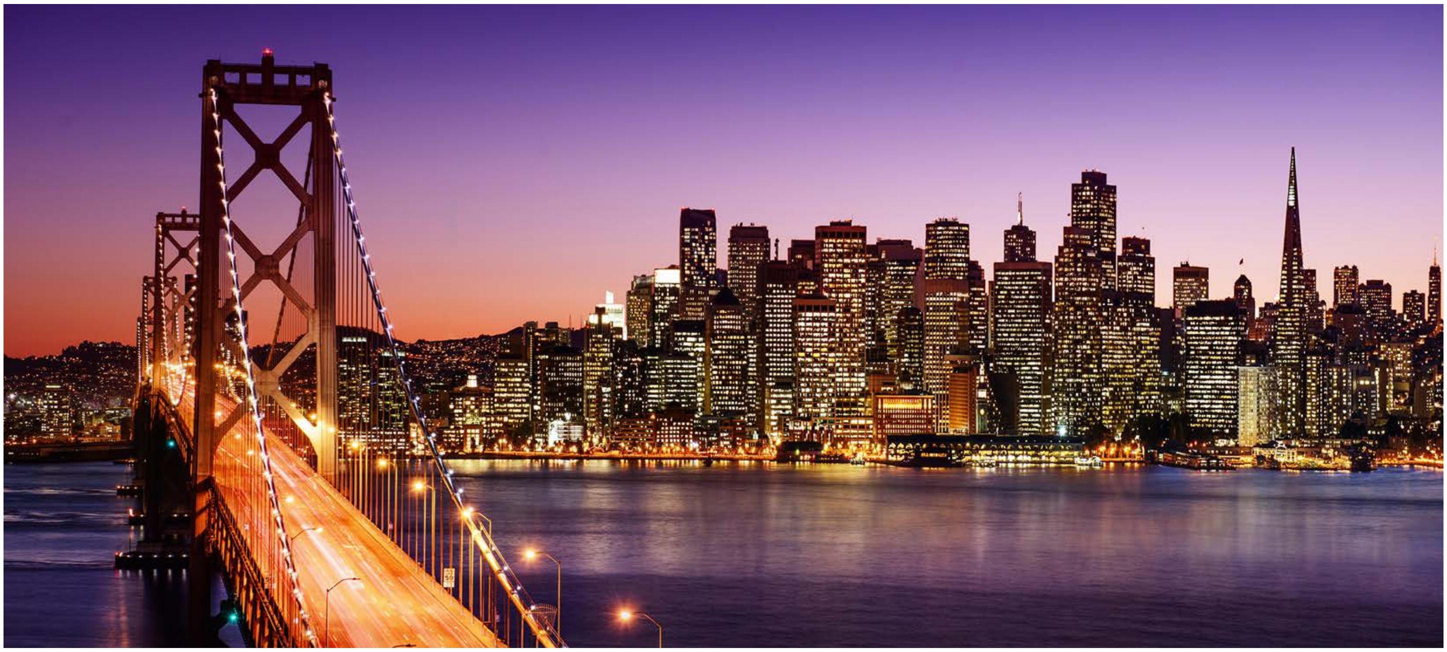

2019 Workshop on Fundamental Needs for Dynamic and Interactive Thermal Storage Solutions for Buildings

Sumanjeet Kaur,[1] Marcus Bianchi,[2] and Nelson James[3]

1 Lawrence Berkeley National Laboratory
2 National Renewable Energy Laboratory
3 Oak Ridge Institute for Science and Education

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June 2020

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Sumanjeet Kaur,[1] Marcus Bianchi,[2] and Nelson James[3]

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Acknowledgments

Thank you to all the invited speakers and participants in the 2019 Workshop on Fundamental Needs for Dynamic and Interactive Thermal Storage Solutions for Buildings. Their contributions, insights, and willingness to share their experiences about the use of thermal energy storage in buildings made the event successful.

