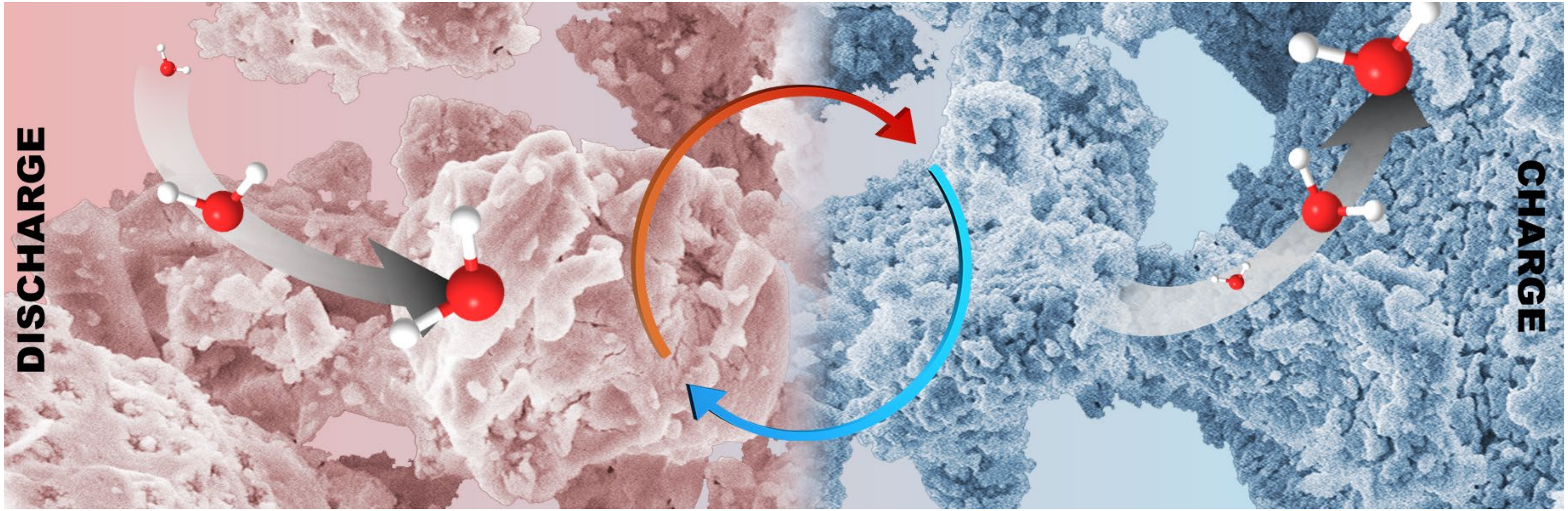
Stable Thermochemical Salt Hydrates for Energy Storage in Buildings



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Project Summary

Timeline:

Start date: 10/1/2020

Planned end date: 09/30/2023

Key Milestones:

1. Down select the most promising thermochemical materials (TCM) with charging temperatures below 100ºC and demonstrate energy densities above 500 kWh/m^3 after cycling. March 2021
2. Synthesize and optimize composite TCM comprising a porous support matrix and an inert binder to achieve thermal reliability >90% after 200 cycles, with energy densities> 250kWh/m^3. Sep 2022
3. Develop a reactor prototype and demonstrate reactor level performance with the following attributes: Energy density > 200 kWh/m^3 , thermal reliability > 90% after > 200 cycles. June 2023
4. Demonstrate cost of <$15/kWh reactor level based on experimental findings and detailed LCOS study. Sep 2023

Budget:

Total Project $ to Date:

- DOE: $403,737
- Cost Share: $ 130,000

Total Project $: $3,000,000

- DOE: $2,400,000
- Cost Share
  - NetEnergy LLC: $525,000
  - University of California, Berkeley : $75,000

Key Partners:

NETEnergy, LLC
University of California, Berkeley
University of Auckland, New Zealand
National Renewable Energy Laboratory

Project Outcome:

Thermal energy storage (TES) solutions offer opportunities to reduce energy consumption, greenhouse gas emissions and cost. Specifically, they **can help reduce the peak load, improve energy efficiency of HVAC systems, and address the intermittency of renewable energy sources by time shifting the load** – all of these are critical towards zero energy buildings.

Thermochemical based TES with high storage capacities (600 kWh/m^3) and negligible self-discharge are uniquely suited as compact, stand-alone units for daily-seasonal storage for residential, district-level or large commercial buildings.

Applications (use cases) include dedicated standalone thermal storage, equipment and heat pumps integrated thermal storage

Team

Materials selection, optimization and characterization

Sumanjeet Kaur (PI)
LBNL

Andrew Martin
LBNL

Mohammed Farid
University of Auckland

Materials to reactor level modeling

Ravi Prasher
LBNL, UCB

Chris Dames
UCB

Scale-up and commercialization

Said Al-Hallaj
NetEnergy, LLC

Mike Pintar
NetEnergy, LLC

System level modeling and techno-economic analysis

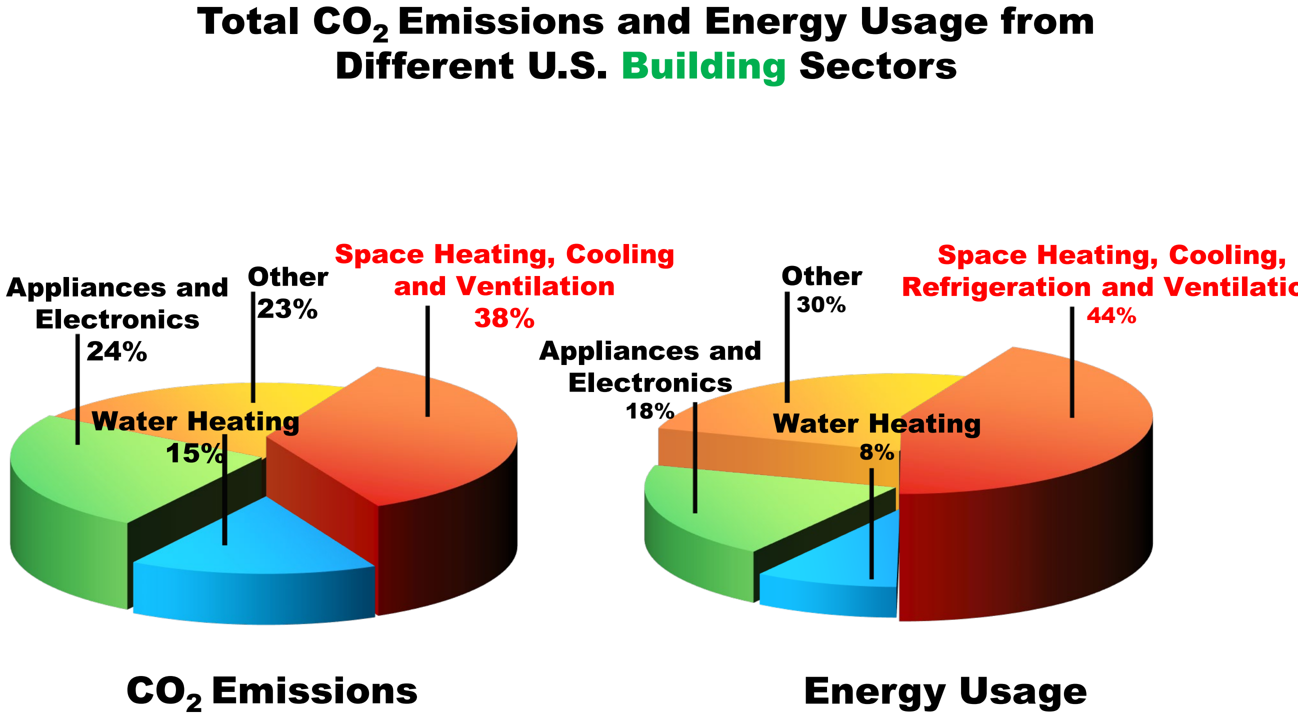
Jason Woods
NREL

Wale Odukomaiya
NREL

Challenge : Energy Storage is Needed

- Buildings dominate primary energy and electricity use in the United States and most of the world. When disaggregated into individual end-uses, thermal loads dominate and are also a major contributors in CO_2 emissions.

