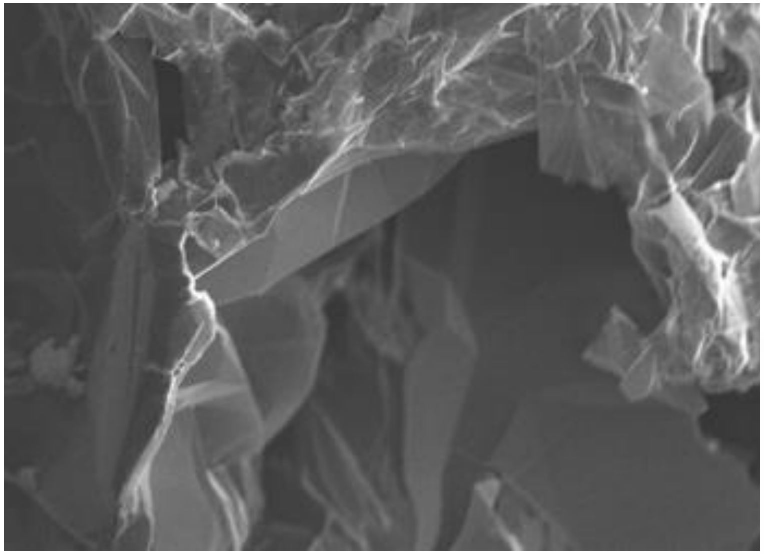
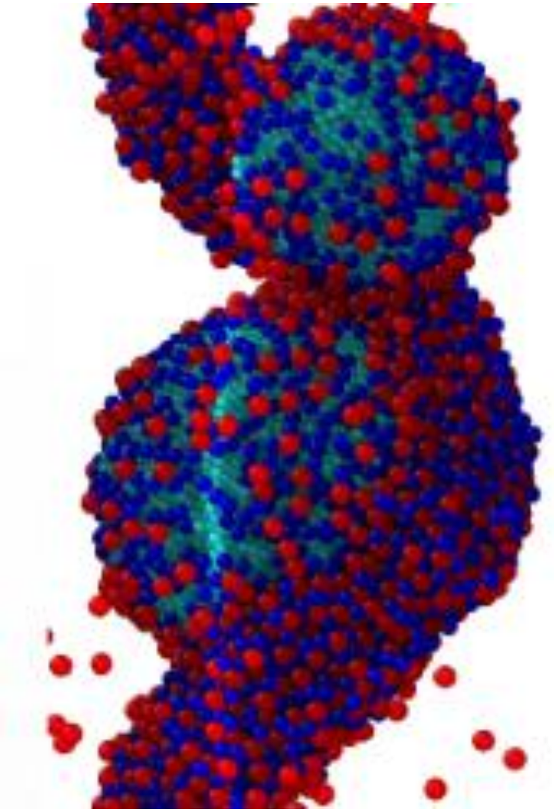
U.S. DEPARTMENT OF ENERGY
Office of ENERGY EFFICIENCY & RENEWABLE ENERGY

Low-cost Composite Phase Change Material





Oak Ridge National Laboratory
Kyle Gluesenkamp, PhD
gluesenkampk@ornl.gov

Project Summary

Timeline:

Start date: 10/1/2018

Planned end date: 9/30/2021

Key Milestones

1. Evaluation of as-received material - Acquire exfoliated graphite, conduct standard characterization, and infuse with salt hydrate and densify; 02/28/2019
2. 3 salt hydrate/CENG composites characterized -– Using commercially available graphite, three different salt hydrates composites are synthesized and evaluated; 03/31/2019

Budget:

Total Project $ to Date:

- DOE: $850k
- Cost Share: $0

Total Project $:

- DOE: $2550k
- Cost Share: $0

Key Partners:

ORNL – Building Technologies Integration Center (BTRIC)
ORNL – Center for Nanophase Materials Science (CNMS)
Georgia Institute of Technology
University of Tennessee, Knoxville

Project Outcome:

When successful, this project will advance the state of the art by realizing a 10x reduction in the cost of deploying phase change materials (PCMs) for building equipment or envelopes.

Multidisciplinary Project Team

Sample synthesis; PCM evaluation

Lead: Gluesenkamp[1]

Team:

Jason Hirschey[3],
Samuel Graham[4],
Tim LaClair[1],
Navin Kumar[2],
Kaushik Biswas[1],
David Keffer[6]

Materials characterization

Lead: Rios[1]

Team:

Yuzhan Li[2],
Michael Kesler[2],
Thomas Proffen[1] ,
Dami Akamo[5],
David Keffer[6]

Principal Investigator:
Gluesenkamp[1]

TBD industry partner(s)

T2M; HVAC Integr.

