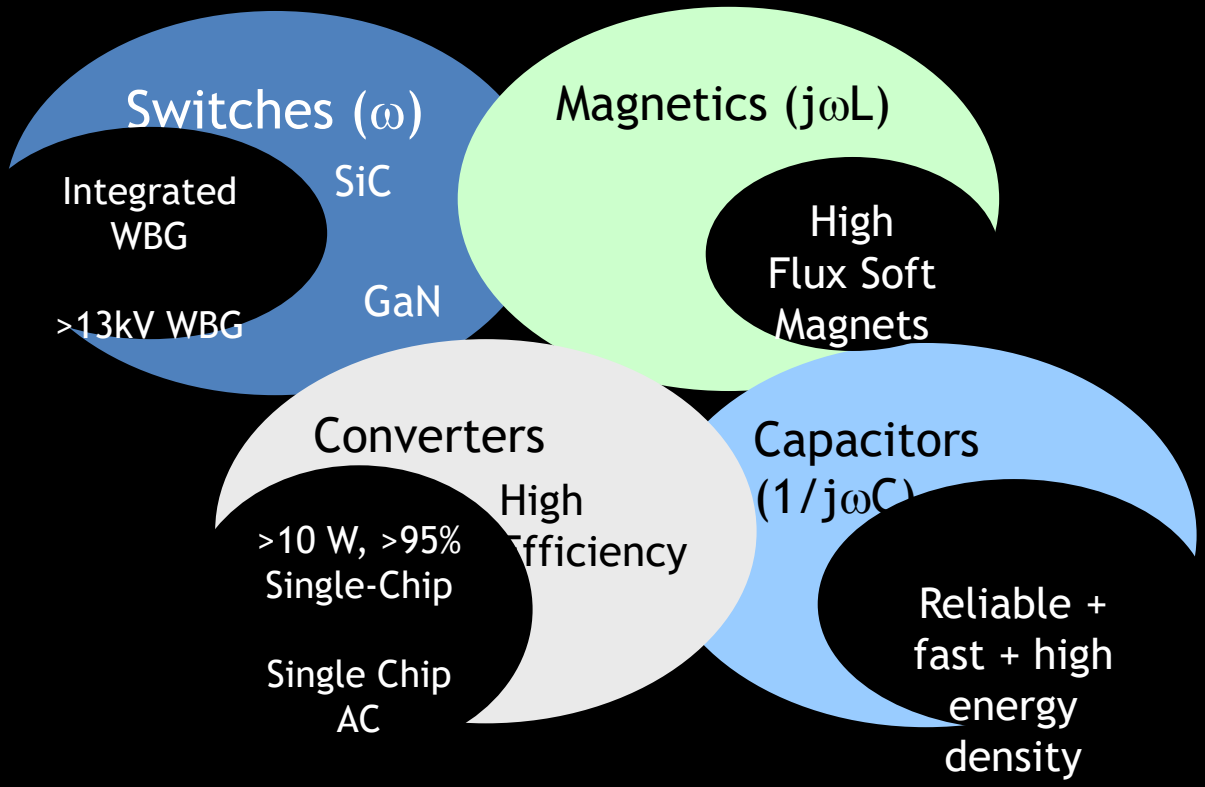
Rare Earth Free Hard Magnetic Materials for Generators & Motors

$Fe_{16}N_2$
"Holy Grail of Magnets"
BH_{max} = 134 MGOe

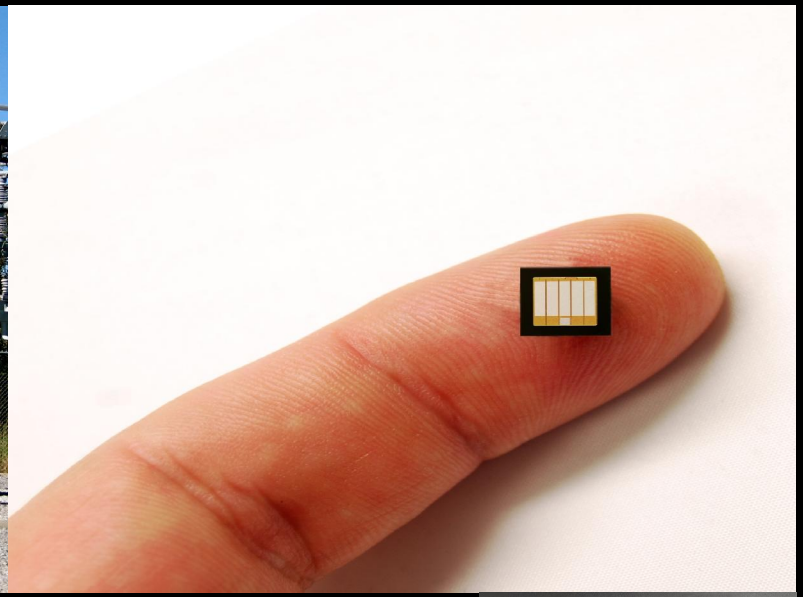




Power Electronics



Power Electronics



8000 lbs, 60 Hz Distribution Transformer

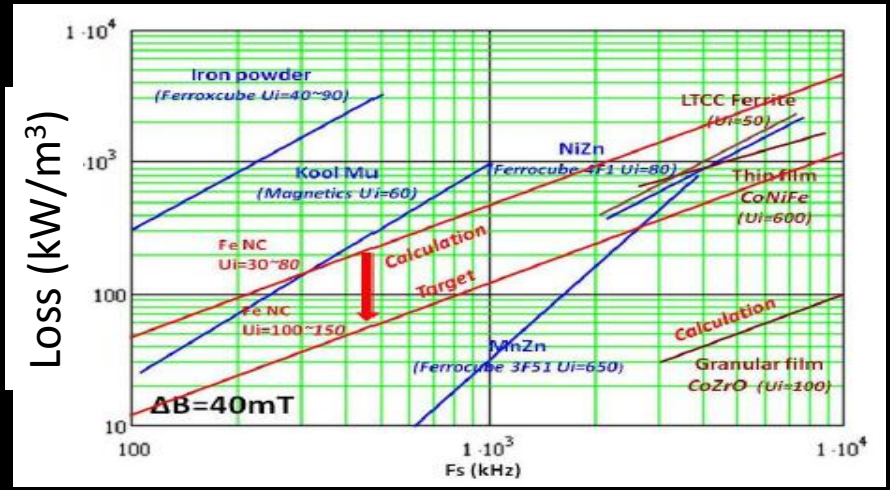
Average Age: 42 years, 2 years beyond projected lifespan

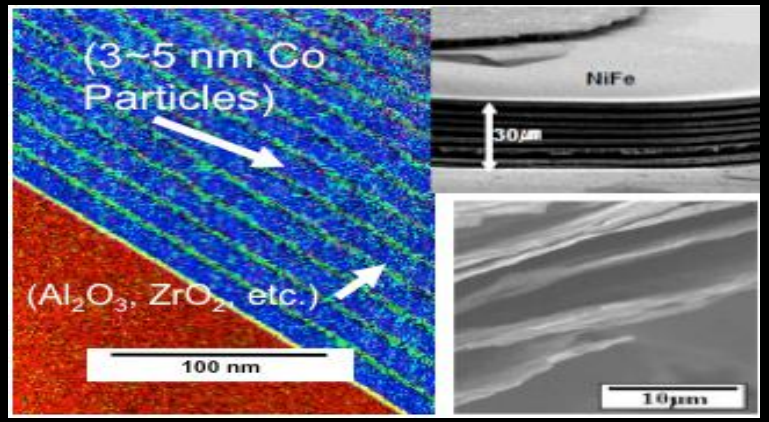
Silicon Carbide IGBT;
15 kV, 100 A;
50 kHz from Cree Inc.