We thank the breakout session leads, Gao Liu, Chris Dames, Judith Vidal, and Anubhav Jain, for facilitating discussions and documenting the findings. In addition, we thank Ravi Prasher and the Lawrence Berkeley National Laboratory (LBNL) for hosting the workshop in Berkeley. We thank Marie Butson for organizing the meeting and facilitating communication.

We also gratefully acknowledge the financial support from LBNL, which enabled us to organize and conduct this workshop.

List of Acronyms

CEC	California Energy Commission
DOE	U.S. Department of Energy
HVAC	heating, ventilating, and air conditioning
LBNL	Lawrence Berkeley National Laboratory
LCOS	levelized cost of storage
NREL	National Renewable Energy Laboratory
NSF	National Science Foundation
ORNL	Oak Ridge National Laboratory
PCM	phase change materials
R&D	research and development
TES	thermal energy storage

Executive Summary

The 2019 Workshop on Fundamental Needs for Dynamic and Interactive Thermal Storage Solutions for Buildings was held at Lawrence Berkeley National Laboratory (LBNL) in Berkeley, California, on November 19–20, 2019. The workshop convened 47 individuals involved in thermal, building, and materials science to present and discuss the use of thermal energy storage (TES) associated with buildings. The goals of the event were to revisit recent breakthroughs and identify future research opportunities in scientific areas related to:

1. Dynamically tunable thermal storage materials that can modify their switching temperature or characteristics to operate optimally in both summer and winter;
2. Thermal circuits elements (analogous to electrical circuits), diodes, switches, and transistors, which could control directional heat and mass transfer and thus provide management over the timing of charging or discharging;
3. Characterization tools and techniques to understand fundamental issues, such as supercooling, metastable phases, slow kinetics, and poor cyclability in TES materials; and
4. Expedite discovery of new materials using computational materials design for thermal energy solutions, combinatorial synthesis, and high throughput characterization.

The workshop comprised a half day of invited talks followed by breakout sessions. The invited talks reviewed the rationale for use of TES in buildings, presented a parallel with electrochemical storage and concentrating solar power thermal storage, and had discussions on materials discovery and characterization. The bulk of the workshop was spent in the breakout sessions where the workshop participants were split into four groups, which were identified to increase the competitiveness of TES technologies: (1) Efficiency; (2) Utilization; (3) Lifetime; and (4) Computational Discovery of Thermal Storage Materials. During the breakout sessions, participants were asked to identify Major Topics, Technological Barriers, Transformational Research Topics, Potential Science Impacts, and Impact on Energy Technology.

The first section of this report, based on Karma Sawyer's[1] invited talk, provides background for the use of TES in buildings. The main part of the report details the findings from the breakout sessions. A final section describes some of the recommendations based on the findings from the breakout sessions.

The workshop identified the following needs:

1. Methods to estimate TES efficiency
2. Effective ways to improve the utilization and flexibility of TES
3. Dynamic tunable storage integrated with thermal switches for better utilization, load flexibility, and integration with the grid
4. Removal of lifetime barriers that impact the performance of TES systems
5. Methods to accurately predict lifetime

[1] Program Manager of Emerging Technologies, Building Technologies Office, U.S. Department of Energy

6. Algorithms (e.g., machine learning) to better manage thermal storage assets and understand economic impacts of new storage technologies
7. Data sets to validate theoretical models or machine learning methods.

A consensus among attendees is the desire to create a larger effort with a consortium of national laboratories, universities, and other research organizations on TES.

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1 Introduction

This report presents the findings of the 2019 Workshop on Fundamental Needs for Dynamic and Interactive Thermal Storage Solutions for Buildings. The workshop was sponsored by and held at Lawrence Berkeley National Laboratory (LBNL) in Berkeley, California, November 19–20, and convened 47 experts in thermal, building, and materials sciences. The following sections detail the rationale, structure, and findings of the workshop.