Lead: Gluesenkamp[1]

Team:

Tim LaClair[1],
Navin Kumar[2],
Bo Shen[1], Jin Dong[1],
Orlando Rios[1],
ORNL TTO

Molecular modeling

Lead: Goswami[1]

Team:

Orlando Rios[1]

Notes:

1. ORNL research staff
2. ORNL postdoctoral researcher
3. Georgia Tech PhD GO! student
4. Georgia Tech professor
5. UTK PhD Bredesen Center student
6. UTK professor

Challenge: Cost Effectiveness

- Traditional PCM solutions:
  - Passive
  - Integrated into wall/floor

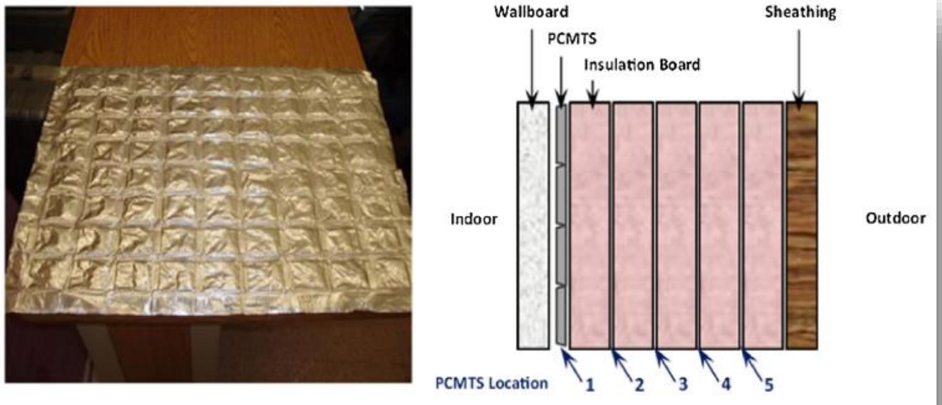


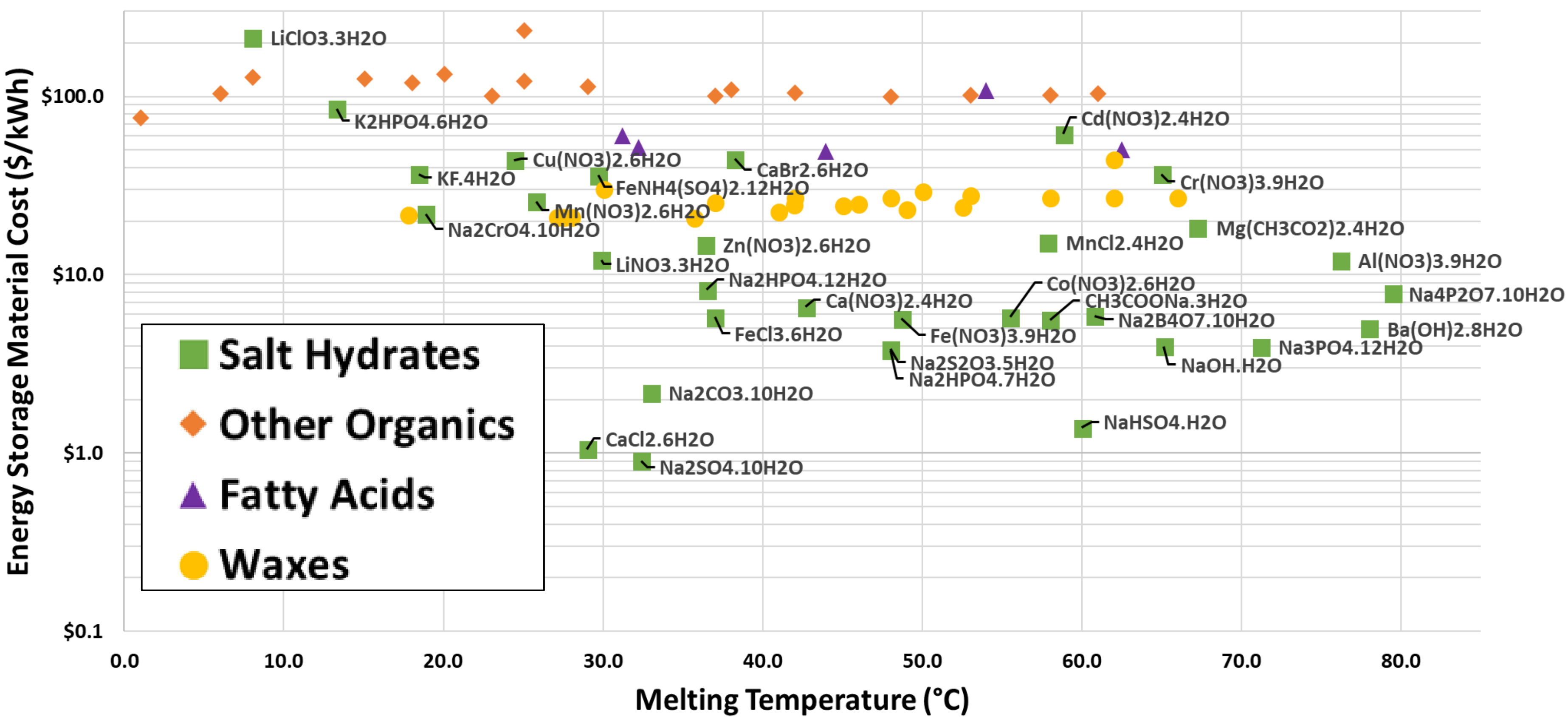
Fig. 37. Sheet of PCM thermal shield PCMTS (left) and wall section showing the PCMTS location (right) [96].