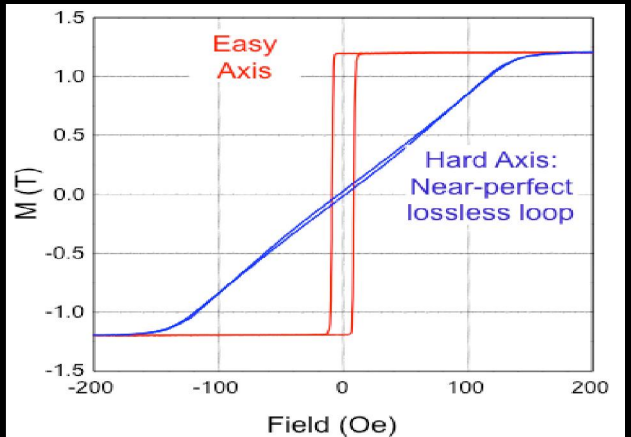
Potentially 100 lbs transformer

Low Loss High Frequency Soft Magnets

SOFT MAGNETS

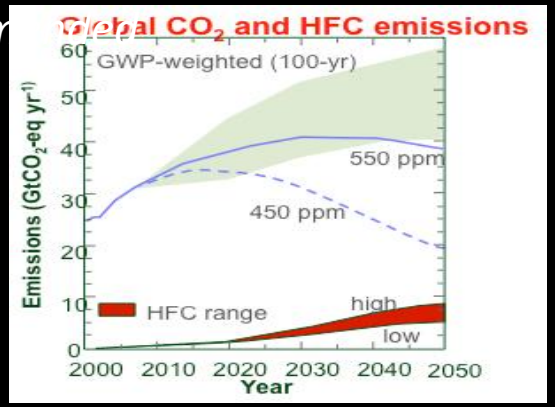




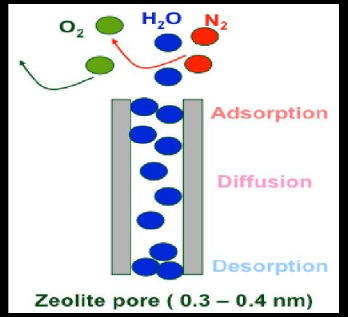


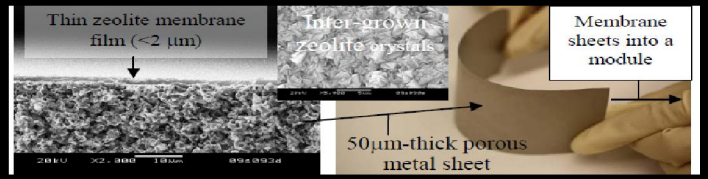
Air Conditioning & Refrigeration

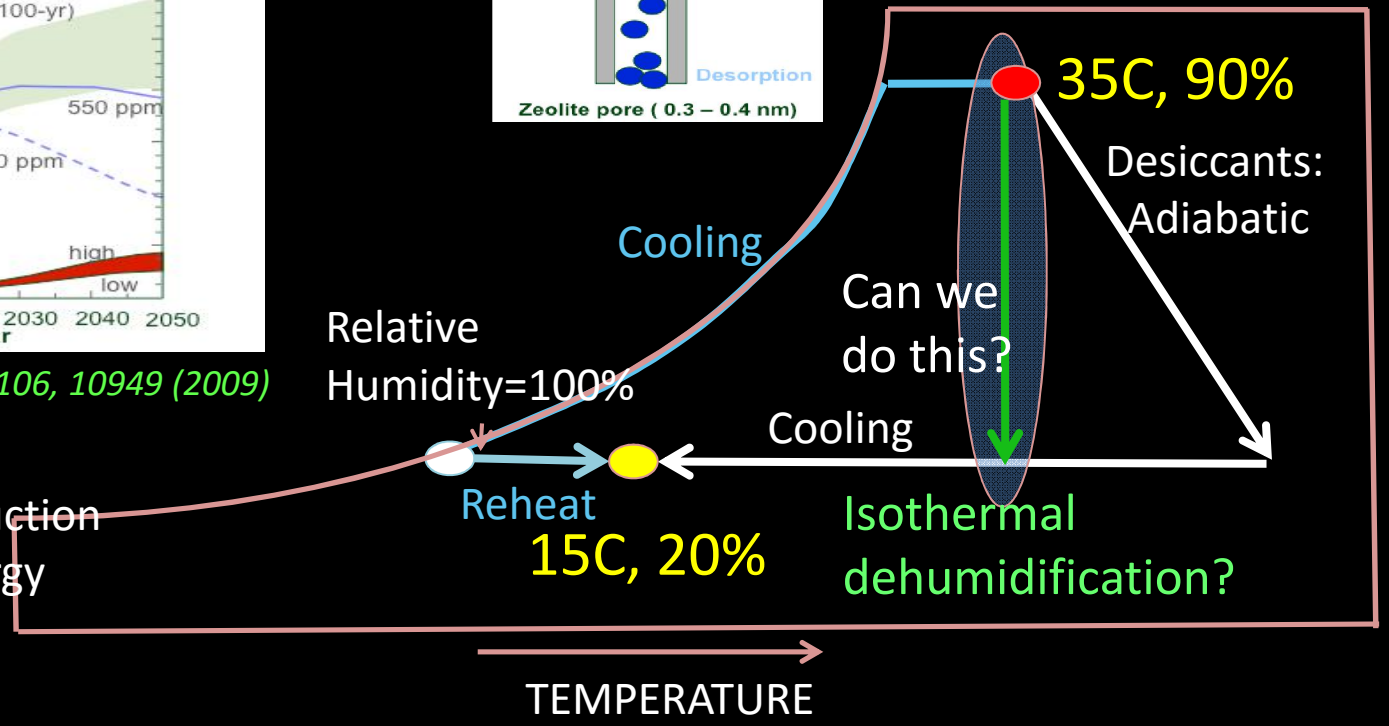
Current refrigerants have GWP over 1000x of CO_2
Montreal Protocol will likely be am



Velders et al, PNAS 106, 10949 (2009)