2 Background

The electrical grid is facing significant transformations. What used to predominantly be a one-directional system, where centralized plants deliver power to end users, is rapidly evolving. As more variable renewable and distributed generation sources are integrated into the electrical grid, the difficulties of reliably matching supply and demand increase. Additionally, growing peak demand and transmission and distribution constraints are also stressing the electrical grid. Energy storage can play a key role in helping to balance supply and demand of electricity. Buildings consume nearly 75% of all the electricity generated in the United States and are responsible for a comparably significant portion of peak power demands (U.S. EIA 2019). Figure 1 displays the variation in end-use electrical consumption for residential and commercial buildings.

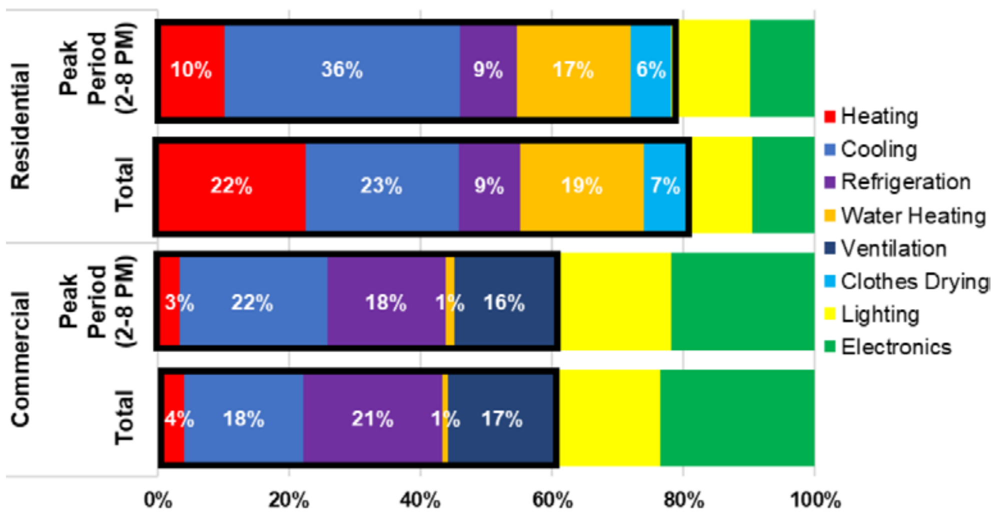

Figure 1. Variation in end-use electrical consumption during peak on off-peak hours for residential and commercial buildings

Figure from U.S. Department of Energy 2019

Many of the solutions that have been investigated for building energy storage have traditionally been thermal mass (e.g., adobe) or phase change (ice storage) and, more recently, electrochemical (e.g., batteries). Because 50% or more of the energy consumed in buildings can be for thermal end uses, thermal energy storage (TES) can also play an important role in facilitating a balanced energy system that is efficient, resilient, and affordable. Systems utilizing hot/chilled water, ice, or other materials have been sold commercially. While readily available, deployment of these traditional TES systems in buildings is still limited. For envelope-based systems, limited adoption is primarily because they charge and discharge passively in response to ambient temperatures and can only shift to off-peak hours either in heating or cooling modes, not both. More generally adoption is limited due to most phase change materials (PCMs) suffer from issues such as supercooling, broad transition temperatures, low energy density, poor heat transfer, degradation with cycling, and high prices. These problems collectively limit increased deployment of TES technologies.

In November 2019, LBNL and the National Renewable Energy Laboratory (NREL) cohosted a two-day workshop to explore ways to revolutionize TES technologies. For TES to make a more significant impact on the energy ecosystem, disruptive solutions are needed that enable control of charging and discharging, as well as address the major shortcomings of existing TES technologies. Stakeholders with a diverse range of expertise, from material science to system integration, participated to ensure recommendations would encompass solutions at all scales.

Batteries and TES technologies should not be looked at as competitors. Rather, they should be treated as complementary systems that can be optimized to work together to service building needs, help integrate distributed energy resources (see Figure 2 for a depiction), and provide services to the electrical grid. Batteries have several advantages from the ability to supply critical electrical loads to the constant price reductions born out of focused research efforts. Leveraging the extensive work that has gone into electrochemical energy storage, insights can be translated to aid TES technology development.