- Problems:
  - *Temperature mismatch*: highly sensitive
  - *High cost*: payback exceeds product life
  - *Poor fire safety*: organic paraffin-based
  - *Intrusiveness; inaccessibility*: integrated into walls
  - *Low utilization*: only useful part of year, hurting economics
  - *Low demand impact*: PCM depleted by afternoon peak

Souayfane et al. (2016). “PCMs for cooling applications in buildings: a review.” *Energy and Buildings* v. 129, 396-431

Bland, et al. (2017). “PCMs for Residential Building Applications.” *Buildings*, v. 7, 78.

Challenge: Cost



Challenge: Technical Issues with Salt Hydrates

- Incongruent melting
  - Water/salt separation with repeated thermal cycling
    - Reduces thermal storage capacity over time
- Large supercooling
  - Unpredictable crystallization, delayed nucleation
    - Large temperature and volumetric fluctuations
- Low thermal conductivity
  - Slow thermal charging/discharging
- Corrosion
  - Liquid phase corrodes packaging
    - Shorten system lifespan
    - Alter chemical composition and thermophysical properties

Approach

Potential to transform energy storage:

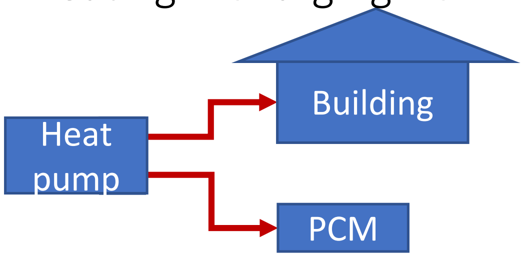
- Billions of dollars have been invested into R&D of electric battery technologies, including
  - As of 2015, nearly $2B from renewable energy
  - As of 2015, nearly $2B from automotive industries
  - From 2017 to 2030, Bloomberg New Energy Finance (2017) predicts that global investments in electrical energy storage will double *6 times*, with
    - $103B invested over this time period
    - $26B in the US
- By contrast, thermal energy storage has seen very little investment
- When this project is successful, a low cost PCM based on ORNL-developed IP can deliver energy storage services more cost effectively than electric batteries

Approach

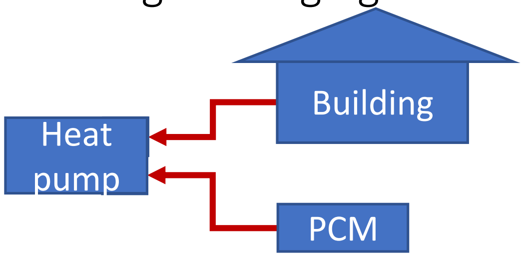
HVAC integration

- HVAC-coupled PCM storage allows a range of possible phase change temperatures to be used.
  - Increases annual utilization factor to improve economics
- Configurations have been modeled and evaluated in ORNL's Heat Pump Design Model (HPDM) software

