Renewable Approaches to Distributed Energy Storage

Eric Toberer

Dept. of Physics, Colorado School of Mines, Golden CO
National Renewable Energy Laboratory, Golden CO
30 minute goals

- Appreciate **grid complexities & need for storage**

- Storage approaches & identify **primary approaches** to distributed storage

- Define challenges & opportunities within **thermal energy storage**

- Consider role of **thermoelectrics materials** and material design strategies

- Thermoelectric search strategies
Today: Storage, the electric grid, and its components

- Current electric grid has **virtually no built-in storage** capacity
- Plants are ramped on and off based on current demand

![Graph showing electric load with Base Load, Intermediate Load, and Peaking Load](image)

- Current demand: Large **base load** with hourly fluctuations due to lifestyle patterns
Addressing fluctuations: Peaking sources today

Gas fired peaker

Pumped hydro
Figure 1: Power requirement versus discharge duration for some applications in today’s energy system

Grid is changing due to falling price of solar electricity

- Factor of 4 drop in installed PV price in last 5 years
- PV now at grid parity w/ non-renewable sources
- 50% of new grid installations are PV!
Challenge of PV and increased grid penetration

- Photovoltaics are considered a **variable** source and when penetration is large, can lead to over-generation
- Base load plants do not want to be throttled down
Need renewable sources of electricity at night

- **Dispatchable** renewable sources needed to smooth out renewable, variable production curve
- Will ultimately lead to reduced carbon-derived base load

If we don’t solve the storage problem, PV’s impact will be limited
A renewable grid

Daytime electricity from PV

Carbon neutral route to address nighttime electricity demand

Need to **time-shift** solar energy into periods where sun is ‘off’

**Unclear** what renewable storage technology will emerge with sufficiently low $/kWh to compete with natural gas peaking plants
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Carbon-neutral storage approaches

Internal energy: Gravity

Example: Pumped hydro

Renewable Source: Indirect solar* 

* wind, PV

“Indirect source” example:

Sunlight

PV
Electricity

Transmission

Uphill pumping

Storage losses

Downhill generation

Transmission

Available Energy

20%

75%

Net: <15%

Pro:
Separate optics from storage

Con:
Additional energy conversion steps lead to reduced overall efficiency

99% of bulk storage capacity worldwide
Carbon-neutral storage approaches

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* wind, PV

Gas Storage Location: Caverns, potentially depleted gas reservoirs (PG&E, ongoing)
Carbon-neutral storage approaches

- Internal energy:
  - Gravity
  - Pressure
  - Electrochemical

- Example:
  - Pumped hydro
  - Compressed air
  - Electrolyzers, batteries

- Renewable Source:
  - Indirect solar
  - Indirect solar
  - Indirect solar

* wind, PV
## Carbon-neutral storage approaches

### Internal energy:
- Gravity
- Pressure
- Electrochemical

### Example:
- Pumped hydro
- Compressed air
- Electrolyzers, batteries

### Renewable Source:
- Indirect solar
- Indirect solar
- Indirect solar* (*wind, PV)

---

![Diagram of carbon-neutral storage systems](image-url)
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# Carbon-neutral storage approaches

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* wind, PV
Figure 3: Maturity of energy storage technologies

## Carbon-neutral storage approaches

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* wind, PV

**To centralize or distribute?**
Why centralized storage technologies?

Storage involving mechanical turbines & generators typically must be large (MW-scale) to achieve high efficiencies due to power block scaling issues & costs which do not scale linearly w/ size.
Why distributed storage technologies?

• Smaller construction costs enable greater iteration rate (faster learning curve)
• Grid security
• Transmission losses & less disruptive to existing grid
• Co-generation opportunities for enhanced efficiency
• Technology can still be centralized (modularity) if desired
Distributed storage approaches

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Distributed storage requires
- efficiency at small scales
- simplicity
- low operation/maintenance costs
- safety
- silence
- small footprint

Today’s focus
30 minute goals

• Appreciate **grid complexities & need for storage**

• Storage approaches & identify **primary approaches** to distributed storage

• Define challenges & opportunities within **thermal energy storage**

• Consider role of **thermoelectrics materials** and material design strategies

• Thermoelectric search strategies
Indirect storage: Thermal storage through refrigeration

Assume smart metering implemented (variable electricity cost):

1. Electricity production approaching overcapacity
2. Refrigerator solidifies phase change material (PCM)
3. Air conditioning transitions PCM back to liquid

Could be implemented today w/ traditional compression refrigeration

In future: Peltier (thermoelectric) coolers
Direct storage: Can we shrink concentrated solar thermal?
Direct storage: Can we shrink concentrated solar thermal?
Modular storage & generation block

- Heat Rejection System
- Thermal Valve
- Phase Change Material
- Heat Pipes
- Container
- Absorber
- Insulation
- TE modules

Concentrated Sunlight
Direct storage: Can we shrink concentrated solar thermal?