Four primary opportunity areas were identified for developments that are needed to increase the competitiveness of TES technologies. These consisted of capital cost reductions, as well as efficiency, utilization, and lifetime improvements.

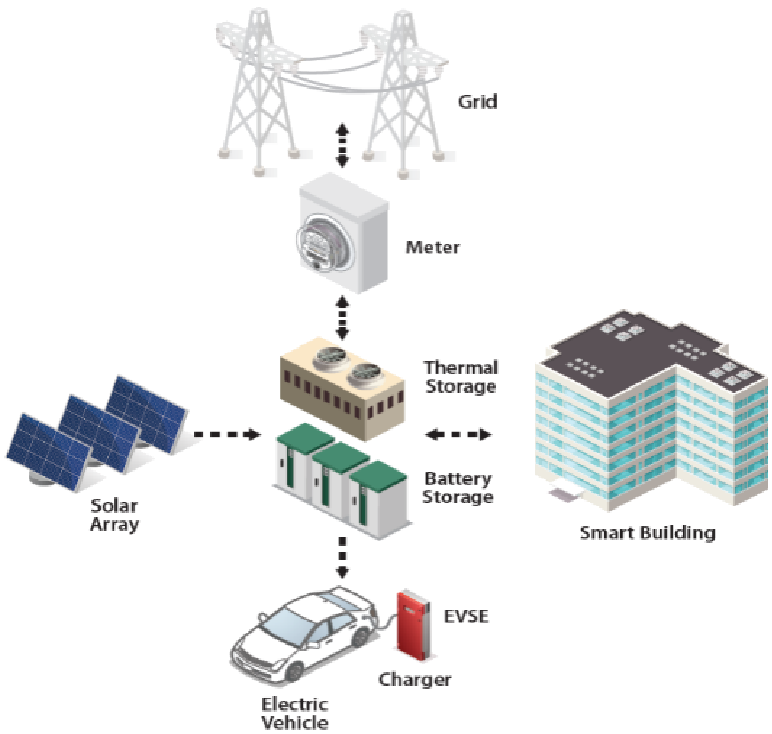

Figure 2. Depiction of integrated energy storage ecosystem
Figure by NREL

2.1 Capital Cost

Many TES approaches require large installations to achieve meaningful amounts of energy storage. This leads to increased capital cost due to increased storage materials as well as materials to house and insulate the storage medium. Water is the most abundant thermal storage material in use today due to its low cost and moderate energy density. Alternative materials have been explored for thermal storage, including various thermophysical- and thermochemical-based transformations. To reduce the size of storage installations, materials with both high energy and power densities for thermal storage are needed. Computationally guided discovery of new materials could aid in the identification of new molecules, materials, and chemistries with high energy density. Also, use of combinatorial synthesis and high throughput characterization for TES materials could expedite realization of these new materials.

2.2 Efficiency

Regardless of what materials are used for TES, some interface between the thermal storage material and the heat source or sink is necessary. As energy is transferred through different forms and across boundaries, losses occur. Thermal resistances and bridges can increase the amount of energy required to charge the storage medium, as well as reduce the energy and power delivery capacity of the thermal storage during discharge. Improved designs and materials may be needed to increase the overall round-trip efficiency of TES.

2.3 Utilization

When thermal loads are present, the increased ability to control when thermal energy is charged/discharged and at what temperatures this occurs can greatly increase the usefulness of thermal storage technologies. PCMs can store appreciable amounts of thermal energy. The phase transition of these materials typically occurs in a narrow band of temperatures. In most building applications, the PCM must be chosen such that it provides cooling or heating use. In much of the United States there is both a heating and cooling season. This means that at times of the year, when the temperature does not cross over the transition temperature range, the PCM is only storing energy in sensible form or a partially melted state. This translates to the storage medium not being fully utilized. Dynamically tunable thermal storage materials that can modify their switching temperature or characteristics to operate optimally in both summer and winter can significantly increase the utilization of the TES.