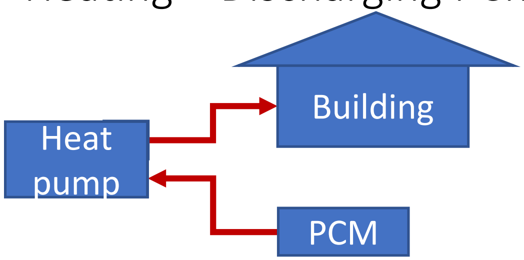
Heating – Charging PCM



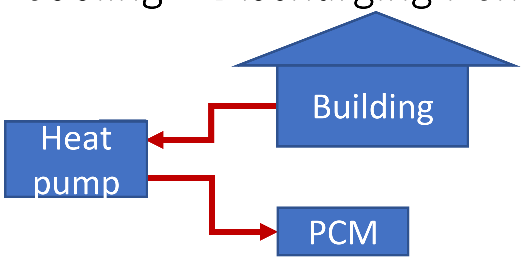
Cooling – Charging PCM



Heating – Discharging PCM

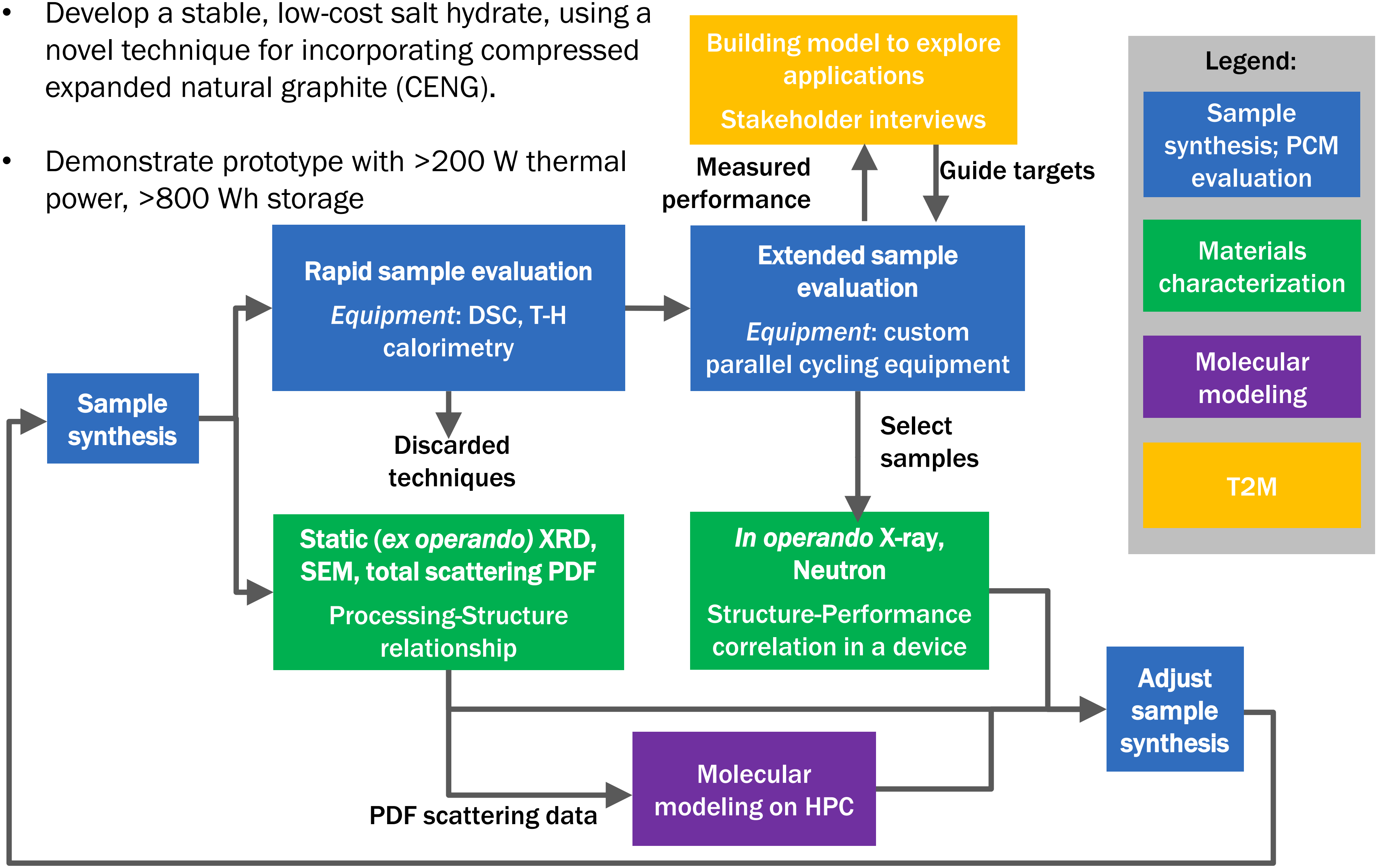


Cooling – Discharging PCM



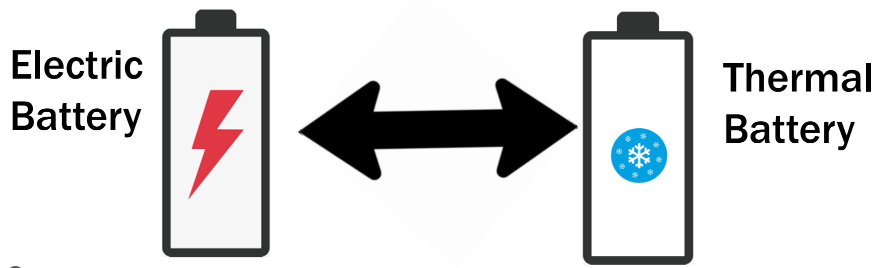
Approach

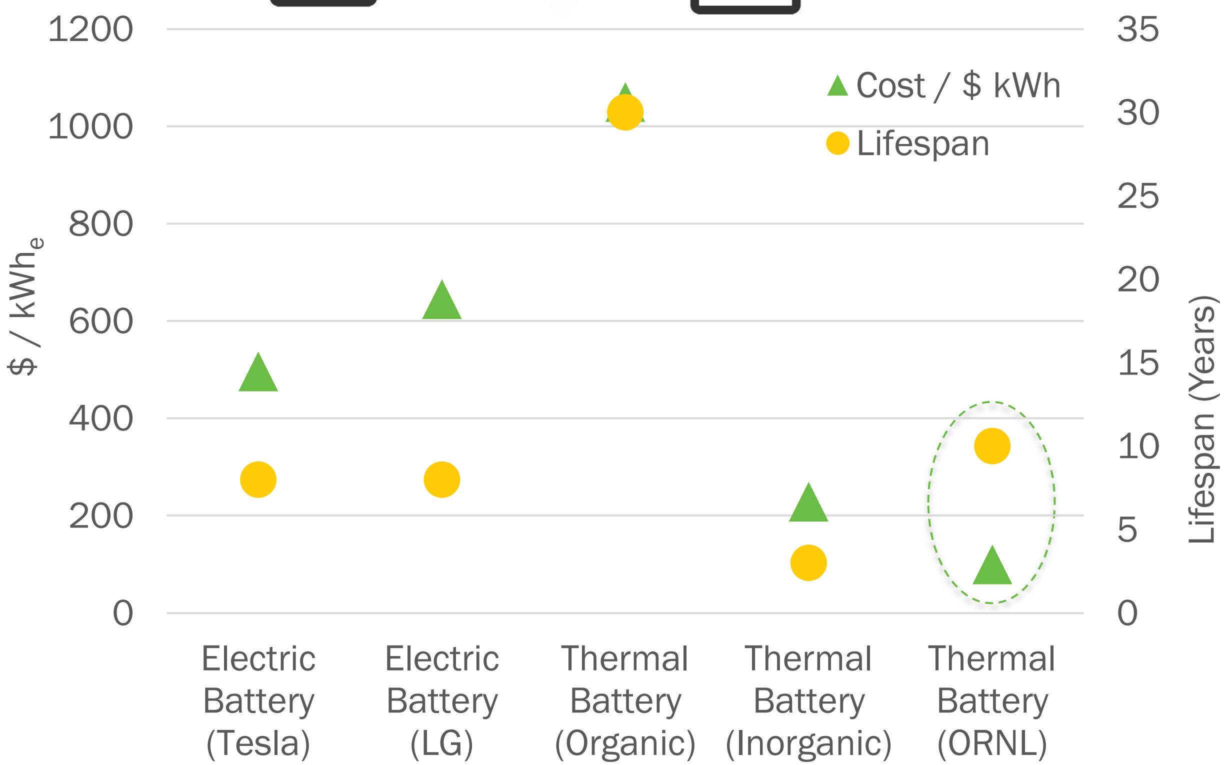
- Develop a stable, low-cost salt hydrate, using a novel technique for incorporating compressed expanded natural graphite (CENG).