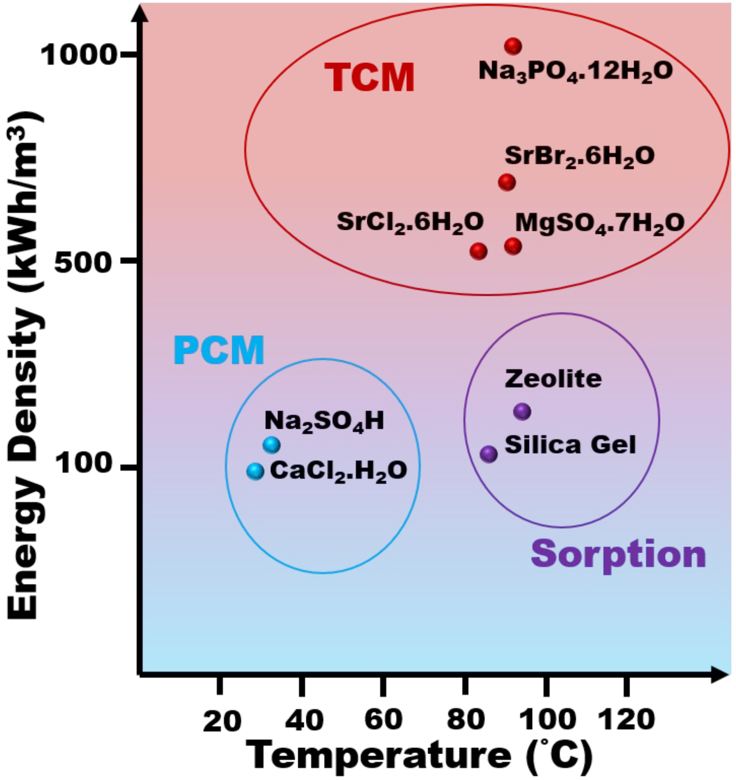
- Much of the heating load in the US is met with fuel-based equipment, such as natural gas furnaces or boilers. **To decarbonize buildings, a significant fraction of this fuel-based equipment will be switched to electric heat pumps.** This will cause the large heating demand to become a dominant part of the grid peak demand, particularly in cool and cold climates where the winter peak is expected to exceed the summer peak.

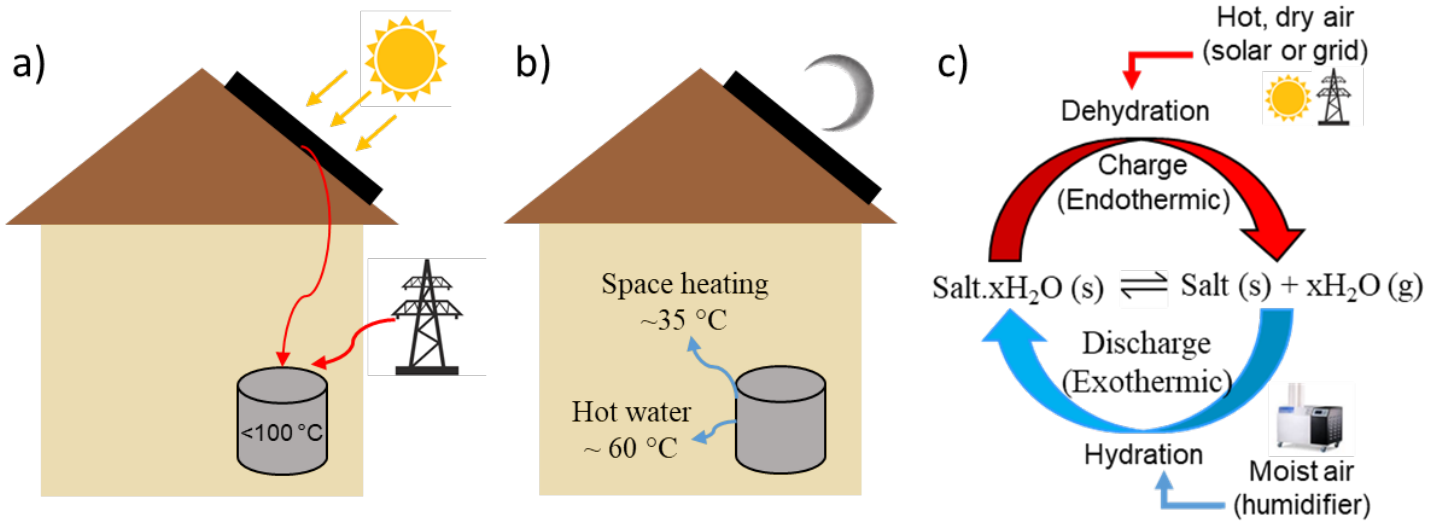


US EIA, Monthly Energy Review, Annual Energy Outlook 2017, Electric Power Monthly, Natural Gas Summary

It is abundantly clear that deeper penetration of renewable electricity will only be possible with scalable, affordable, and sustainable energy storage. **Because heating and cooling are projected to account for more than 50% of the energy demand in buildings, we believe that on-site TES for buildings is a sustainable, scalable and affordable energy storage solution.**

Approach: Thermal Energy Storage for on-site Storage





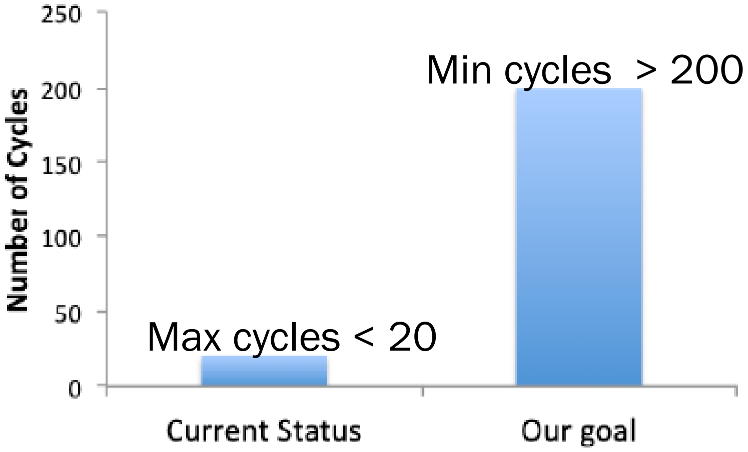
a) TCMs can be charged using solar energy or grid electricity. b) Energy stored in TCM can be discharged at desired T for thermal end-uses. c) Reversible solid-gas reactions (salt hydrate) in an open system.