Another challenge to TES utilization is the fact that heat flows tend to occur through passive components with the primary means of control being inputs from devices controlled through electrical switches. A revolution in electrical devices occurred with the introduction of nonlinear components such as diodes and transistors. Thermal circuits elements (analogous to electrical circuits) diodes, switches, and transistors, which could control directional heat and mass transfer and thus provide management over the timing of charging or discharging, could lead to a paradigm shift in thermal energy utilization.

2.4 Lifetime

One of the most vital aspects of any investment in building technologies is that it must last for multiple years (ideally the lifetime of the building or equipment that the TES is integrated with). The longer the storage systems lasts, the more useful charge and discharge cycles the owner will get out of the investment. Though they still have their own degradation mechanisms, TES materials are believed to be able to outlast electrochemically based battery technologies. Use of new characterization tools and techniques to understand and solve the fundamental issues, such as the presence of non-equilibrium phases, slow kinetics, and poor cyclability in TES devices, can significantly improve the economics of these technologies.

3 Workshop Structure

The workshop was conducted over two days at LBNL. As discussed previously, four primary opportunity areas were identified for developments needed to increase the competitiveness of TES technologies. Breakout sessions were organized around these four topics:

1. Efficiency
2. Utilization
3. Lifetime
4. Computational Discovery of Thermal Storage Materials.

3.1 Participants

The organizers identified individuals from academia, industry, and research institutions, representing a large spectrum of areas that are directly or indirectly involved in TES research. Representatives from the U.S. Department of Energy (DOE), California Energy Commission (CEC), and the National Science Foundation (NSF) attended the workshop. The attendees have background in one of the following areas:

- Thermal storage
- Building science
- Nanoscale thermal transport
- Materials science
- Mechanical cooling and heating systems (heating, ventilating, and air conditioning [HVAC]).

Appendix B presents a list of the participants and their affiliation.

3.2 Invited Talks

On the first day, after the welcome from Mike Witherell (LBNL Director) and Ravi Prasher (LBNL Associate Director), a series of invited talks were delivered to establish the current state of the art and objectives of the workshop. Table 1 lists the subjects and speakers invited to present at the workshop.

Karma Sawyer started by setting the stage for the need of TES. Robin Goodhand presented the efforts by the CEC in energy storage. Robert Kostecki provided a historical perspective of electrochemical storage and how some of the lessons could be applied to TES research. Judith Vidal described the uses of TES in concentrating solar power. Anubhav Jain discussed the process of computational material discovery and how it could apply to TES materials. Kyle Gluesenkamp, Navin Kumar, and Eli Rotenberg all discussed characterization techniques for TES materials.

Table 1. Invited Talks Titles and Speakers

Title	Speaker
Scientific and Technological Challenges in Thermal Storage—Why are we here? Review of goals/objectives, challenges, research and development (R&D) needs, and opportunities	Karma Sawyer, Program Manager, Emerging Technologies, Office of Energy Efficiency and Renewable Energy, DOE
Energy Systems Integration and Energy Storage	Robin Goodhand, Electric Generation System Specialist, CEC
History of Electrochemical Storage	Robert Kostecki, Scientific Division Director, Energy Storage Group, LBNL
Evolution, Progress, and Challenges of Thermal Storage in Concentrated Solar Power	Judith Vidal, Group Manager, Building Energy Science, NREL
Computational Material Discovery	Anubhav Jain, Chemist Staff Scientist/Engineer, Applied Energy Materials Group, LBNL
Challenges with Current Characterization Techniques for Thermal Energy Storage Materials	Kyle Gluesenkamp, Senior R&D Scientist, and Navin Kumar, postdoctoral researcher, Oak Ridge National Laboratory (ORNL)
New Characterization Techniques for Thermal Energy Storage Materials	Eli Rotenberg, Senior Scientist, Program Lead Angle-Resolved Photoemission Spectroscopy (ARPES), Photon Science Operations, LBNL
NSF Perspective on Thermal Energy Storage	Ying Sun, Program Director, Thermal Transport Processes, Engineering/Chemical, Bioengineering, Environmental and Transport Systems (ENG/CBET), NSF

3.3 Breakouts

Marcus Bianchi and Sumanjeet Kaur briefly introduced the structure of the breakout sessions, creating teams in the following areas with the associated moderators (Table 2).