- Demonstrate prototype with >200 W thermal power, >800 Wh storage



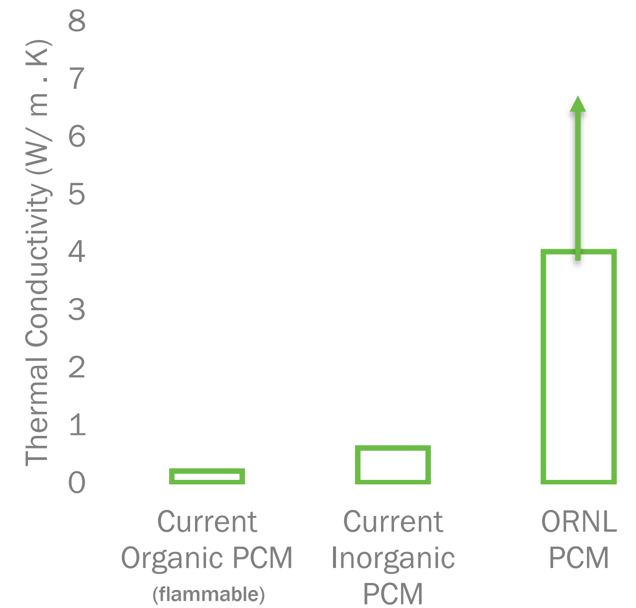
Impact

- When this project is successful, a low cost PCM based on ORNL-developed IP can deliver electric-equivalent storage more cost effectively than electric batteries





Computed for 5 kWh$_t$ = 1 kWh$_e$



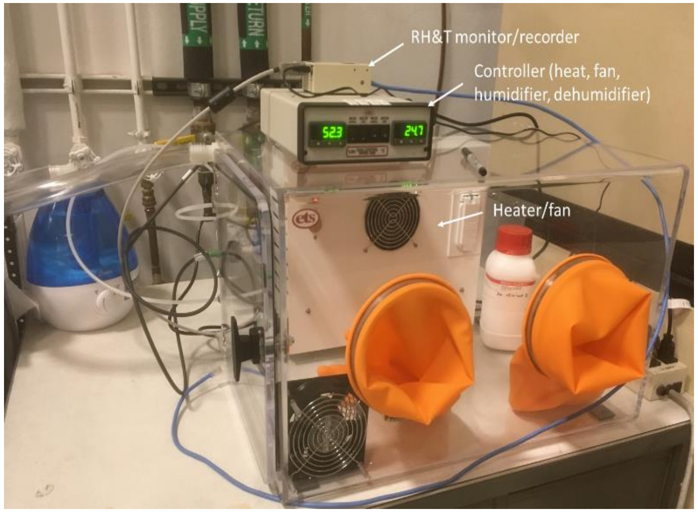
Project outcomes:

- *Demonstrate the stability >100 cycles and cost of PCM < $2/ kWh*
- Demonstrate prototype with >200 W thermal power, >800 Wh storage

Progress

Sample synthesis

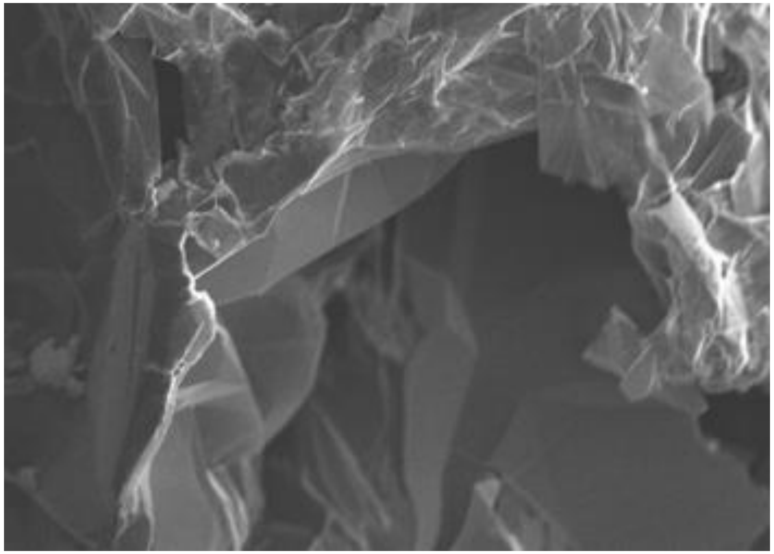
- Composite samples have been created
- Patent was filed on composition of matter and technique for creating it
- Sample handling procedure developed for XRD, SEM, and PDF evaluations



Humidity controlled glovebox for sample transfers

Compressed graphite-salt "puck" before sealing with water vapor impermeable film.

Graphite-salt composite packed in bag

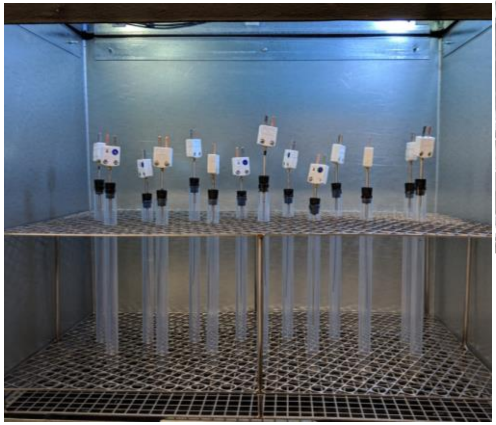


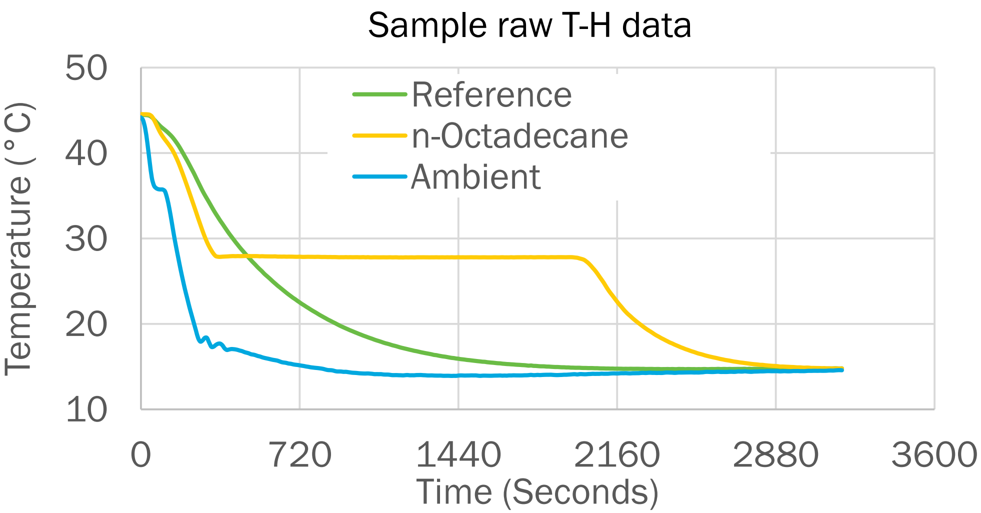
SEM image of composite sample

Progress

Temperature-history calorimetry

- Accelerated thermal cycling with in-situ temperature, latent heat, heat capacity measurement for PCMs.
- Accuracy ± 3–6% of latent heat.
- Large sample throughput
  - Simultaneous evaluation of up to 150 samples
  - 24/7 operation
- Temperature range: -20°C to 60°C