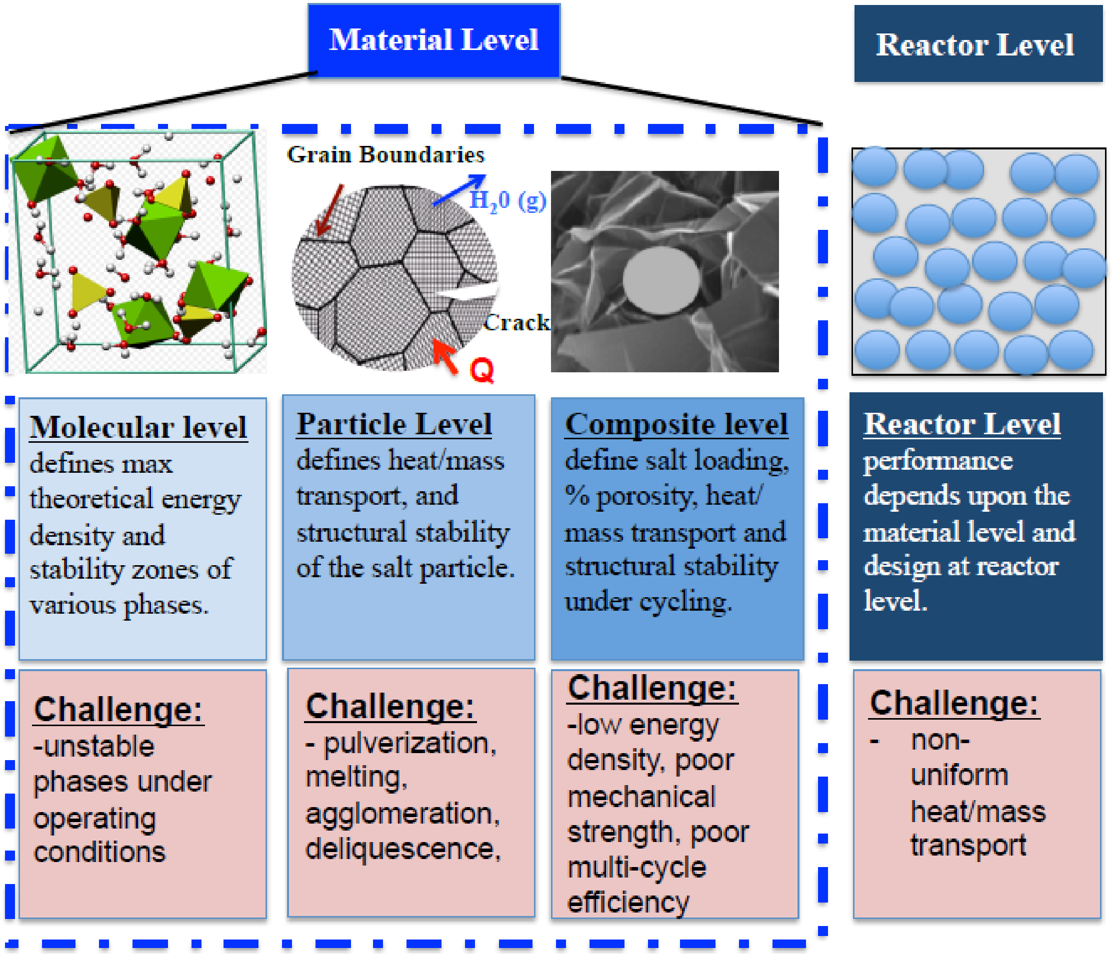
- Phase Change Materials (PCMs) and sorption-based storage have energy density in the ranges of ~100 kWh/m^3
- Thermochemical Materials (TCMs), comprising a reactive pair of inorganic salt and water vapor, have higher theoretical energy densities of ~500 kWh/m^3 and negligible self-discharge as energy is stored in chemical bonds, making them ***uniquely suited as compact, stand-alone solutions for daily-seasonal energy storage in buildings***

Approach: Bottom-up Optimization from Material to Reactor Level

State of the art: Poor Multi-cycling Performance for TCMs

- TCMs suffer from instabilities at the material (salt particles) and reactor level (packed beds of salt), resulting in poor multi-cycle efficiency.
- So far the TCM based storage is optimized for seasonal: number of charge/discharge cycles per year to only *one* (charge in summer and discharge in winter). Has **high-levelized cost of storage**.