Table 2. Breakout Topics and Moderators

Topic	Moderator
Efficiency	Gao Liu, LBNL
Utilization	Chris Dames, UC Berkeley
Lifetime	Judith Vidal, NREL
Computational Discovery of Thermal Storage Materials	Anubhav Jain, LBNL

Based on their backgrounds, we created groups of participants for each breakout topic for the first two hours of discussions. While the moderators stayed with the same topics, in the second breakout meeting (one and a half hours), attendees were encouraged to change breakout topics to increase the generation of new concepts and ideas.

4 Breakout Session Key Findings

4.1 Efficiency

During the breakout sessions of both the first and second days, the groups discussed different aspects of efficiency. Here is a summary of the discussion.

4.1.1 How to Define TES Efficiency?

- How to connect microscale material properties measured by differential scanning calorimetry to bulk material properties?
- At which level should efficiency be defined? System level, materials plus encapsulation, or in a building installation?
- Is time scale important for measuring and defining the efficiency? Daily versus seasonal?
- Does power density need to be considered when defining efficiency?
- Does hysteresis need to be considered? How does hysteresis interplay with power impact the efficiency measurement?
- How does transition temperature range impact the efficiency?
- Should it be defined as life cycle efficiency (first cycle to last cycle)?
- What mathematical definitions should be used to define efficiency of TES?
- Need measurement standardization for the efficiency from micro to system levels to assist and stimulate the development of this area.

4.1.2 Findings

Table 3 shows the summary of results of this breakout session as organized by Dr. Gao Liu (moderator). Two major themes were discussed by the participants: interface thermal contact resistance and reversibility. Two critical highlights:

- The community needs a comprehensive standard in targets and measurement methods to better quantify the "building thermal efficiency." These definitions can help to bridge fundamental thermal science to the applied building efficiency. It is an important component to an applied oriented research program.
- More focused fundamental research needs to be performed on the understanding of thermal transport in composite materials and their interfaces and tune-able materials as such forward-looking directions.

Table 3. TES Efficiency: Major Topics, Technological Barriers, Transformational Research Topics, Potential Science Impacts, and Impact on Energy Technology

Major Topics	**Technological Barriers**	**Transformational Research Topics**	**Potential Science Impacts**	**Impact on Energy Technology**
Transport at Interfaces (Thermal and Mass)	1. Poor thermal and mass transport at interfaces 2. Lack of understanding of changes in contact areas and morphologies at interfaces with cycling and effect of these on transport 3. Lack of predictive models at system levels which incorporates interfaces and changes at interfaces 4. Difficult to generalize, as the transport has strong dependence on geometry.	1. Heat loss factor and transport at the interface 2. Impedance factors 3. Moisture and water in HVAC 4. Mechanical degradation 5. Contact and morphology 6. Thermal and mass transport.	1. Understand heat transport at the atomic and interface level 2. Move the knowledge level from ideal system to practical hybrid system, such as large scale and composite materials 3. Develop predictive mathematical models for the hybrid materials and system.	1. Improve efficiency 2. Controlled large-scale processing of the interface 3. Accurate prediction of the system performance in multiple length scale and in system level 4. Better overall control in the materials and system level.
Reversibility	1. Phase segregation of the thermal storage material 2. Need for better understanding of the phase evolution, namely the effect of rate of cooling and heating 3. Is it thermodynamically limited or kinetically limited process? 4. Lack of understanding of supercooling* at system level.	1. New strategies to control segregation 2. New chemistries to lower activation energy for thermochemical storage 3. Use of adaptive and dynamic controls to enhance reversibility 4. Nucleation control strategies to overcome supercooling 5. Need for in-situ cycling characterization 6. Experiments that allow accelerated cycling and	1. Reversibility of PCMs 2. Stability of materials under repeated thermal cycles 3. Thermal degradation mechanisms and prevention 4. Nucleation and supercooling at large scale.	1. At the large scale, allowing construction of the thermal storage system with predictive and long lifetime 2. At a device level, thermal diode and switch 3. Circular economy based on regeneration of the storage materials.