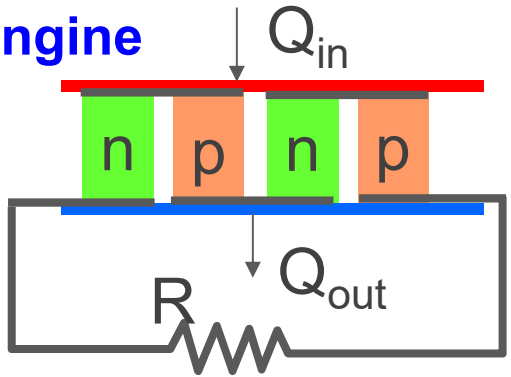


Up to 50% reduction in primary energy consumption

Thermoelectric Power Generation (Xternal combustion engine) & Cooling

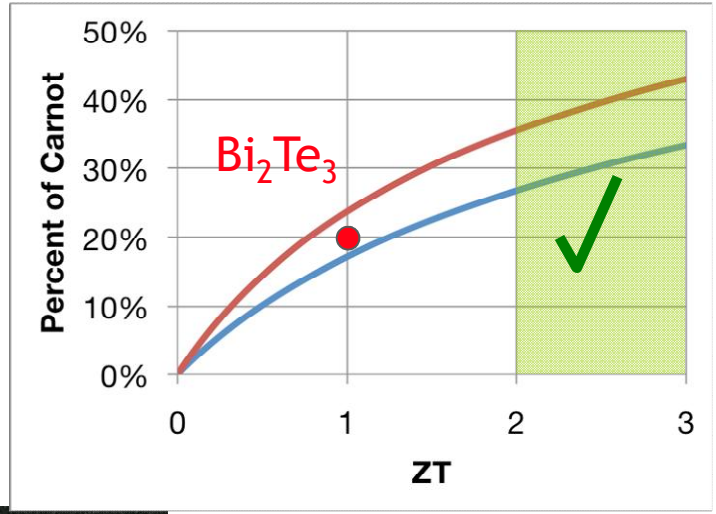
Biomass, LPG

Engine

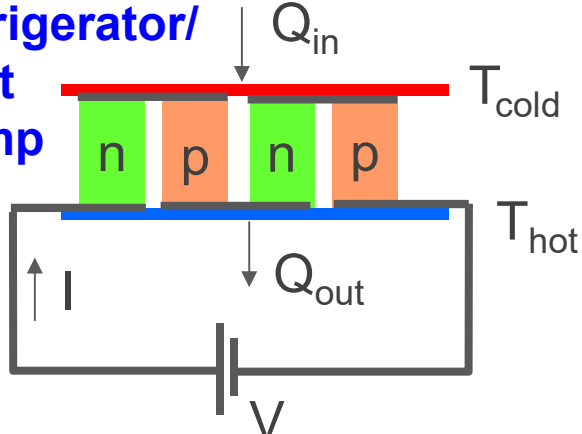


Seebeck Coefficient, S = V/⊗T

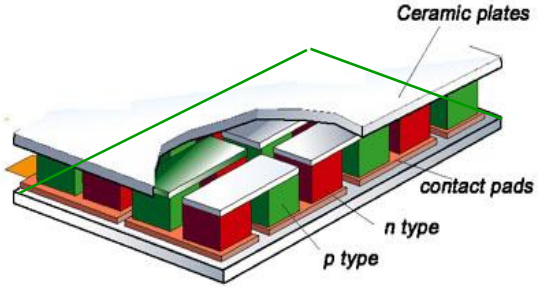
$$ZT = \frac{S^2 \sigma T}{k}$$



Refrigerator/ Heat Pump



Bismuth Telluride



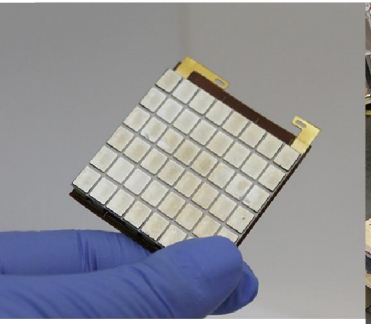
Power Generation & Cooling Systems

POWER PRACTICAL

Power Pot = $70

chotukool

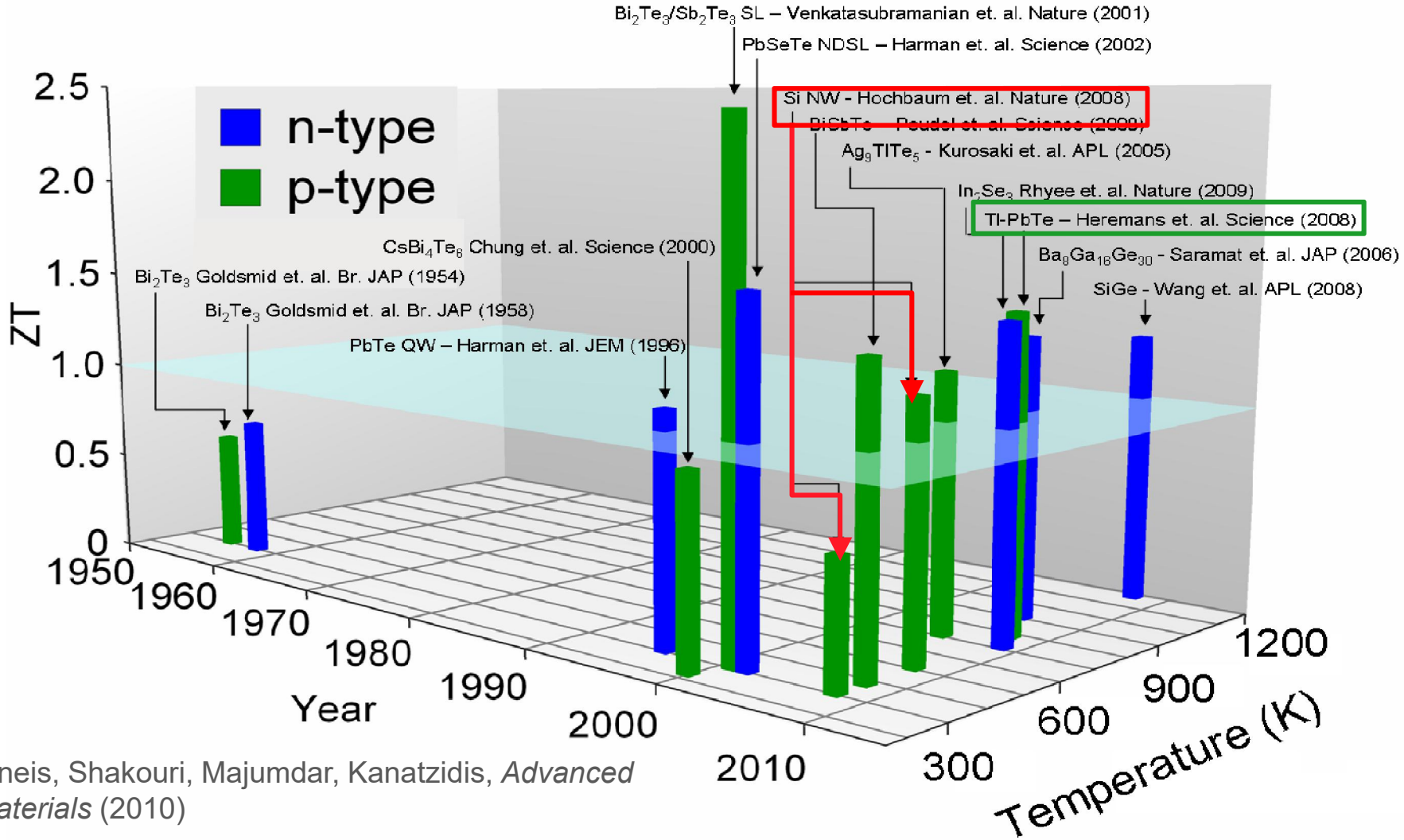
alphabet energy



System level cost target = $1/W

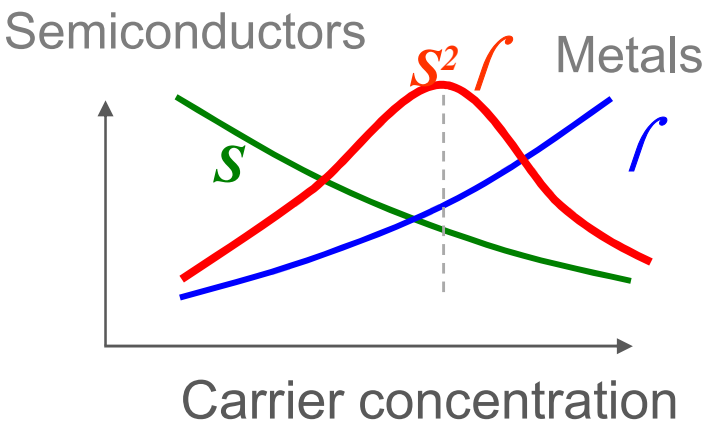
Balance of system cost > TE device cost

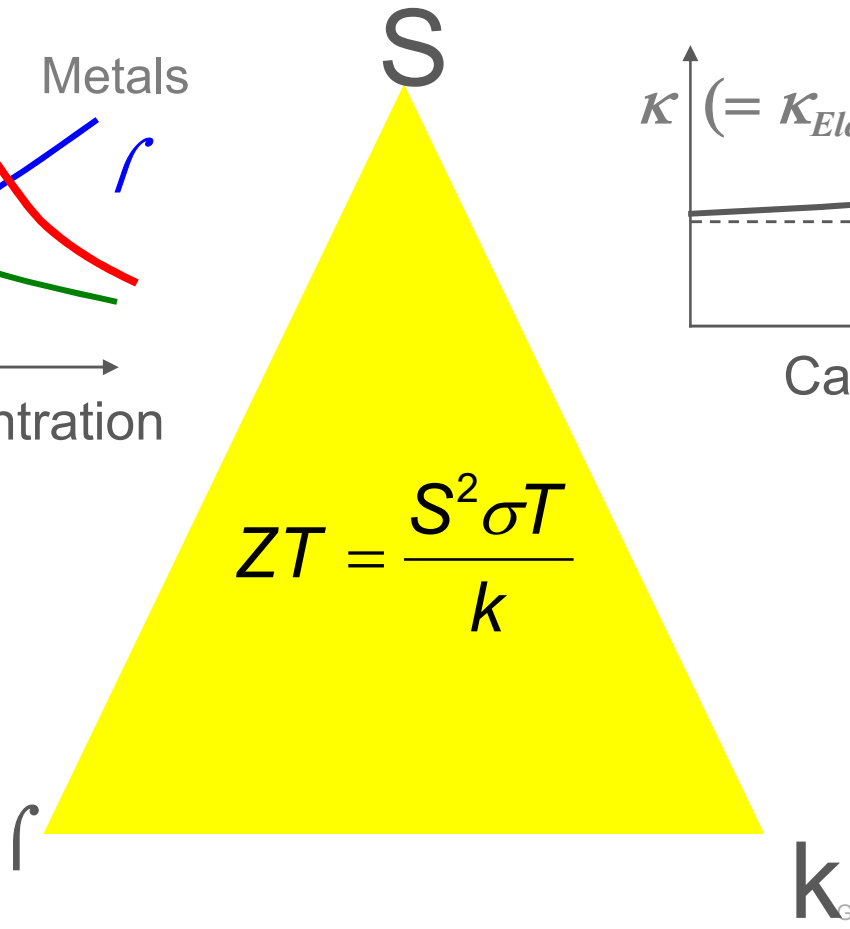
Device efficiency matters

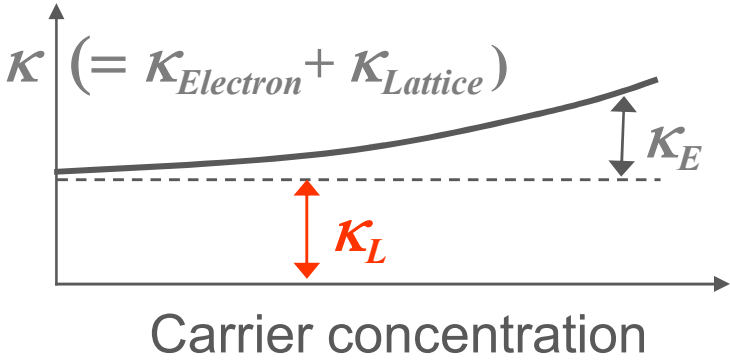


Vineis, Shakouri, Majumdar, Kanatzidis, *Advanced Materials* (2010)

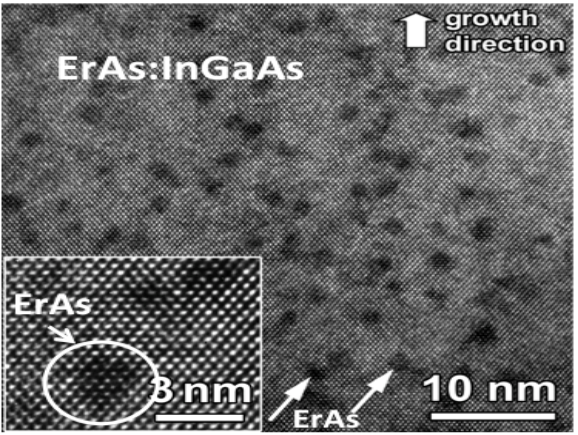
Bermuda Triangle of Thermoelectrics





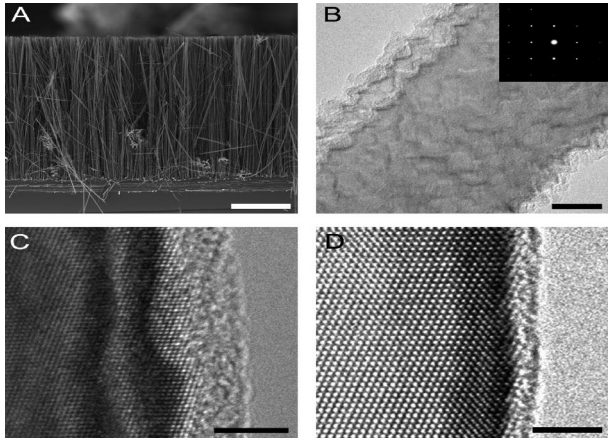


III-V Semiconductors



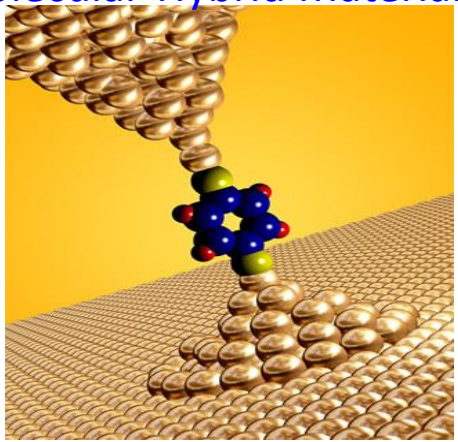
A. Shakouri, T. Sands(Purdue), J. Bowers, A. Gossard, S. Stemmer (UCSB), R. Ram (MIT), J. Zide (Delaware)