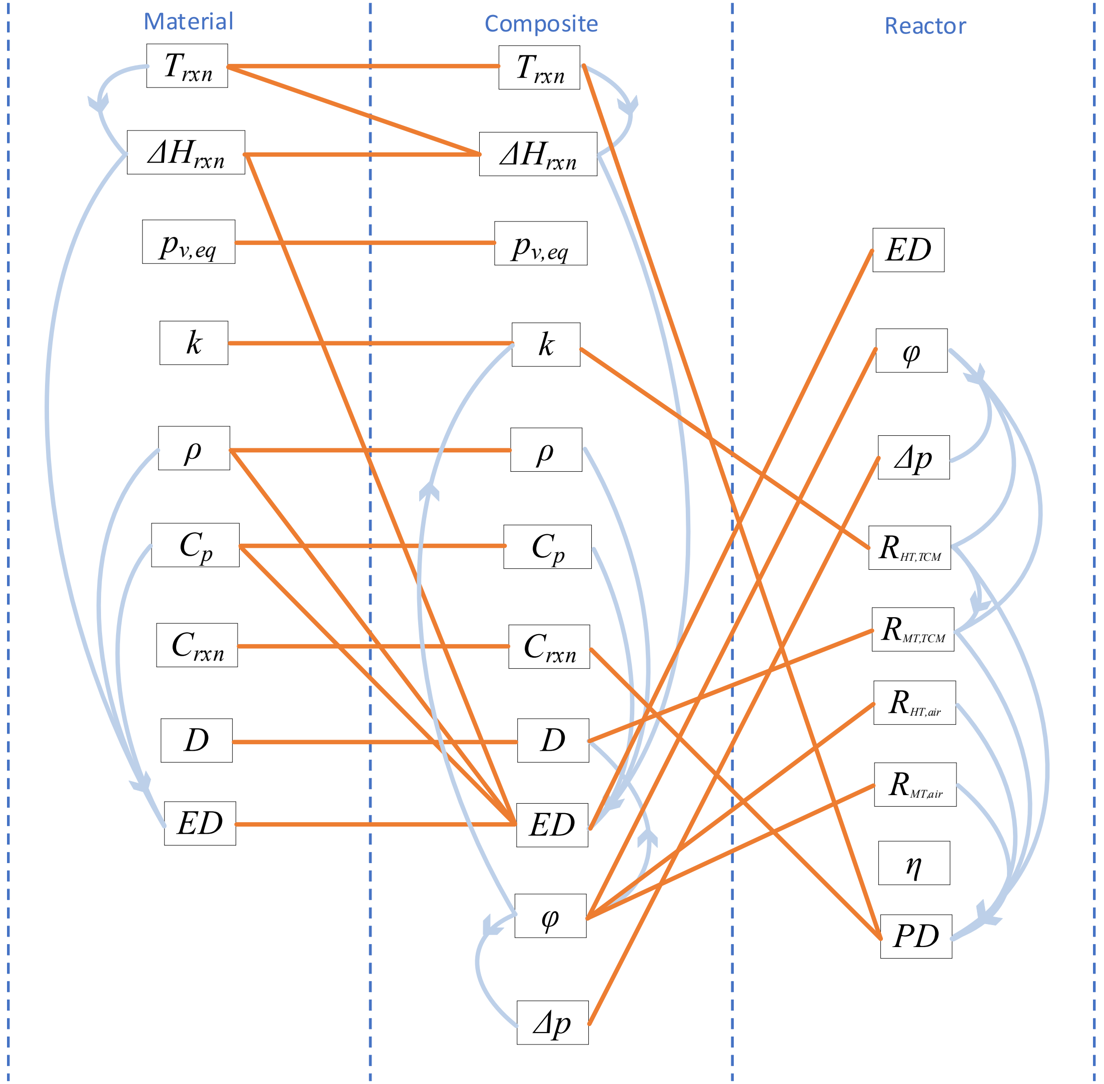




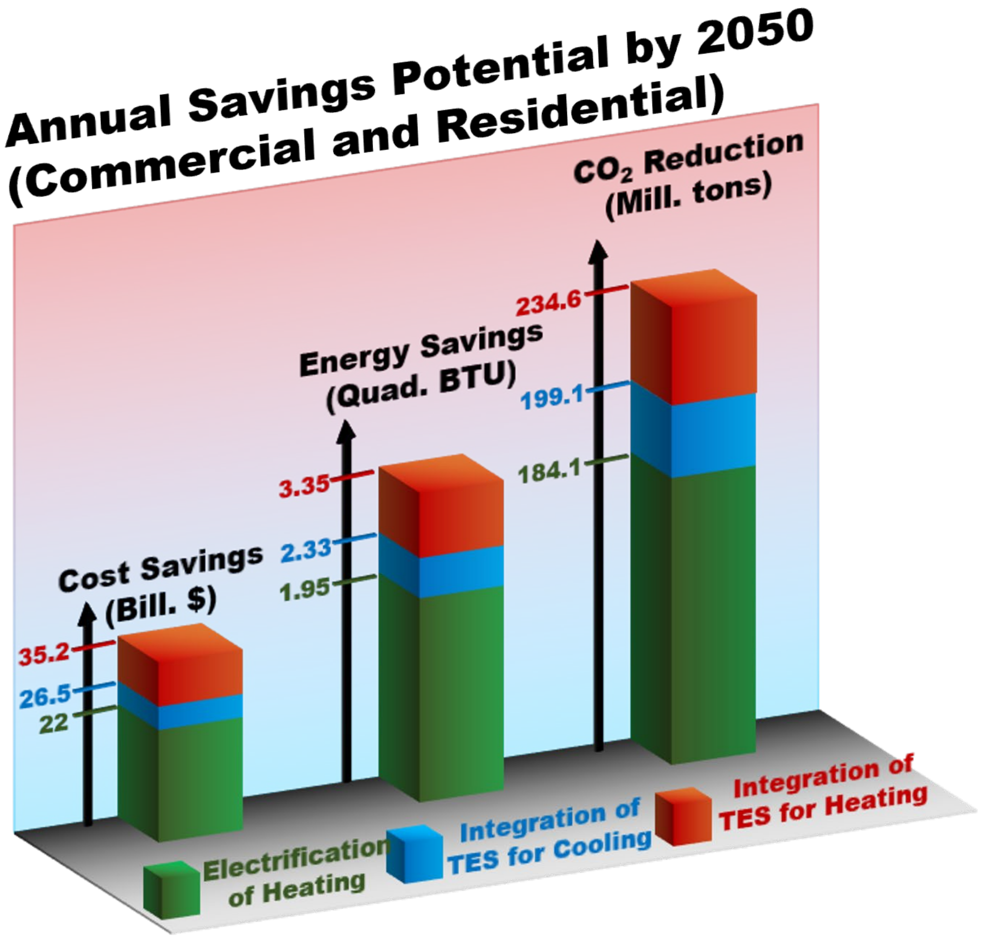
Our goal is to use bottom-up approach to design, optimize and develop TCM based energy storage for buildings by addressing the chemical instabilities of the salt at material (and composite) level as well as optimizing the performance for heat and mass transport at reactor level.

Approach: Optimization from Material to Reactor Level

Parameter	Symbol	Scale (M-material, C-composite, R-reactor)		
		M	C	R
Enthalpy of reaction	ΔH_{rxn} [J/g]	X	X	
Diffusion coefficient	D [-]	X	X	
Equilibrium vapor pressure	$p_{v,eq}$ [Pa] = f(T)	X	X	
Thermal conductivity	k [W/m·K]	X	X	
Deliquescence point	RH_{del} [-] = f(T_{del})	X	X	
Density	ρ [kg/m^3]	X	X	
Specific heat capacity	C_p [J/g·K]	X	X	
Reaction constant	C_{rxn} [1/s]	X	X	
Thermal expansion coefficient	C_{TE} [1/K]	X	X	
Volume change (due to reaction)	ΔV_{rxn} [-]	X	X	
Compressive strength	σ [Pa]	X	X	
Porosity	φ [-]		X	
Energy density	ED [kWh/m^3]	X	X	X
Specific energy	SE [kWh/kg]	X	X	X
Power density	PD [kW/m^3]	X	X	X
Specific power	SP [kW/kg]	X	X	X
Reaction temperature	T_{rxn} [°C] = f($p_{v,eq}$)	X	X	X
Cycle life (utilization)	N_{cyc} [-]	X	X	X
Reaction advancement (SOC)	X [-]	X	X	X
Tortuosity	τ [-]		X	X
Pressure drop	Δp [Pa]		X	X
Bulk density	BD [kg/m^3]			X
TCM heat transfer resistance	$R_{HT,TCM}$ [m^2·K/W]			X
TCM mass transfer resistance	$R_{MT,TCM}$ [m^2·K/W]			X
Air-side heat transfer resistance	$R_{HT,air}$ [m^2·K/W]			X
Air-side mass transfer resistance	$R_{MT,air}$ [m^2·K/W]			X
Roundtrip efficiency	η [-]			X



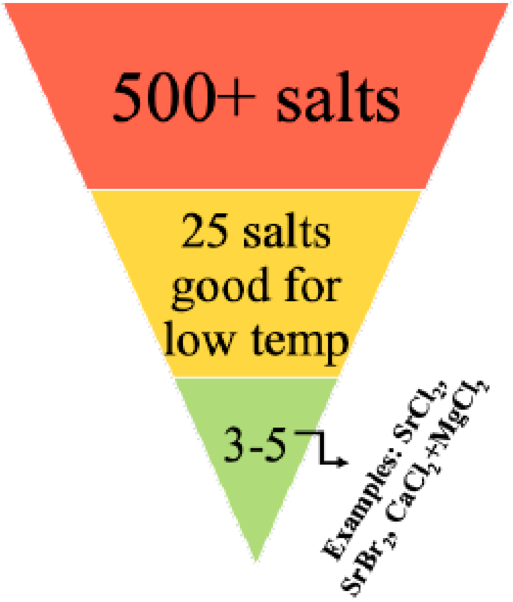
Impact



- Cost effective energy storage is a critical enabler needed for the large-scale deployment of renewable energy.
- By increasing the utilization, we aim to significantly reduce levelized cost of storage (LCOS) of TCM based TES with a goal of reaching DOE target of less than $0.05/kWh.
- Our group has conducted preliminary analysis for heating and cooling in residential and commercial buildings using NREL's Scout tool for TCM-heat pumps hybrid systems.
- As shown in Figure, preliminary results indicate a potential annual savings of the hybrid system: $35.2 Billion, 3.35 Quadrillion BTUs and 234.6 Million tons reduction of CO_2.