<table>
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<th>Need to satisfy:</th>
<th>Solution</th>
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<tbody>
<tr>
<td>efficiency at small scales</td>
<td>Turbine</td>
</tr>
<tr>
<td>silence</td>
<td>Solid state thermoelectric generator</td>
</tr>
<tr>
<td>simplicity</td>
<td>Pumped working fluid</td>
</tr>
<tr>
<td>low operation/maintenance costs</td>
<td>“static” system, minimal moving parts</td>
</tr>
<tr>
<td>safety</td>
<td>Non-flammable working fluid</td>
</tr>
<tr>
<td>small footprint</td>
<td>Sensible heat storage</td>
</tr>
<tr>
<td></td>
<td>Phase change material with high latent heat</td>
</tr>
<tr>
<td>dispatchability</td>
<td>Pumped working fluid</td>
</tr>
<tr>
<td></td>
<td>“thermal valve”</td>
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**Solar Thermoelectricity via Advanced Latent Heat Storage (STEALS)**
Thermoelectric generators

Overall system design driven largely by thermoelectric generators

- Efficiency driven by Carnot and material terms:

\[ \eta = \eta_{\text{Carnot}} \eta_{\text{Materials}} \]

\[ \eta_{\text{Carnot}} = \frac{T_{\text{hot}} - T_{\text{cold}}}{T_{\text{hot}}} \]

- Maximize \( T_{\text{hot}} \) for efficiency
- However, \( T_{\text{hot}} \) impacts radiation, material selection & corrosion

Compromise:
~600C (steel rather than exotic alloys)
Still good efficiencies
Thermoelectric generators

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Compromise:
~600C (steel rather than exotic alloys)
Still good efficiencies
Phase change material (PCM)

Storage capacity:  Aluminum example
Specific heat:  0.9 J/gK
Heat of fusion:  400 J/g

Initially, it would appear that with a storage temperature of 600°C, specific heat stores more energy.

Energy vs exergy - ability to do work w/ stored energy

Carnot efficiency
-> 0% as T storage approaches T ambient
Phase change material (PCM)

Latent heat storage at 600°C:

**Molten salts** (e.g. CaCl₂/KCl eutectic)
- Economically viable corrosion solutions exist
- Low thermal conductivity

**Metals** (e.g. aluminum-silicon eutectic)
- High thermal conductivity
- Economically viable corrosion solutions unknown

30 year lifetimes....?
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Motivation - Electrical energy production

Thermoelectric materials directly convert the flow of heat into electrical power

Seebeck effect
Known since 1821

\[ \alpha = \frac{\Delta V}{\Delta T} \]

Voltage
Temperature gradient

\( \Delta V \)

\( h^+ \) →

\( e^- \) →

Diffuse!
Efficiency: Want maximum power for a given transfer of heat (heat is our fuel)

Two sources of loss:
  • electrical resistance  -> $P = \frac{V^2}{R}$
  • thermal shorting

Material efficiency: Transport

Figure of merit ($z$) =

$$zT = \frac{\alpha^2 T}{\rho \kappa}$$

Seebeck coefficient\(^2\)

- electrical resistivity
- thermal conductivity

Avoid parasitic heat loss. All heat transferred should be creating current.
Thermoelectrics and generator efficiency

Thermoelectric figure of merit: $zT$

$$zT = \frac{\alpha^2 \sigma T}{\kappa}$$

- $\alpha$ - Seebeck coeff.
- $\sigma$ - Electrical conductivity
- $\kappa$ - Thermal conductivity

Generators based on materials with average $zT > 2$ would be transformative!
Thermoelectrics and generator efficiency

Thermoelectric figure of merit: \( zT \)

\[
zT = \frac{\alpha^2 \sigma T}{\kappa}
\]

Generators based on materials with average \( zT > 2 \) would be transformative!