Si Nanowires



Peidong Yang, Joel Moore (UCB, LBL)

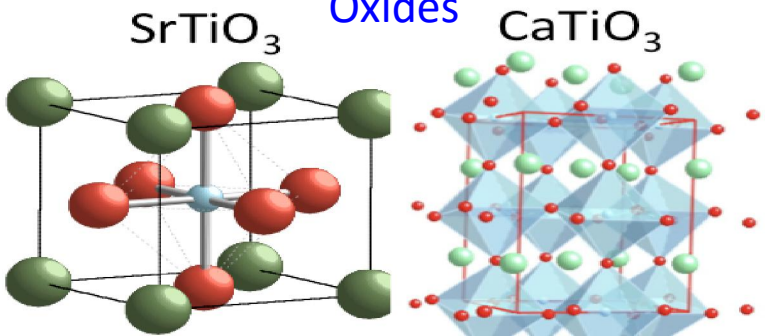
Molecular-Hybrid Materials



Rachel Segalman, J. Urban (LBL, UCB)

Reddy et al., *Science* (2007)

Oxides

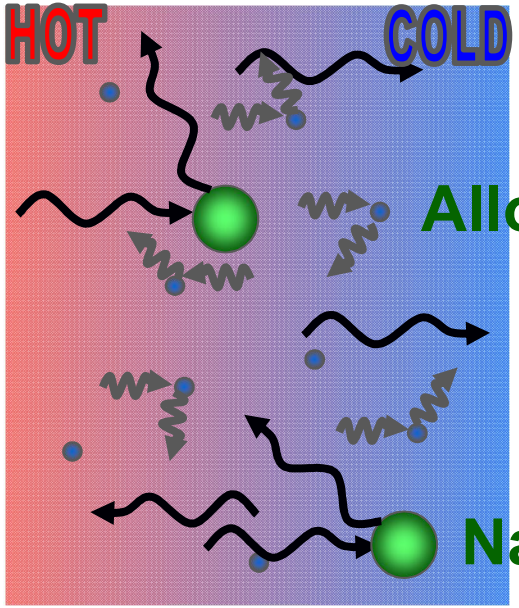


R. Ramesh (UCB, LBL)

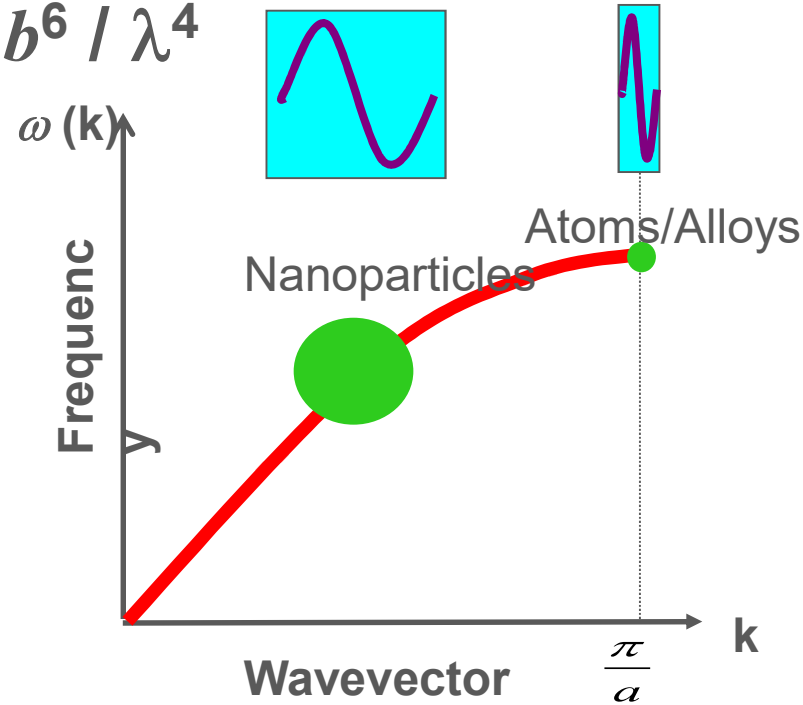
DOE
NSF
ONR
DARPA
AFOSR

Phonon Scattering Using Nanostructures

Rayleigh scattering regime: $\sigma \sim b^6 / \lambda^4$



Kim et al., *Phys. Rev. Lett.* (2006)



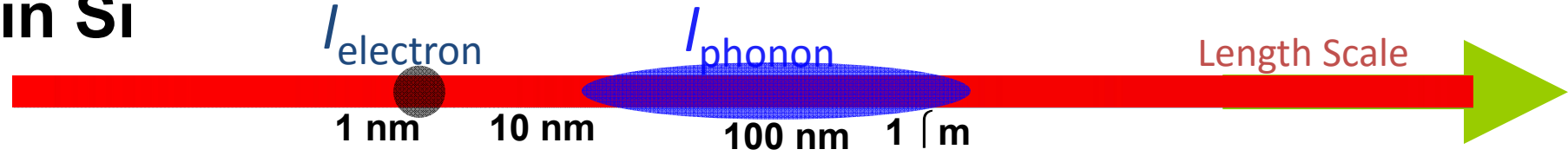
Short wavelength phonon

Mid/Long wavelength phonon

Typical *b*: Alloy — 1 Å

Nanoparticle — 1~4 nm

Electron & Phonon Mean Free Path Differences in Si



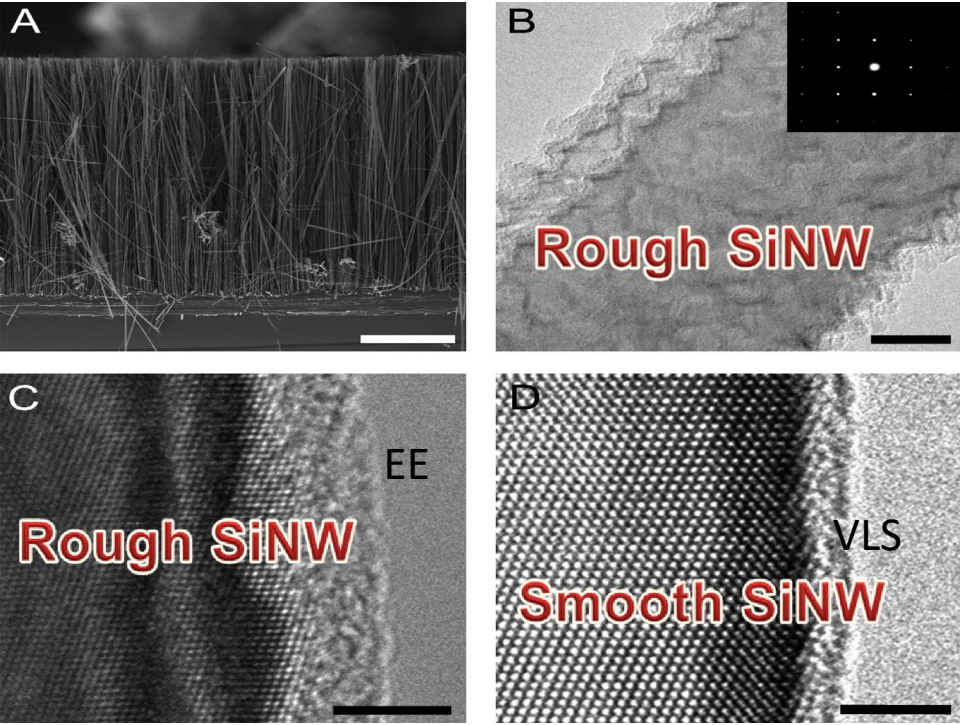
$l_{electron} < l_{phonon}$

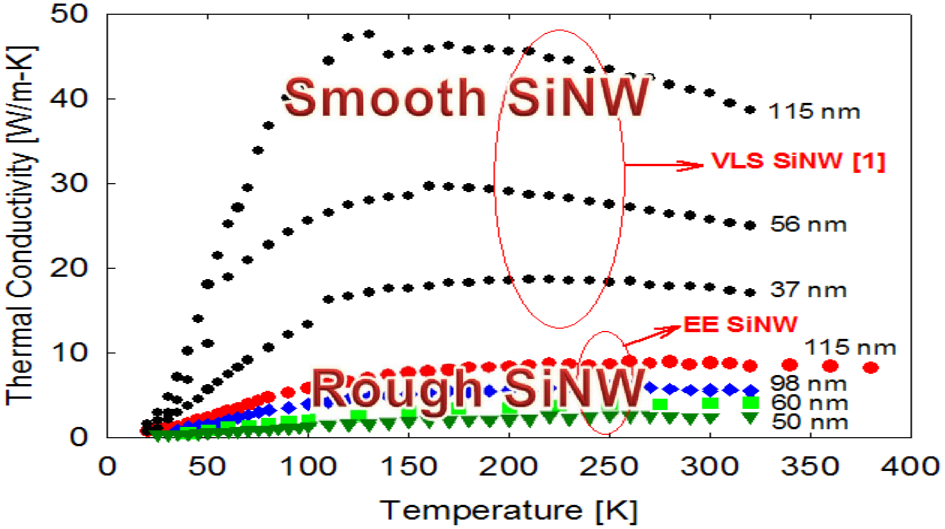
Ju and Goodson, "Phonon Scattering in Silicon Films of Thickness Below 100 nm," *Applied Physics Letters*, Vol. 74, pp. 3005-3007 (1999).