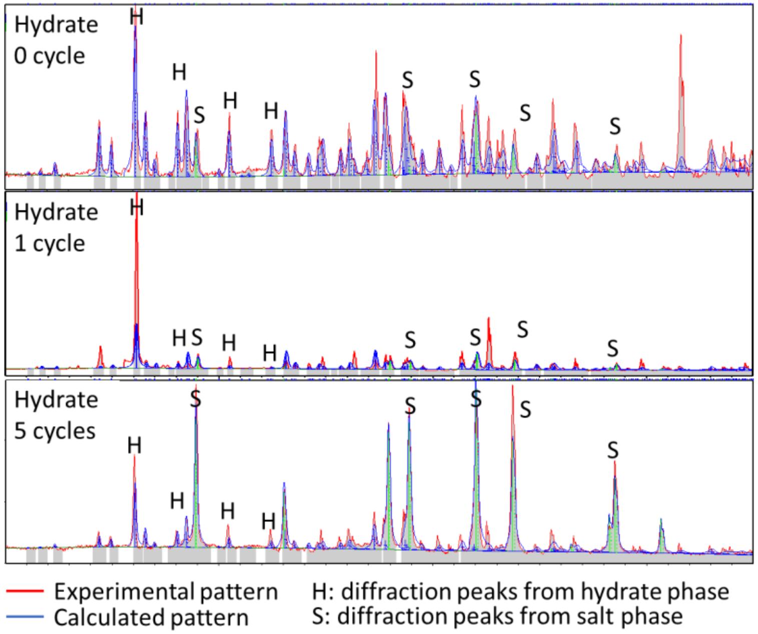


$$H_{fs} = \frac{m_W Cp_W + m_{tw} Cp_{tw}}{m_p} \frac{A_1}{A_1'} (T_0 - T_m)$$

Progress

XRD Characterization

- Rietveld method for quantitative phase analysis
- Thermal degradation with cycling
- New PCM degradation evaluation technique
- Outlines the degradation mechanism
  - By-product of degradation
  - Quantifies the rate of degradation



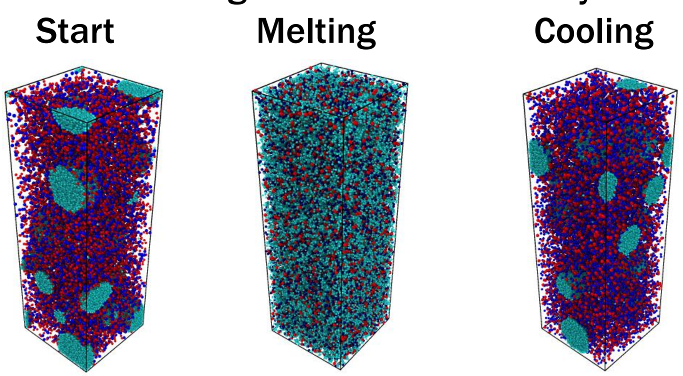
Sample	Pure hydrate		Composite 1		Composite 2		Composite 3		Composite 4	
	Hydrate	salt	Hydrate	salt	Hydrate	salt	Hydrate	salt	Hydrate	salt
Cycle-0	94.2	5.8	88.4	11.6	97.9	2.1	91.9	8.1	48.3	51.7
Cycle-1	86.7	13.3	59.8	40.2	92.4	7.6	1.3	98.7	7.6	92.4
Cycle-5	23.0	77.0	49.7	50.3	78.5	21.5	0	100	0.8	99.2