How do we design materials with desired transport properties?
Thermoelectrics and generator efficiency

Thermoelectric figure of merit: $zT$

$$zT = \frac{\alpha^2 \sigma T}{\kappa}$$

Generators based on materials with average $zT > 2$ would be transformative!

How do we design materials with desired transport properties?
Controlling transport - Landauer approach

Electrical conductivity & “transport function” (isotropic assumption)

\[ \sigma = e^2 \int dE \left( -\frac{\partial f(E)}{\partial E} \right) \Sigma \]

\[ \Sigma = v^2 \tau_e g \]

How many (g), how fast (v) & how long (τ)?

Weighed by partial state occupation (-df/dE)

<table>
<thead>
<tr>
<th>( E )</th>
<th>Energy</th>
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<tbody>
<tr>
<td>( \Sigma )</td>
<td>Transport function</td>
</tr>
<tr>
<td>( g(E) )</td>
<td>density of states</td>
</tr>
<tr>
<td>( f(E) )</td>
<td>Fermi distribution</td>
</tr>
<tr>
<td>( \tau_e )</td>
<td>carrier relaxation time</td>
</tr>
<tr>
<td>( v )</td>
<td>Group velocity</td>
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Even in simplest form, material design in reciprocal space and charge carrier and phonon scattering

Chemical intuition lacking....
Controlling transport – Landauer approach

Electrical conductivity:

\[ \Sigma = v^2 \tau g \]
\[ \sigma = e^2 \int dE \left( -\frac{\partial f(E)}{\partial E} \right) \Sigma \]
Controlling transport - Landauer approach

$\Sigma = v^2 \tau_e g$

Seebeck coefficient is similar:

$$\alpha = \frac{e}{\sigma T} \int dE \left( -\frac{df}{dE} \right) \Sigma (E - E_F)$$

Transport Distribution Function

$\Sigma(E) = v^2 \tau g$

Transport Coefficients

$-\frac{df}{dE} \Sigma$

$-\frac{df}{dE} \frac{\Sigma(E-E_F)}{\sigma}$

$-\frac{df}{dE} \frac{\Sigma(E-E_F)^2}{K_e}$
Insight from Landauer approach

Seek to maximize both $\Sigma$’s magnitude and asymmetry (about $E_F$)

**Conductivity**  **Seebeck coef**

\[
\Sigma(E) = v^2 \tau g
\]
Insight from Landauer approach

Seek to maximize both $\Sigma$’s magnitude and asymmetry (about $E_F$)

- Conductivity
- Seebeck coef

Non-parabolic bands (to date, largely detrimental)
Insight from Landauer approach

Seek to maximize both $\Sigma$’s magnitude and asymmetry (about $E_F$)

\[ \Sigma(E) = v^2 \tau g \]

Conductivity  Seebeck coef

Resonant states:
Alloying to *insert* electronic states at specific energies (e.g. Tl-PbTe)
Resonant states (e.g. Tl-PbTe)

Resonant states

Pro: Enhanced g near band edge

Con: Decrease in mobility due to increased scattering

Bloch spectral function for states near band edge

Tl resonant states

Wiendlocha DOI: 10.1103/PhysRevB.88.205205
Electron filtering to enhance $\Sigma$ asymmetry

Superlattice limits mobility of low energy electrons due to quantum well formation
Increasing $\Sigma$ through band degeneracy

Symmetry leads to multiple band extrema
Increase $g$ without decreasing $\nu$
May decrease $\tau$ due to inter-valley scattering
Thermal conductivity - Debye Callaway Approach

\[ \kappa_L = \frac{1}{3} \int d\omega \ C \ v_g^2 \ \tau \]

| \(C\) | Heat capacity |
| \(v\) | Group velocity |
| \(\tau\) | phonon relaxation time |

Low lattice thermal conductivity (phonon transport) achieved by:
- reducing the group velocity (\(v\))
- inducing scattering sources
Structural complexity and low thermal conductivity

Group velocity: \( v_g = \frac{d\omega}{dk} \)

Roufosse & Klemens *PRB* 1973
Toberer, Zevalkink, Snyder, *J. Mater. Chem* 2011
Structural complexity and low thermal conductivity

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Structural complexity and low thermal conductivity

Theory:
\( \kappa_L \propto n^{-2/3} \)

n: # atoms primitive cell

Expectation that structurally complex crystalline materials will have incredibly low thermal conductivity.