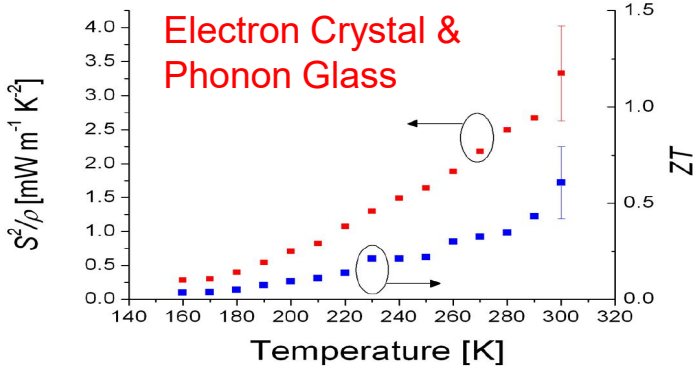
Bulk Silicon

	l_{phonon} (nm)	k (W/m-K)	$S^2\sigma$ (W/m-K^2)	ZT	Abundance
Si	~100-1000 nm	140	0.0047	0.01	27%
Bi_2Te_3	~1 nm	1.4	0.0037	0.8	Bi: 48 ppb Te: 5 ppb

Smooth and Rough Si Nanowires





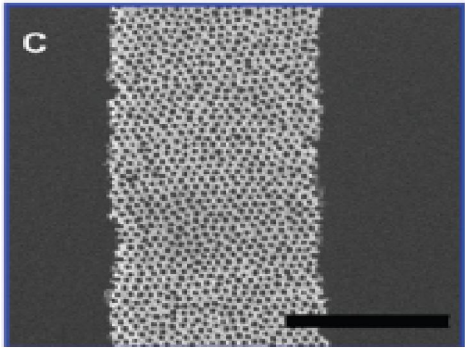


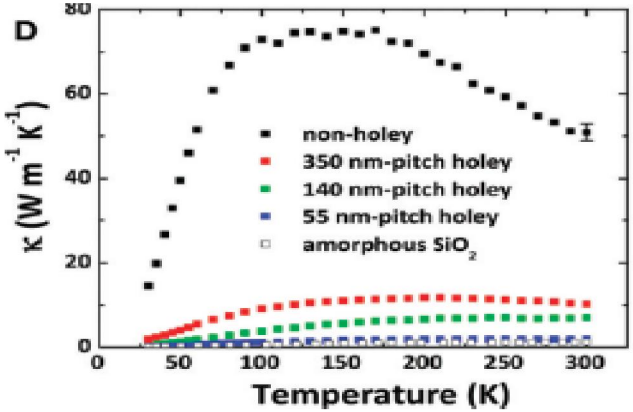
alphabet energy

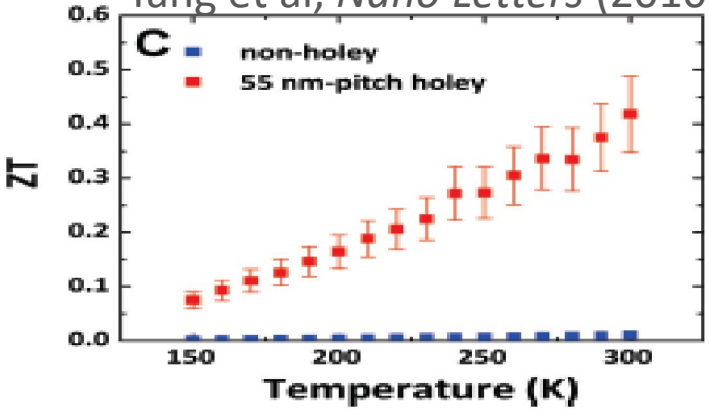
Hochbaum et al., *Nature* (2008)

Holey Silicon

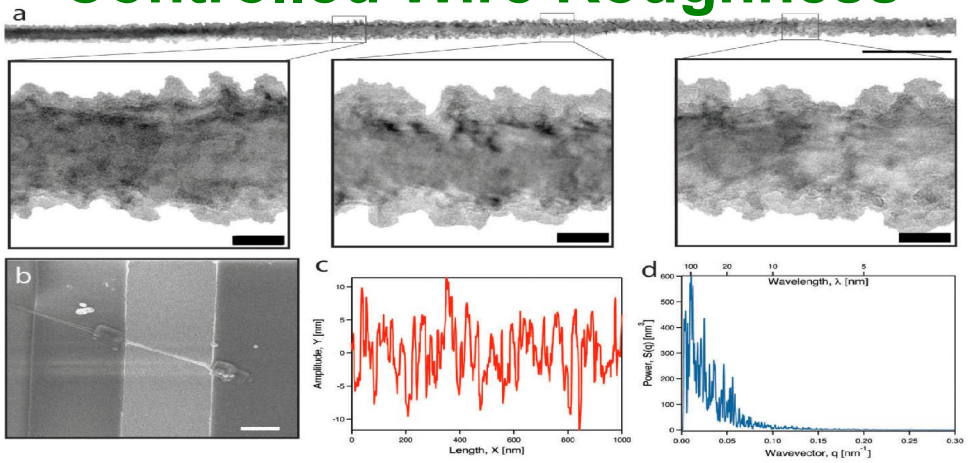
Tang et al, *Nano Letters* (2010)







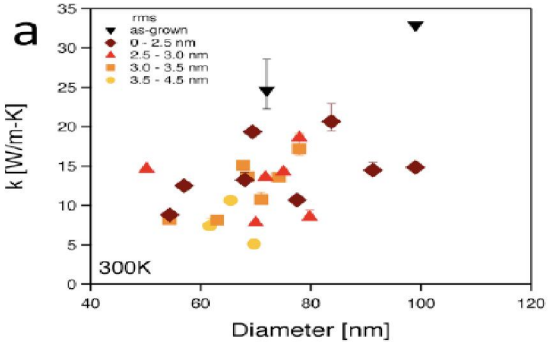
Controlled Wire Roughness

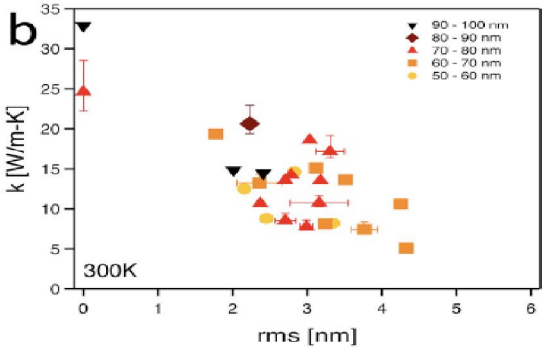


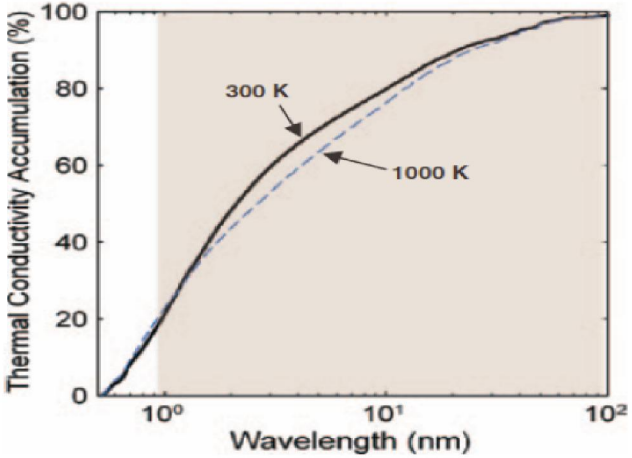
Roughness Parameters

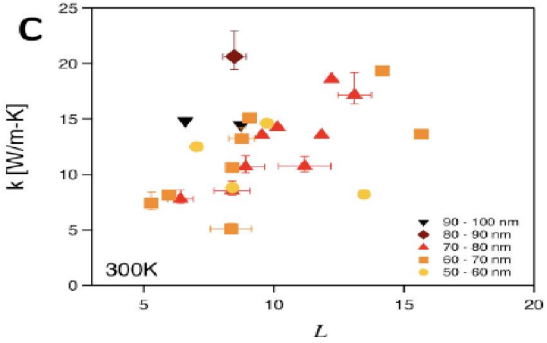
σ: Rms height

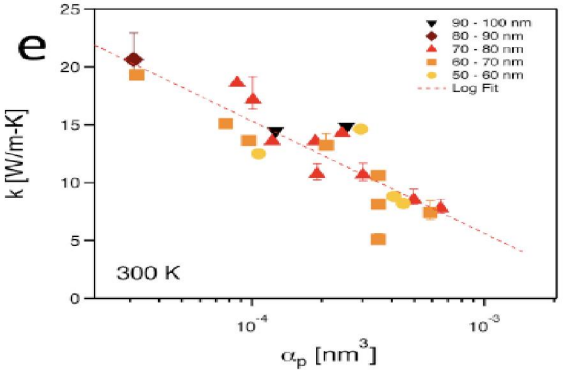
L: Autocorrelation length

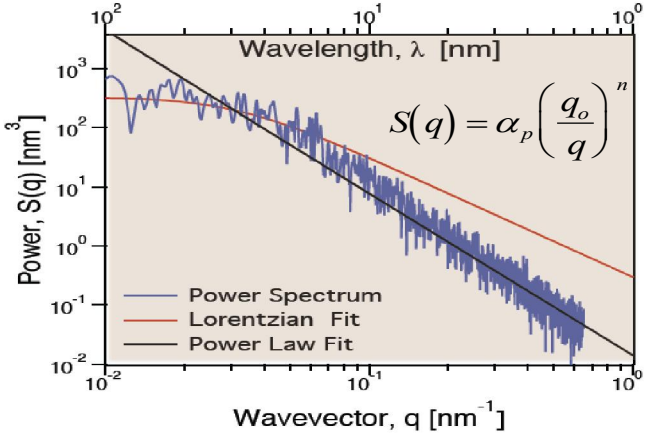












J. Lim, K. Hippalgaonkar, S. C. Andrews, A. Majumdar, P. Yang, *Nano Letters* (2012)

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 <$30/t$CO_2$ with a carbon price >$40/t$CO_2$