Progress

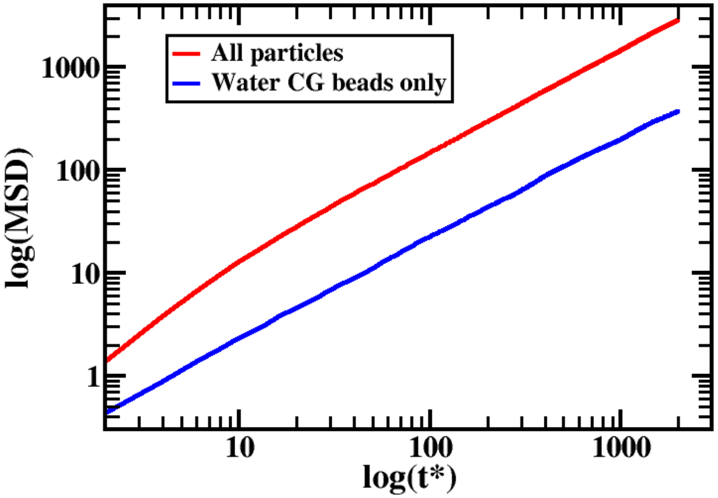
MD Simulation

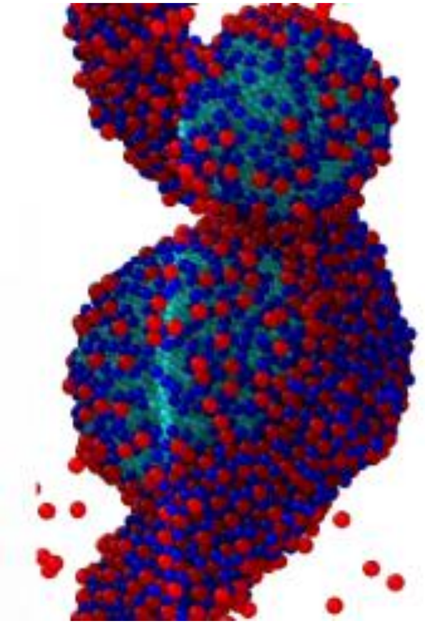
- Coarse–grain simulation of Na_2SO_4 + H_2O
- Understand the basic mechanism of phase-separation in the PCM
- Excellent phase separation under gravity and viscosity
  - Two phase separation: Hydrous and anhydrous

Phase Change structures in **78K** system



- 78K system vs. 28K System
  - Smaller system shows
  - Viscosity-dependent phase reversibility
- Ostwald ripening
  - Water motion is separate from all particles





Stakeholder Engagement: early stage project

- Multi-institution team

- **Outreach to potential industry partners**
  - Discussions held with **5 thermal storage companies**
  - Coordination established with **2 graphite suppliers**
  - Discussions ongoing with **3 HVAC OEMs**

Stakeholder Engagement (continued)

- **Inventions**
  - Jason R. Hirschey, Yuzhan Li, Tim Laclair, Anne Mallow, Kyle R. Gluesenkamp, Orlando Rios, Monojoy Goswami, and Samuel Graham (2019). *Composite thermal batteries: robust low-cost composite phase change energy storage with high transient power*. Oak Ridge National Laboratory Invention Disclosure 201804349. Provisional patent filed March, 2019.
  - Gluesenkamp, K.R., Tim LaClair, Jeffrey Munk, Jin Dong (2018). *Thermal storage system for residential space conditioning*. ORNL Invention Disclosure 201804095, DOE S-138,762.
- **Reports and Publications**
  - Manuscript submitted: "Review of Stability and Thermal Conductivity Enhancements for Salt Hydrates"
  - Monojoy Goswami, "Beyond petascale—HPC and polymeric materials design", presented to *American Physical Society March Meeting*, Boston, MA, March 3-8, 2019.
  - Jin Dong, Bo Shen, Jeffrey Munk, Kyle R. Gluesenkamp, Tim Laclair, and Teja Kuruganti (accepted). "Novel PCM Integration with Electrical Heat Pump for Demand Response," *IEEE Power & Energy Society General Meeting 2019*, Atlanta GA, August 4-8, 2019 (Accepted).
  - Three abstracts submitted to European Congress and Exhibition on Advanced materials and Processes (EUROMAT 2019).

Remaining Project Work

- Evaluate and publish different PCM characterization techniques, including:
  - Large scale parallel T-H calorimetry
  - XRD-based degradation
- Develop CENG-PCM and characterize on micro-level
- Perform technoeconomic analysis for applications
- Develop and characterize system prototype at the macro level

Thank You

Oak Ridge National Laboratory
Kyle R. Gluesenkamp, PhD
gluesenkampk@ornl.gov

REFERENCE SLIDES

Project Budget

Project Budget: $850k/yr, FY19-21
Variances: None
Cost to Date: $297k
Additional Funding: None

Budget History					
FY 2018 (past)		FY 2019 (current)		FY 2020 – FY 2021 (planned)	
DOE	Cost-share	DOE	Cost-share	DOE	Cost-share
0	0	$850k	0	$1700k	0

Project Plan and Schedule

Project Schedule												
Project Start: October 2018		Completed Work										
Projected End: September 2021		Active Task (in progress work)										
	◆	Milestone/Deliverable (Originally Planned)										
	◆	Milestone/Deliverable (Actual)										
	FY2019				FY2020				FY2021			
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												
Q2 Milestone 1: Characterization CENG-PCM												
Q2 Milestone 2: Three different CENG -PCM characterized and cycle and Review Paper of Salt Hydrate												
Current/Future Work												
Q4 Milestone 3: Preliminary technoeconomic analysis												
Q4 Milestone 4: Publish standard characterization												
Q4 Milestone 4: One Composite Evaluation (Go/No-Go)												
Q2 Milestone 5: Evaluation of milled + passivated material												
Q3 Milestone 6: Refine technoeconomic analysis												
Q4 Milestone 7: New material exploration												
Q4 Milestone 8: 50 W HX prototype fabraciated												
Q4 Milestone 4: One Composite Evaluation (Go/No-Go)												
Q1 Milestone 9: MD Simulations reported												
Q3 Milestone 10: Cycling and latent heat evaluation												
Q4 Milestone 11: Project Wrap Up												
Q4 Milestone 12: Scaled Up Prototype Evaluation												