Roufosse & Klemens *PRB* 1973
Toberer, Zevalkink, Snyder, *J. Mater. Chem* 2011
Experimental validation

Structural complexity proves to be a good predictor of $\kappa_L$ for similar compounds (e.g. antimonides)!

Roufosse & Klemens *PRB* 1973
Toberer, Zevalkink, Snyder, *J. Mater. Chem* 2011
Beyond low group velocity: Phonon scattering

Primary sources of phonon scattering?
- Other phonons - Unklapp (phonon-phonon) scattering
- Point defects (mass disorder, strain fields)
- Extended defects and nanostructures

Opportunities both within and beyond the unit cell to design materials with strong phonon scattering

Point defects in SnSe - Strain field formation

\[ \Delta_{SAD} = 0.38 \]

\[ \Delta_{SAD} = 2.96 \]
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New search methodologies needed!

Computationally driven search approaches
Known non-intermetallic compounds and TE materials

~50,000 unique crystalline compounds (excluding intermetallics) within the Inorganic Crystal Structure Database (ICSD)

Only a small fraction have been considered for TE performance!

Yan et al EES 2015
Current approach: Serendipity & intuition

... also known as ...

*fishing*

However, TE design is a **reciprocal (momentum) space** problem. Minimal intuition for reciprocal space.....
Current approach: Serendipity & intuition

... also known as ...

fishing

Grand Challenge: New paradigms for material discovery & design needed!
Discovery methodology

Known and stable hypothetical compounds: >100,000
+ stable alloys: >>100,000

Identify semiconductors*: >10,000

Estimate TE properties from calculations: >1,000 candidates

Validation:
- Improved calc.
- Doping
- Scattering
- Experiment

* Building off of NREL’s Center for Inverse Design codes for photovoltaics
Discovery methodology

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Framing the problem: Alternative metrics

Boltzmann transport equations

\[ zT = \frac{\alpha^2 \sigma T}{\kappa} \]

E\textsubscript{F} optimization (doping)

\[ \beta \propto \frac{\mu N m^{*3/2}}{\kappa_L} \]

Intrinsic material properties

\( \mu \) - mobility
\( N \) - number of band minima/maxima
\( m^* \) - band effective mass
\( \kappa_L \) - lattice thermal conductivity

Separating out doping enables improved structure-property database development and data mining

Alternative metric for material discovery

\[ zT = \frac{\alpha^2 \sigma T}{\kappa} \]

Boltzmann transport equations

**EF optimization (doping)**

**Intrinsic material properties**

\[ \beta \propto \frac{\mu N m^{*3/2}}{\kappa_L} \]

- High \( \beta \) is a necessary but insufficient criteria for high \( zT \).
- Potentially easier to search for \( \beta \) than for “dopability”
- \( \beta \) doesn’t solve the problem of scattering

Snyder & Toberer Nature Mat. 2008
Applying $\beta$ to high throughput calculations

Ground state:
- Electronic band structure ($k$)
- Phonon band structure ($q$)

Coupling:
- Electron scattering rates ($k + q$)
- Phonon scattering rates ($q_1 + q_2$)

$\beta \propto \mu N m^{3/2}$
Applying $\beta$ to high throughput calculations

**Goal:** Develop **semi-empirical models** for mobility ($\mu$) and $\kappa_L$ which correlate **ground-state** DFT calculations & structural data (.cif file) with experimental measurements.

Source experimental data:
- Known thermoelectric materials
- Classic III-V and II-VI semiconductors
- Oxides

Too little experimental data for machine learning, use theory driven models instead.