Thank you!

nature materials

December 2013 LETTERS

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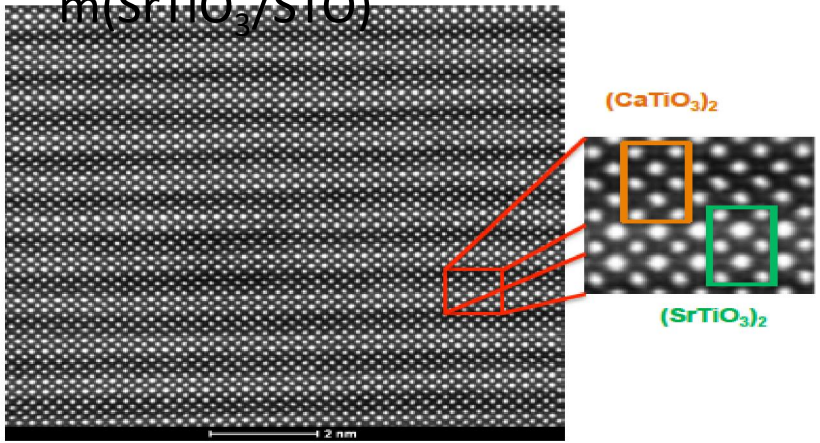
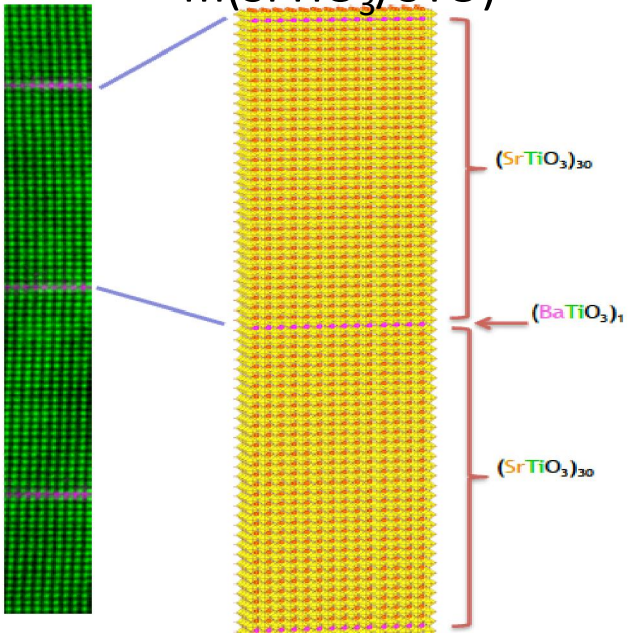
Crossover from incoherent to coherent phonon scattering in epitaxial oxide superlattices

Jayakanth Ravichandran[1,2†‡], Ajay K. Yadav[2,3‡], Ramez Cheaito[4‡], Pim B. Rossen[3], Arsen Soukiassian[5], S. J. Suresha[2], John C. Duda[4], Brian M. Foley[4], Che-Hui Lee[5], Ye Zhu[6], Arthur W. Lichtenberger[7], Joel E. Moore[2,8], David A. Muller[6,9], Darrell G. Schlom[5,9], Patrick E. Hopkins[4], Arun Majumdar[10], R. Ramesh[1,2,3,8,11*] and Mark A. Zurbuchen

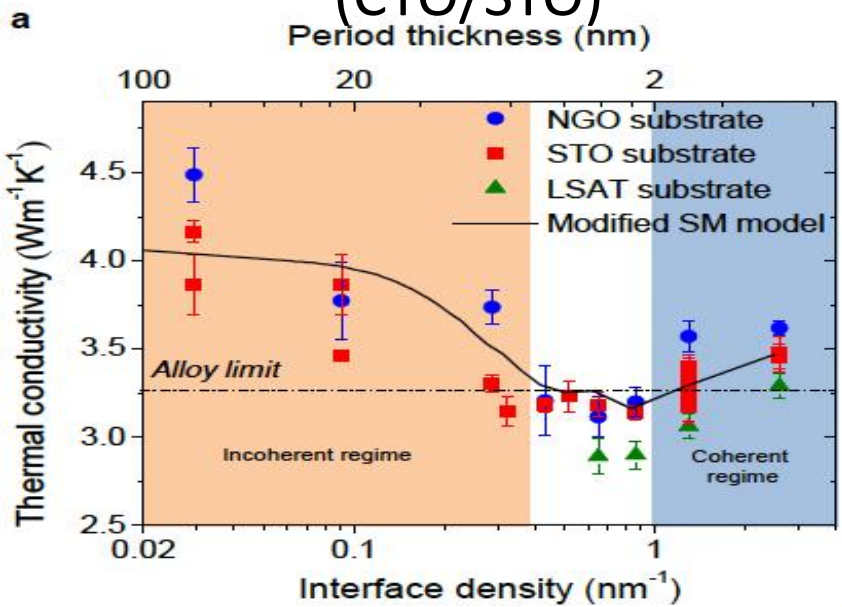
n($BaTiO_3$/BTO) : m($SrTiO_3$/STO)

n($CaTiO_3$/CTO): m($SrTiO_3$/STO)

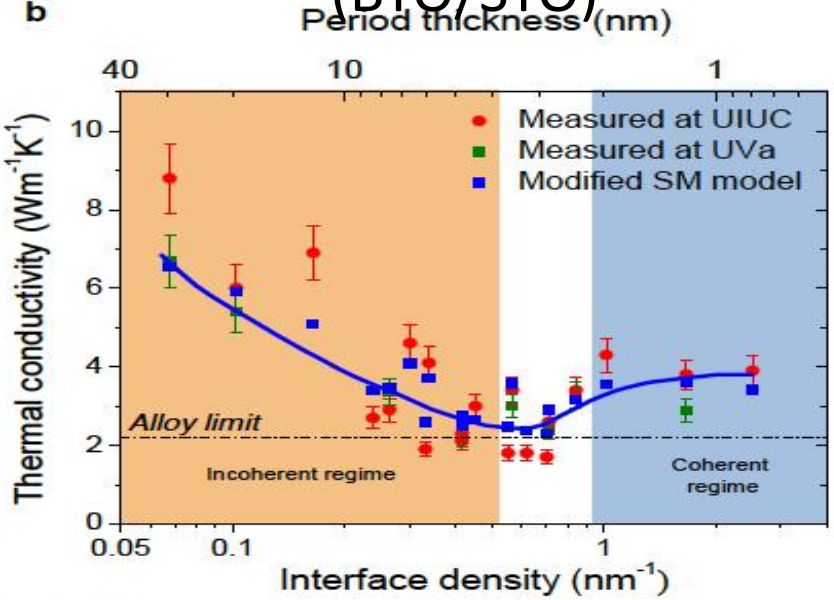


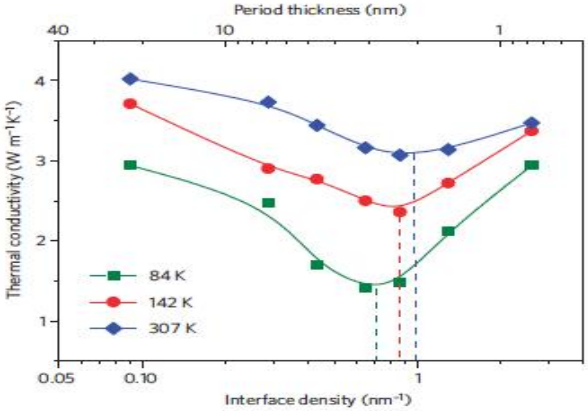


(CTO/STO)



(BTO/STO)



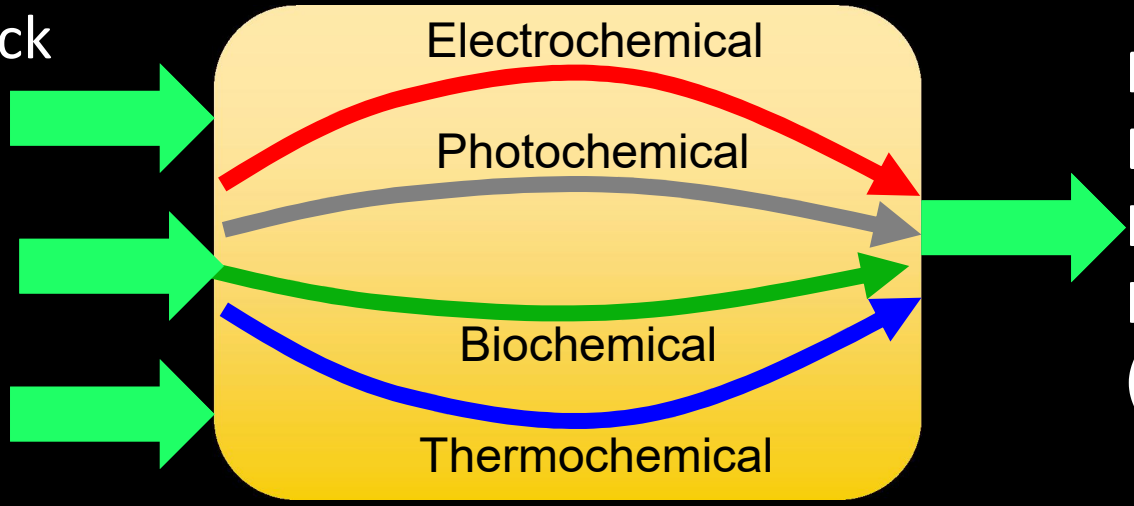


What is our Haber-Bosch like challenge?