Progress: Salt Selection and Characterization

Down-selection of Compatible Salt Hydrates



Salt Selection Criteria:

- Non-toxic and non-flammable
- Charging temperature <100°C
- Fast reaction kinetics
- Energy density >500 kWh/m^3
- Deliquescence relative humidity (DRH) >40%RH to prevent over-hydration
- High cyclability
- $T_{melting} > T_{dehydration}$ to ensure solid stability
- Material cost <$2/kg

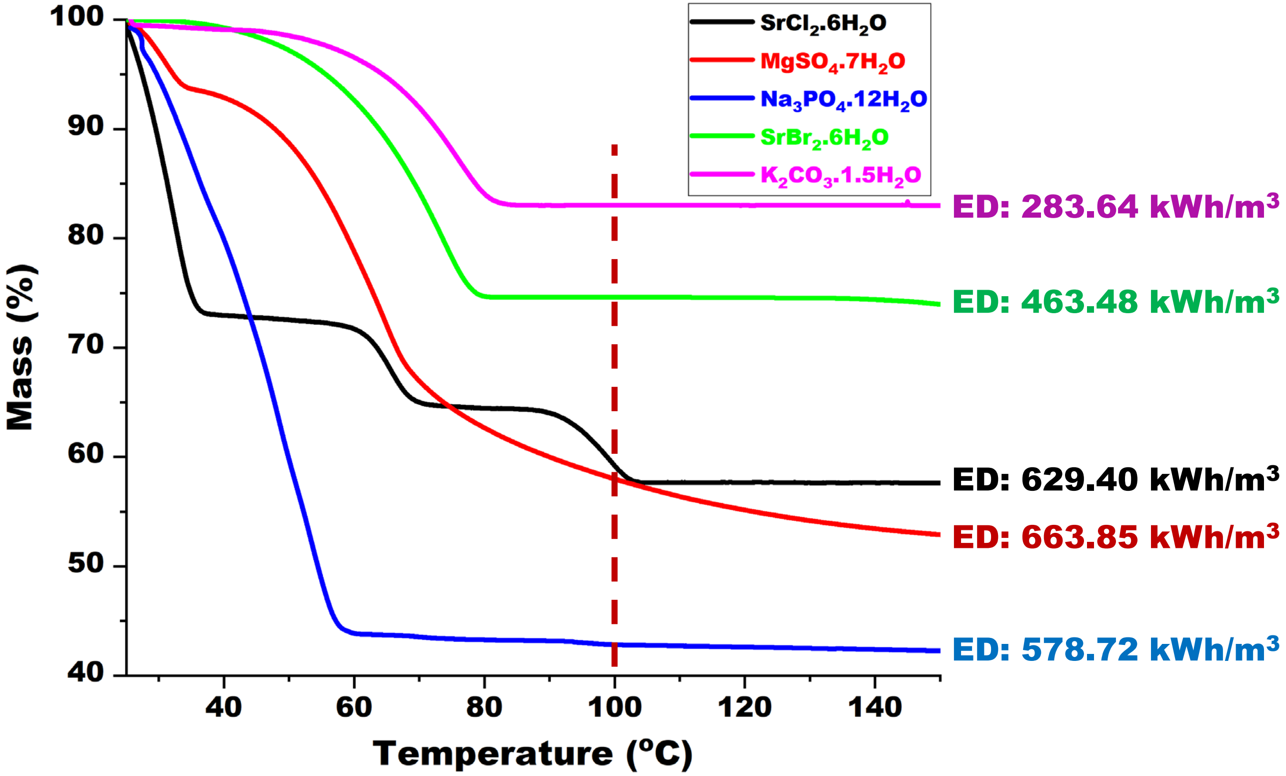
From 25 salts good for low temp, 5 salt hydrates were down selected which met our selection criteria.

Example

Salt	Dehydration temperature (°C)	Dehydration steps	Cyclability	Density of hydrated material (kg m^{-3})	Energy density (kWh m^{-3})	Energy of reaction (kJ mol$^{-1}_{salt}$)	Energy of reaction (kJ mol$^{-1}_{water}$)	Cost per kg (USD)	Cost of power (USD/kWh)	Comments
$SrCl_2.6H_2O$	42-50	$SrCl_2.6H_2O \rightarrow SrCl_2.2H_2O + 4\ H_2O$	Composite of $SrCl_2$ and pumice stable for 10 cycles in lab-scale reactor	1930	560	285	57	0.65 (anhydrous) 0.1 (hydrate)	0.35	• Reversible reaction achievable • Lower energy density than $SrBr_2$ unless dehydration temperature above 128 °C
	86	$SrCl_2.2H_2O \rightarrow SrCl_2.H_2O + H_2O$								

Progress: Salt Selection (cont'd)

Salt Selection And Powder Characterization

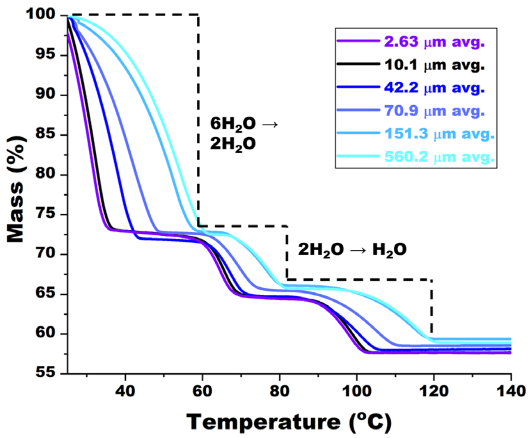


- Selected salts were characterized to show that the operating temperature and energy density matches the requirement.
- Out of 5 down-selected salts, $SrCl_2.6H_2O$ shows the most promising behavior and thus selected as the main workhorse of this project.

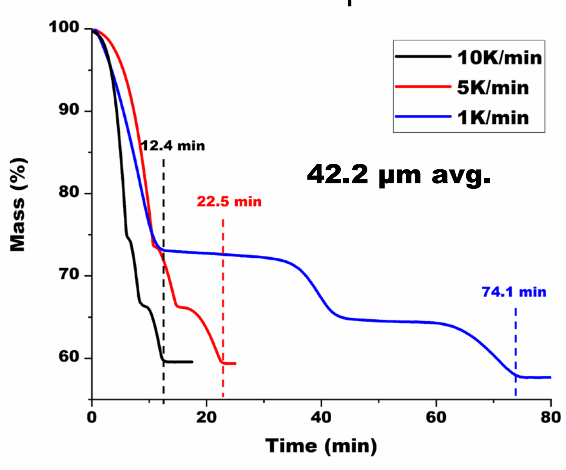
Progress: Fundamental Analysis and Optimization