Ground state:
- Electronic band structure ($k$)
- Phonon band structure ($q$)

Coupling:
- Electron scattering rates ($k + q$)
- Phonon scattering rates ($q_1 + q_2$)
Semi-empirical approach to lattice thermal conductivity

Can we down-select materials without knowledge of anharmonicity or $\nu_g(k)$?

$$\kappa_L \propto C \nu_g^2 \tau$$

$\kappa_L \sim \frac{1}{n^x} \frac{B^x}{d^x} B^{x*}$

- $C$ - optical modes have extremely low velocity, effectively decreasing available heat capacity
- $\nu$ - acoustic branch carries heat, using low frequency approximation - speed of sound $\nu_s$
- $\tau$ - Expectation that stiffer lattices have lower phonon-phonon coupling

$n = \text{number of atoms in primitive cell}$
$B = \text{bulk modulus}$
$d = \text{density}$

* - plus small optical phonon term

Yan et al EES 2015
Semi-empirical approach to lattice thermal conductivity

Calculate via:

- DFT bulk modulus ($B$)
- known mass density ($d$)
- # atoms in primitive cell ($n$)

\[ \kappa_L \propto C \nu_g^2 \tau \]

\[ \kappa_L \sim \frac{1}{n^x} \frac{B^x}{d^x} B^x + \text{minimum term for optical modes} \]

Trying not to over fit the data!!
Similar approach applied to mobility

Yan et al EES 2015
Development of high throughput descriptors for $\beta$

\[ \beta \propto \frac{\mu N m^*^{3/2}}{K_L} \]

From .cif:
- $n$ - number of atoms in primitive cell
- $d$ - density

From DFT:
- $N$ - band degeneracy
- $m^*_b$ - band effective mass
- $B$ - bulk modulus

\[ \beta_{SE} \approx \frac{n^a d^b N^c}{m^*_d B^e} \]

Yan et al EES 2015
Comparison between $\beta_{\text{exp}}$ and $\beta_{\text{SE}}$

- Semi-empirical $\beta$ as accurate as experimental in predicting TE performance
- $\text{Mg}_2\text{Si}$ and p-$\text{PbTe}$ underestimated due to doping (Bi) and T-dependent effects

Yan et al EES 2015
Compounds: (~2,000 unique structures from ICSD & 10 TE materials)
- Stoichiometric
- No H, O
- No more than 10 atoms in primitive cell
- No row 7, La, Ac, Noble gases

DFT Calculations:
- ~4000 k-points
- Magnetic systems - compared non-magnetic, ferromagnetic and antiferromagnetic configurations and chose lowest energy spin configuration

Yield:
~600 semiconductors
Downselected remaining semiconductors to $E_g < 2$ eV:
~450 compounds remain
Trial high-throughput calculations - valence band

\[ \beta_{SE} \propto \frac{\mu N m^{3/2}}{\kappa_L} \]

Bubble area indicates \( \beta_{SE} \)

Bi\(_2\)Te\(_3\), PbTe, PbSe PbS all in top 4% of down-selected compounds

Yan et al EES 2015
Trial high-throughput calculations - conduction band

\[ \beta_{SE} \propto \frac{\mu N m^{*3/2}}{\kappa_L} \]

Bubble area indicates \( \beta_{SE} \)

Yan et al EES 2015
Expanding the search - 1,600 semiconductors

Atom count: up to 30 in primitive cell
Pnictides, oxides, chalcogenides

\[ \mu_n (\text{cm}^2 \text{V}^{-1} \text{s}^{-1}) \]

\[ \kappa_L (\text{Wm}^{-1} \text{K}^{-1}) \]

\[ \mu_e (\text{cm}^2 \text{V}^{-1} \text{s}^{-1}) \]

\[ \kappa_L (\text{Wm}^{-1} \text{K}^{-1}) \]

\( N_b \):

- 1
- 2
- 3
- 4
- 5
- 6
- 7
- 8
- >9
Thermoelectric material design: Looking forward

Beginning to design charge & phonon transport:

A solid state heat engine with >25% efficiency would transform energy storage.

Things get even neater in:
- Anisotropic materials
- Correlated systems
Not discussed:
- Solid state refrigeration (Peltier cooling)
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<tr>
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<th>1(^{st}) step:</th>
<th>2(^{st}) step:</th>
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<tr>
<td></td>
<td>Solar reduction ((\sim) 1500°C)</td>
<td>Non-solar oxidation ((\sim) 900°C)</td>
</tr>
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</table>

\[
\delta O_2 \rightarrow CeO_2-\delta \rightarrow \delta H_2, \delta CO \rightarrow H_2O, CO_2 \rightarrow \text{Syn gas?}
\]

Chemical: Solar biofuels, thermochemical

Direct abs.
Example of Band Degeneracy: p-type PbTe

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Temperature (K)

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arXiv:1404.1807v3