CO_2 feedstock at $/tC

H_2O

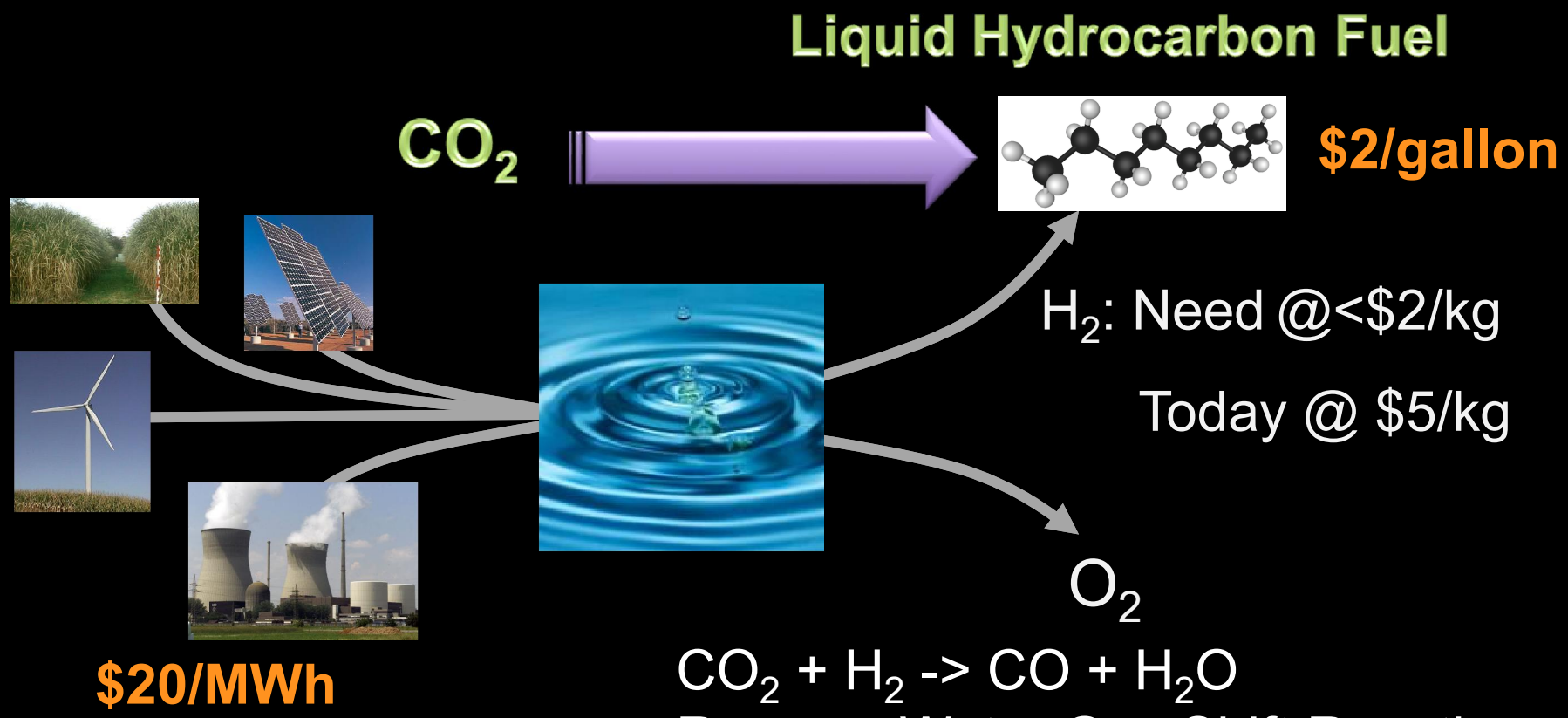
Carbon-free energy at $/kWh



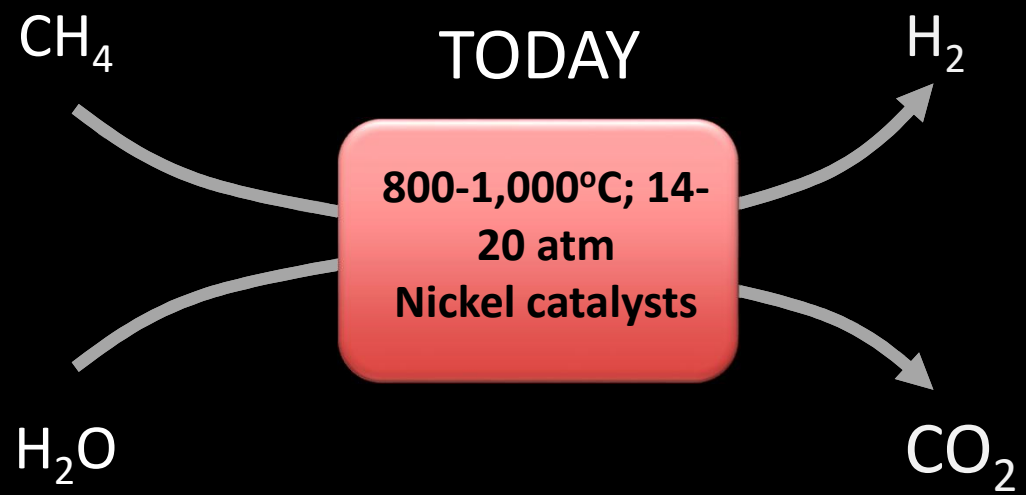
Methanol
Ethanol
Hydrogen
Hydocarbon
($/kg; $/L)

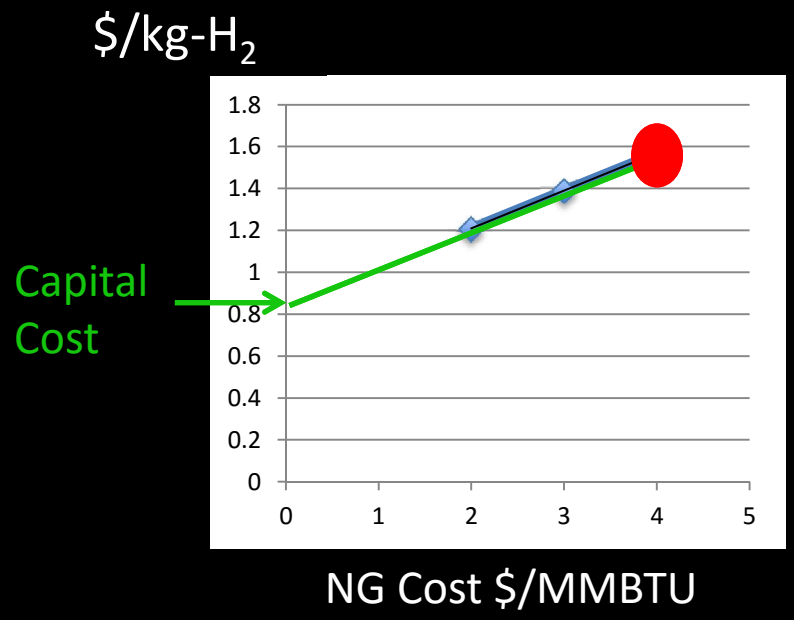



A grand challenge….



H_2 production: Steam Reforming of Natural Gas

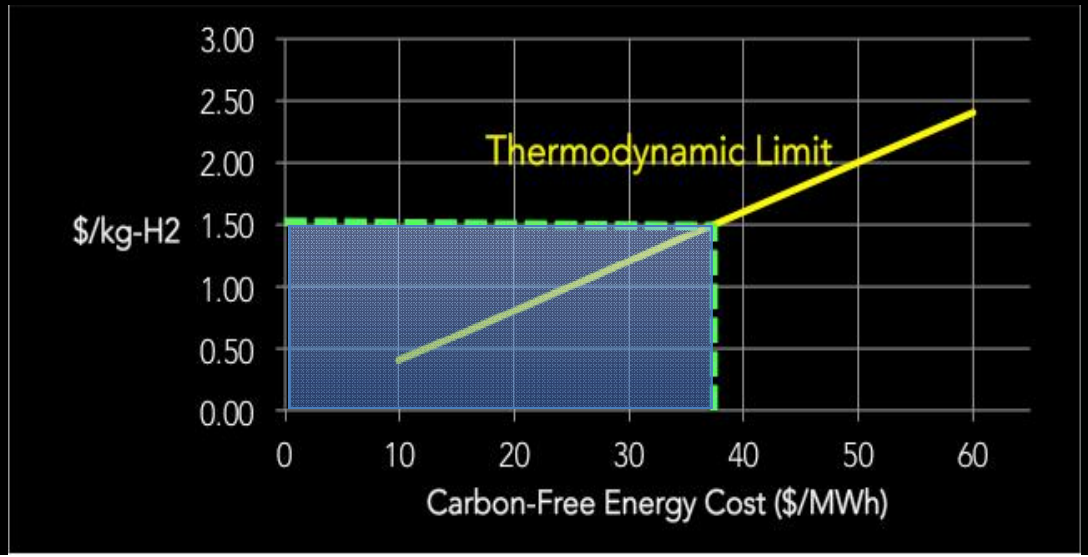


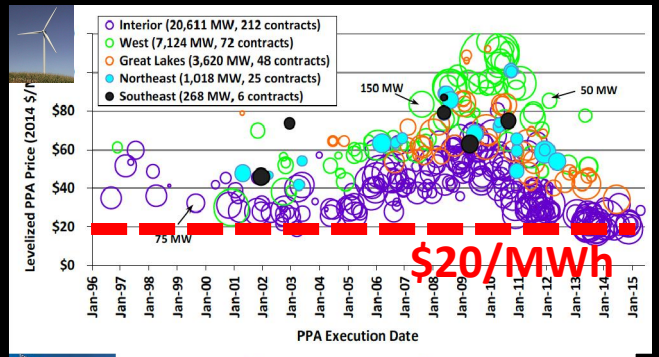


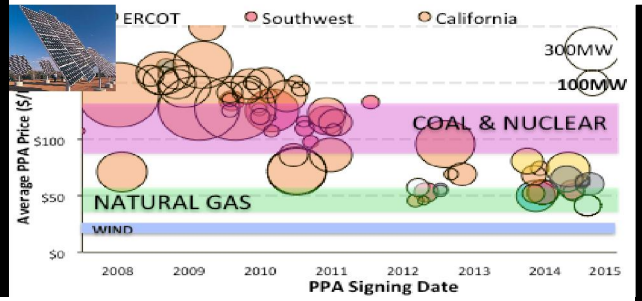
How do we produce carbon-neutral H_2 at <$2/kg at scale?