Materials Level Optimization and Studies

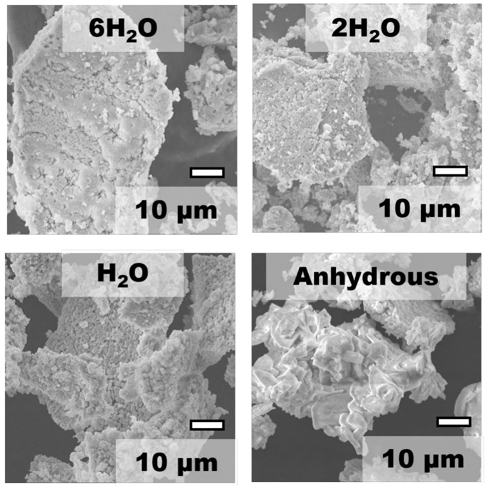
Effect of particle size

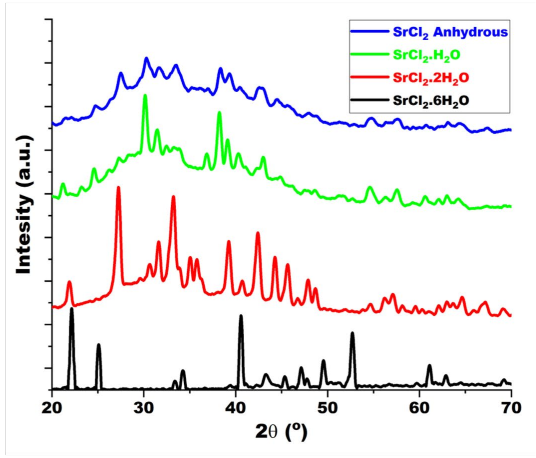


Effect of ramp rate



Effect of depth of discharge

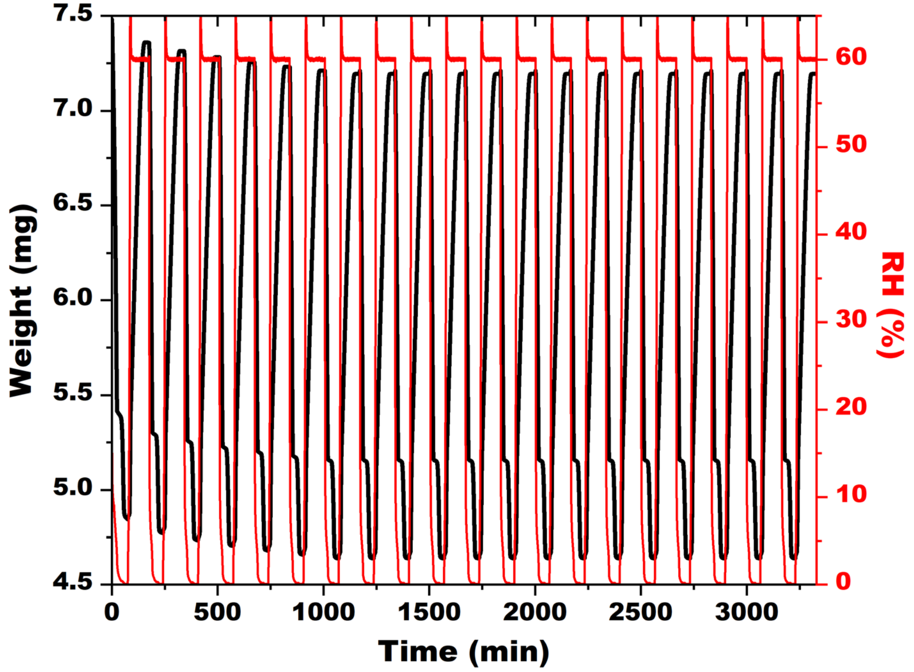


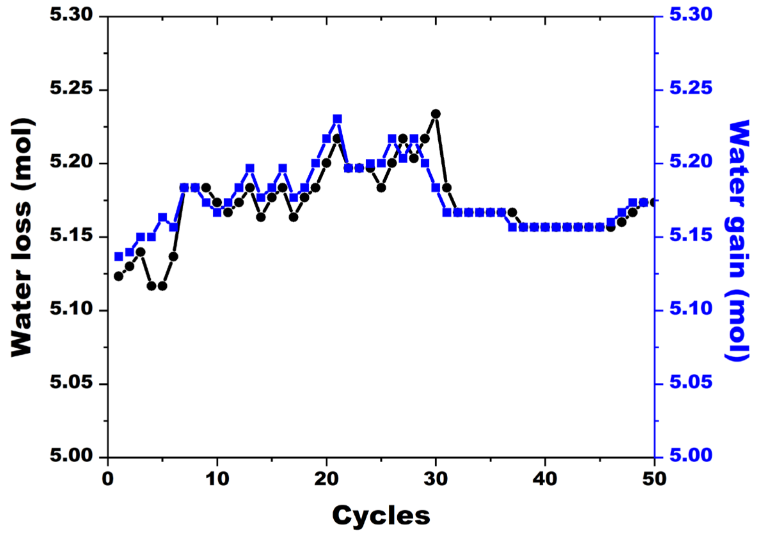


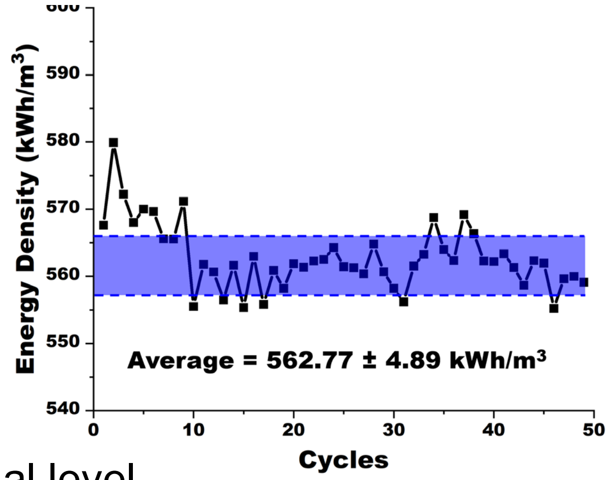
- Performance optimization are done from the materials scale where fundamental analysis are done to investigate morphological and kinetic behaviors of the salt hydrates.
- Key Findings: Optimal particle size required, understanding of ramp rate and depth of charge is critical.

Progress: Material Level Stability

Materials Level Stability (50 cycles, $SrCl_2.6H_2O$ <-> $1H_2O$)





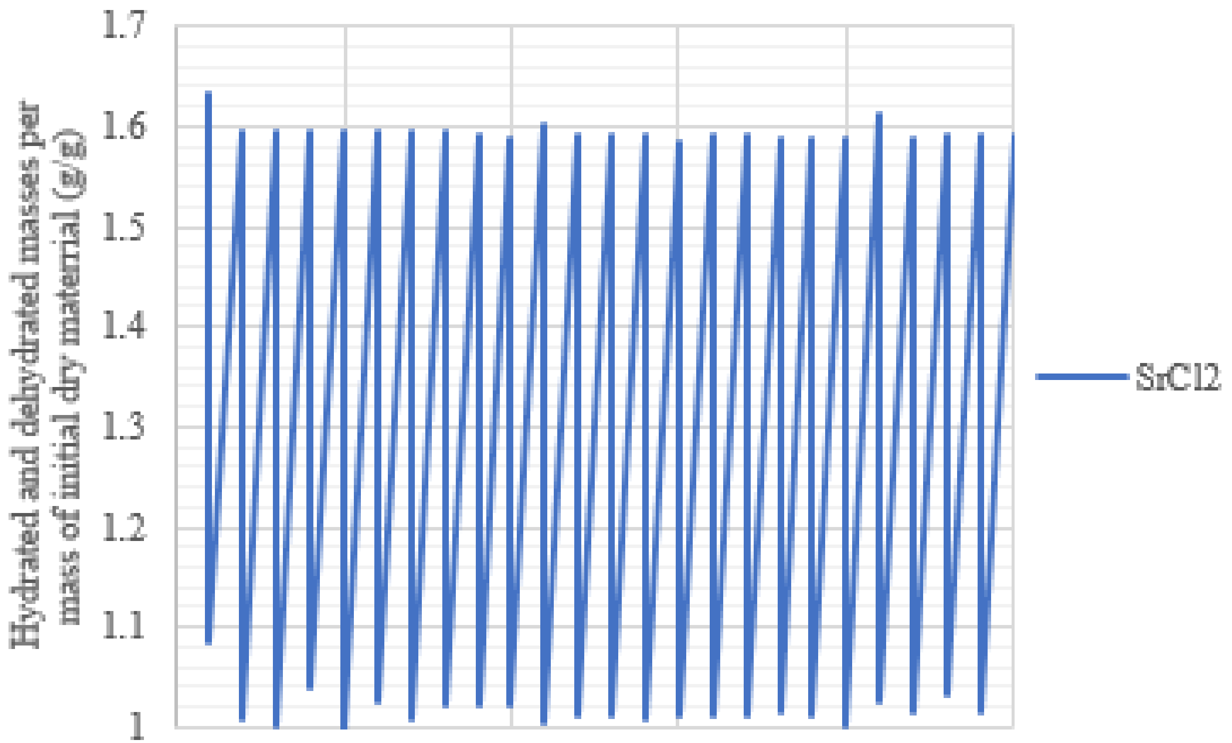


- Selected salts display reliable stability for 50 cycles in the material level.
- Deviation in water uptake and energy density is marginal with an average of 562.77 kWh/m^3*

*Calculation done using bulk density

Progress: Scaling Stability

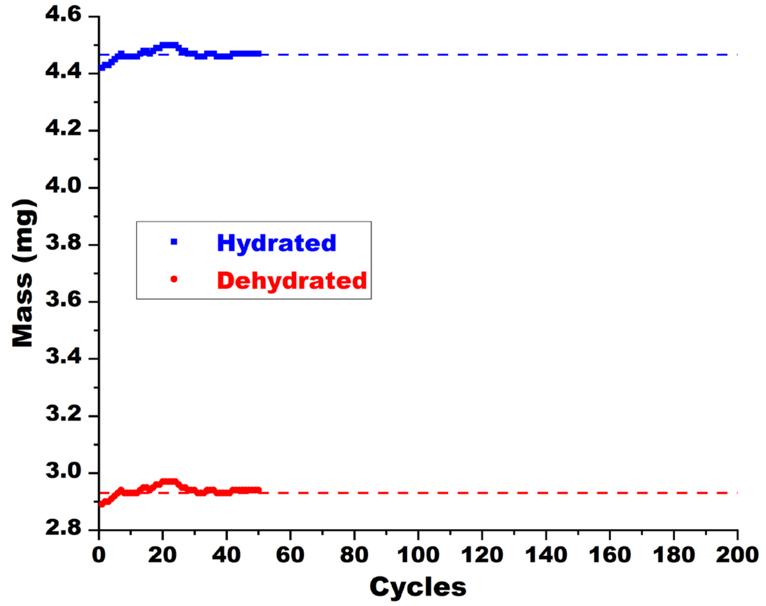
Film Level Stability

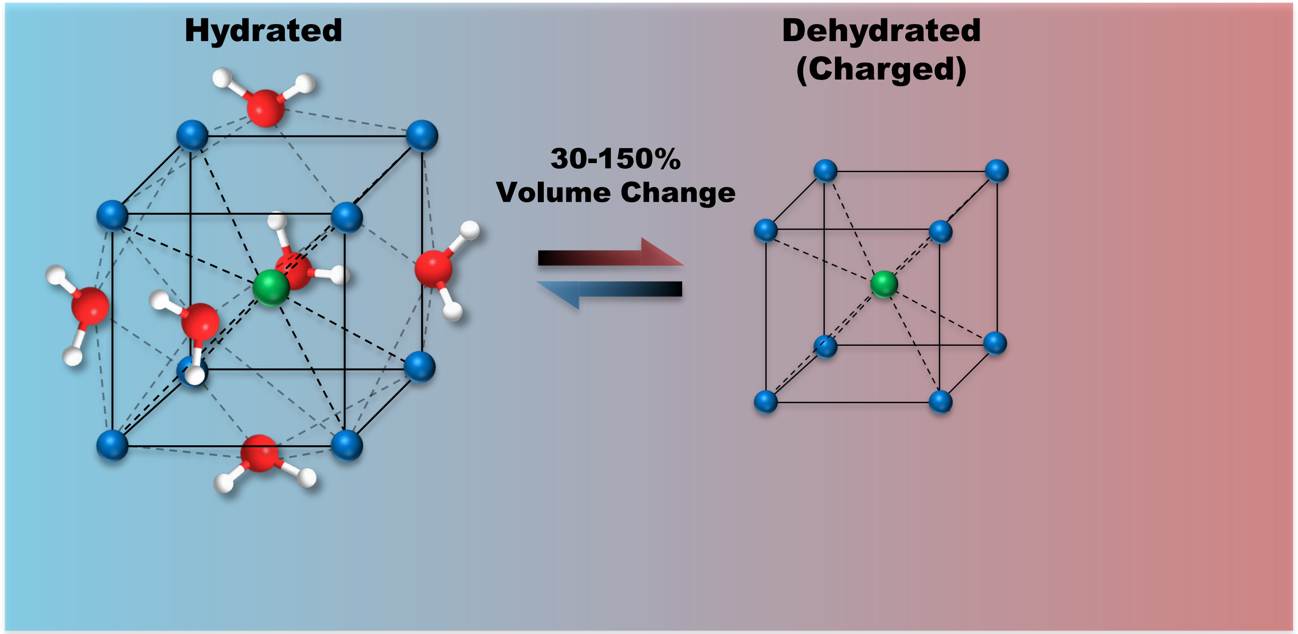


- Stability in the material level translates to a larger scale (film, with more mass)
- Most of the down-selected salts ($MgSO_4.7H_2O$, $SrBr_2.6H_2O$ and $Na_3PO_4.12H_2O$) display relatively stable performance >30 cycles in the film form with constant water intake and output.

Progress: Materials Level Stability Summary

Mass Evolution Projected to 200 Cycles



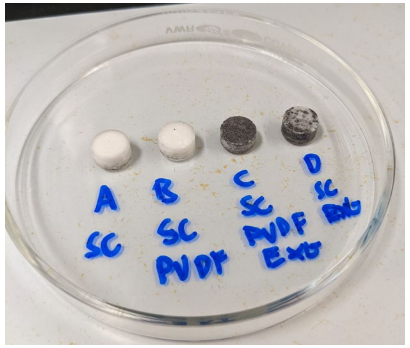


- Projected mass evolution within 50 cycles show at materials level show no degradation trend and thus projected approximately linear for the rest to 200 cycles.
- Stability in the materials level, **however, does not reflect end-product stability (composites or slabs).** Given there are no restriction of space in loose particles/powders, the mechanical stability is not being tested.