Thermodynamic & Cost Limits

$H_2O = H_2 + ½ O_2$; ΔH = 286 KJ/mol = 40 kWh/kg-H_2



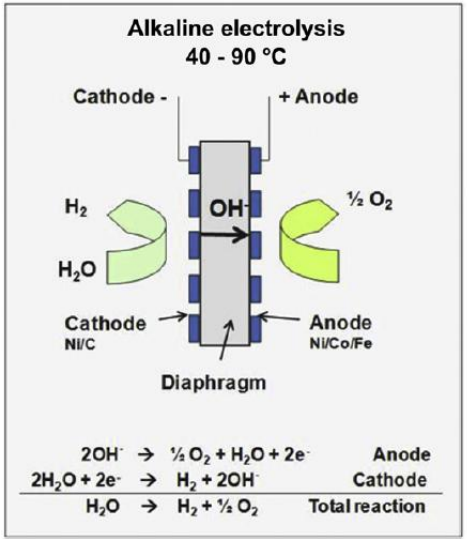


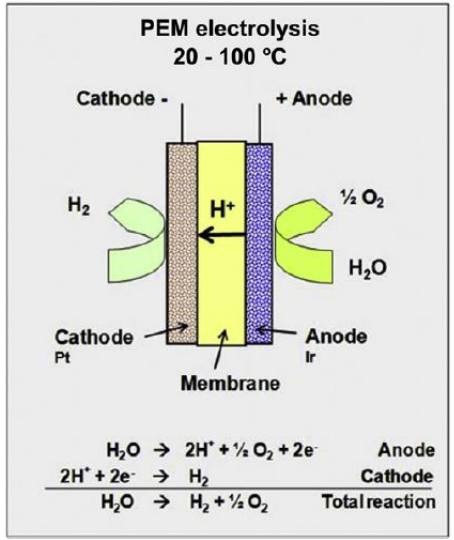


Biomass

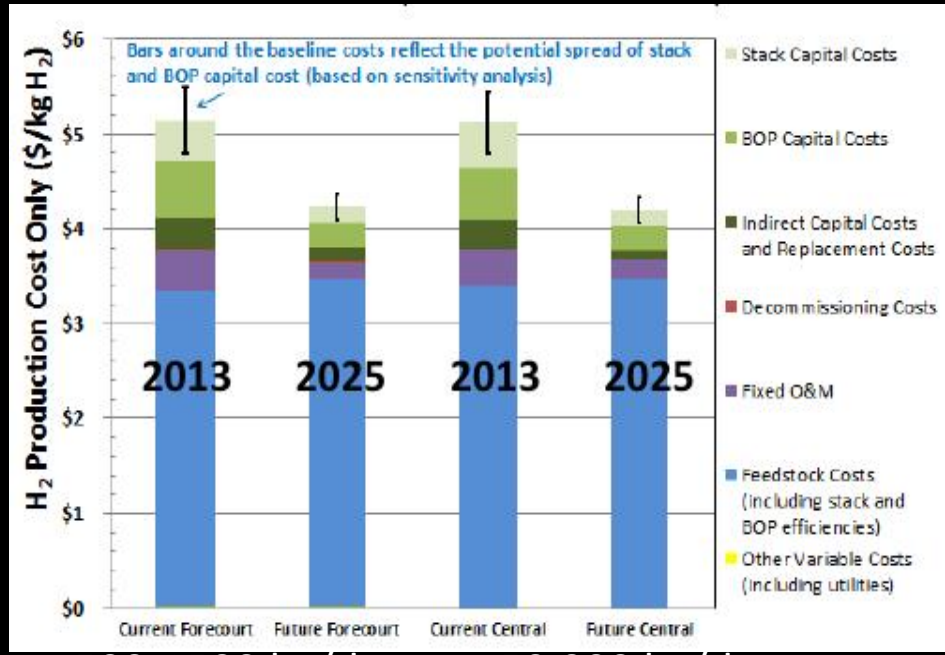
- Calorific Value: 7000 BTU/lb = 15400 BTU/kg = 4.50 kWh/kg-bm
- Cost = $65/ton = $0.065/kg-bm
- Energy Cost = $15/MWh

Electrochemical Pathway





Negligible economies of scale



$\Delta H = 55$ kWh/kg-H_2

TODAY: \$5/kg-H_2

OPTIMISTIC LIMIT: \$2/kg-H_2

500-1500 kg/day 50,000 kg/day

How can we beat the \$2/kg-H_2 limit at scale with new system design?

Thermochemical Pathway

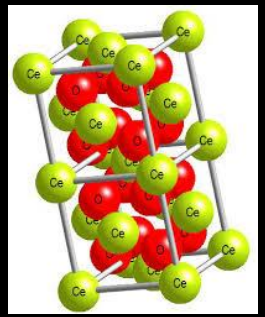
STATE-OF-THE-ART

Medium = 600 °C

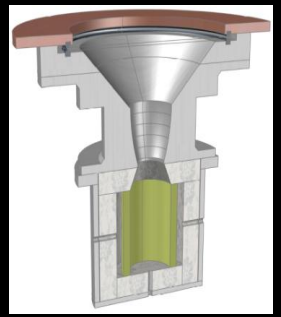
Hot = 1,500 °C

CeO_2

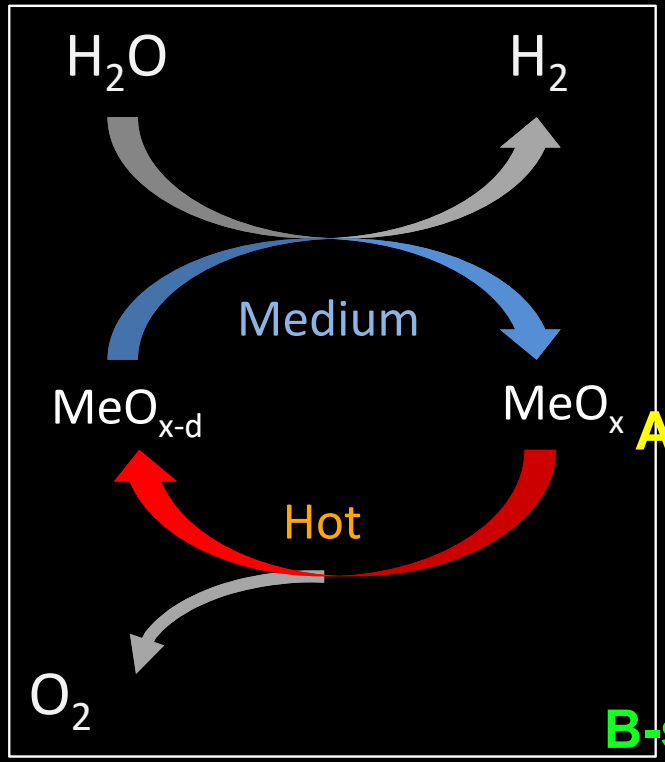
< 1% η_{Carnot}



Material



Reactor



FUTURE

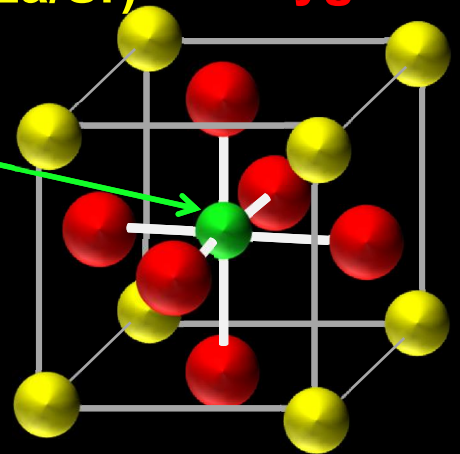
Medium = 600 °C

Hot = 800 °C

Fluidized bed reactor?

- Matching heat input to chemistry
- Heat recuperation

PEROVSKITE



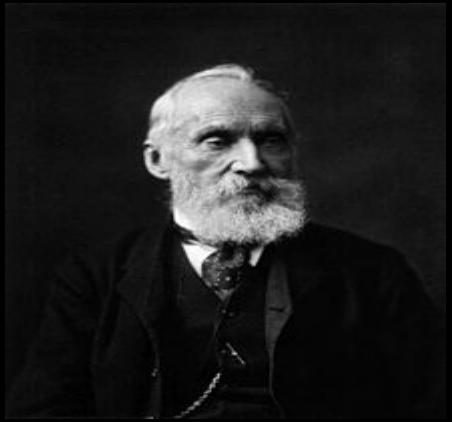
(In)Famous Predictions from the Past

“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