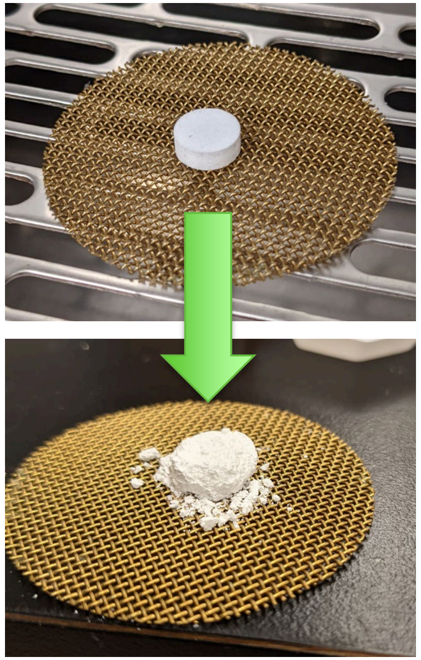
Critical to test cyclability at slab level

Ongoing Project Work: Scaling-Up to Composites

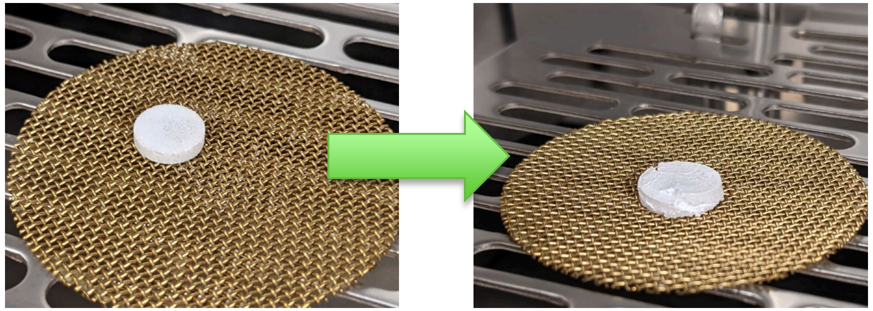
Development and optimization of a three-component composite TCM



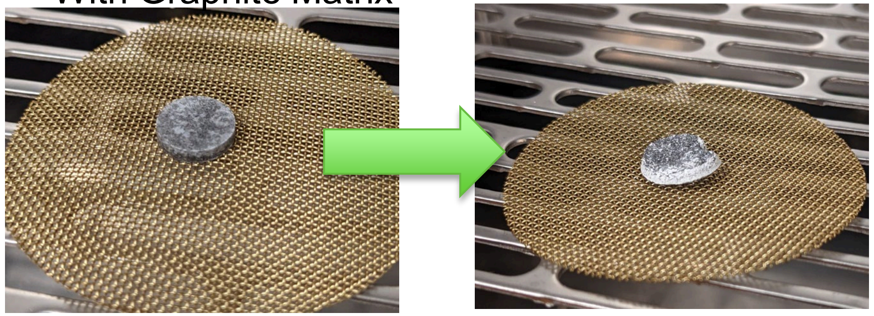
Without Binders



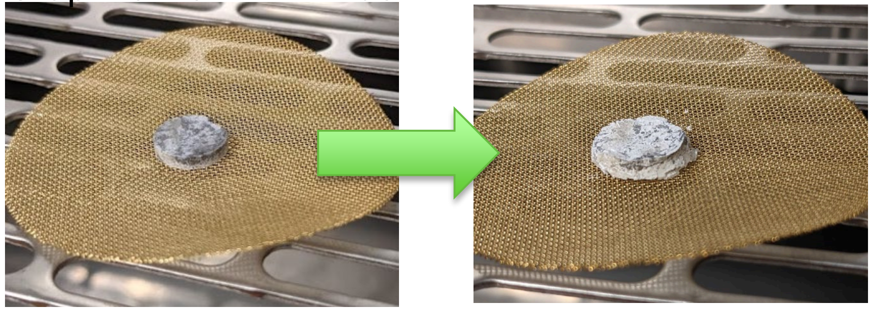
With Binders



With Graphite Matrix



Graphite Matrix + Binder



- Incorporation of binders or expanded graphite matrix help stabilize salt hydrate pucks mechanically.
- Current studies being done to optimize the mechanical stability and performance.

Future Work: Optimization of Composites and Building Reactor Prototype

Tasks	Q4 2021	Q1 2022	Q2 2022	Q3 2022	Q4 2022	Q1 2023	Q2 2023	Q3 2023
Development of three-component composite TCM								
Investigations of binder and matrix to optimize composite performance								
Coupled thermo-chemical mechanical model of TCM composites								
6” x 6” TCM Slab optimization								
Built Reactor Prototype: Design and Testing of thermochemical reactor								
Techno-economic model development								

Stakeholder Engagement

Claus Daniel

Sr. Fellow and Innovation Theme Leader for Sustainability at Carrier

Robert Comparin

Vice President Research at Emerson Commercial and Residential Solutions

Louis Storino

Principal Civil Engineer and Treasurer of Illinois Water Environmental Association (IWEA)

Warren C. Jones

Chief Executive officer at BluePath Finance LLC

- We will conduct biannually meetings with the advisory board members and report on the discussions/ guidance from committee in the quarterly reports.
- The board will guide us on research direction, technology development, target cost, scalability and marketability.
- First advisory board meeting is scheduled on August 13, 2021

Thank You

Lawrence Berkeley National Laboratory, UC Berkeley, NETEnergy. LLC, National Renewable Energy Laboratory
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REFERENCE SLIDES

Project Budget

Project Budget: $2,400,000 over 3 years with $600,000 cost share
Variances: Late hire of postdocs and students due to COVID
Cost to Date (till July 2021): $533,737 (Fed +Cost Share)
Additional Funding: Cost Share partners: NetEnergy LLC and UC Berkeley

Budget History					
FY 2020-Fy2021 (current)		FY 2021- Fy2022 (planned)		FY 2022 – FY2023 (planned)	
DOE	Cost-share	DOE	Cost-share	DOE	Cost-share
800,000	200,000	800,000	200,000	800,000	200,000

Project Plan and Schedule

Project Schedule												
Project Start: Oct 1, 2020		Completed Work										
Projected End: Sep 30, 2023		Active Task (in progress work)										
	◆	Milestone/Deliverable (Originally Planned) use for										
	◆	Milestone/Deliverable (Actual) use when met on time										
	FY2021				FY2022				FY2023			
Task	Q1 (Oct-Dec)	Q2 (Jan-Mar)	Q3 (Apr-Jun)	Q4 (Jul-Sep)	Q1 (Oct-Dec)	Q2 (Jan-Mar)	Q3 (Apr-Jun)	Q4 (Jul-Sep)	Q1 (Oct-Dec)	Q2 (Jan-Mar)	Q3 (Apr-Jun)	Q4 (Jul-Sep)
Past Work												
Q1 Milestone: : Selection of thermochemical salt hydrates	◆											
Q2 Milestone: : Investigation and characterization of pristine salts		◆										
Q3 Milestone: Characterization and Cycling			◆									
Q4 Milestone: Conduct LCOS												
Q4 Milestone: Thermochemical Modeling												
Q4 Milestone: Form TAC			◆									
Current/Future Work												
Milestone 5.1.1 Report on properties of graphite host matrix using various techniques. (Net Energy Inc + LBNL)												
Milestone 5.1.2 Report on properties of other host matrix such as vermiculite using various techniques. (Net Energy Inc +LBNL)												
Milestone 5.2.1 Down-select the most promising binders and demonstrate 5X better mechanical properties (failure stress) compared to non-binder composite after 50 cycles. (LBNL)												