Major Topics	Technological Barriers	Transformational Research Topics	Potential Science Impacts	Impact on Energy Technology
		quantification of degradation and/or determination of degradation mechanisms in situ.		
Material Properties, for Example: Type of Storage (Sensible, Latent, Thermochemical), Transition Temperature Range, Hysteresis	1. Need for systematic material characterization and standard reporting of materials properties in literature 2. Can new scientific approaches yield step function changes in energy density? 3. Can hysteresis losses be minimized in PCMs to maximize round-trip efficiency?	1. Explore thermal storage including various thermophysical- and thermochemical-based transformations 2. Explore materials using computational methods to aid in the discovery of new TES materials, which have both high energy and power densities for thermal storage. A potential path to achieve this includes the design of new molecules/materials/chemistries with high energy density	Lead to the development of new materials	1. Accelerated materials discovery could be a game-changer for TES as it can significantly reduce the footprint of storage 2. Standardized reporting of materials properties will accelerate the research.

4.2 Utilization

Prof. Chris Dames moderated this session. The discussions during this breakout session can be grouped under the categories of temporal, such as tunable PCMs and thermal switch, spatial and crosscutting ideas, including complex optimization and codesign.

1. **PCM with tunable phase transition temperature**. High risk and fundamentally challenging, but high impact if successful. Probably many ways of attacking this problem (e.g., voltage-controlled phase change temperature).
2. **Thermal switches for building applications.** This is relatively difficult, especially from the perspective of plausible cost and scalability. For envelope integrated, the cost levels are quite challenging. Switching ratio and high off-state resistance are the leading technical challenges, along with cyclability. Can the interfacial thermal resistance be tuned to act as thermal switch? It remains to be seen if such ideas can be economically viable to achieve the metrics ultimately needed for buildings.
3. **Crosscutting**
    - **A. System-level modeling and complex optimization,** the co-design ideas. Need simple model building blocks to feed into the higher-level models. Can machine learning/artificial intelligence aspects be fruitful here?
    - **B. High throughput metrology seems important.** Also, this community might be ripe for some round-robin studies on relevant materials.
    - **C. Composites to enhance the effective thermal conductivity, diffusivity, of** TES
    - **D. Innovative business models** ("heating and cooling as a service")
    - **E. Human comfort and psychological aspects** (i.e., $T_{perceived}$ not equal to T_{actual}) are quite intriguing and worthy of research somewhere.

Table 4 shows the summary of results of this breakout session as organized by Prof. Chris Dames.

Table 4. Utilization: Major Topics, Technological Barriers, Transformational Research Topics, Potential Science Impacts, and Impact on Energy Technology

Major Topics	Technological Barriers	Transformational Research Topics	Potential Science Impacts	Impact on Energy Technology
Tunable Phase Transition Temperature (T_{PT})	1. PCM with dynamically tunable T_{PT} does not exist today 2. Can we generate enough enthalpy change (ΔH), or, more likely, entropy change (ΔS) from external stimuli to yield desirable (ΔT_{PT}) (i.e., 5-10°C)? 3. What are the possible control mechanisms to change the T_{PT} (pressure, electrical, thermal, magnetic, optical)? 4. What are the energy costs of applying the external stimuli? 5. How fast can we do it, and what is the optimal time scale? 6. Could tunable transitions lead to materials lifetime issues?	1. Identify the most plausible mechanisms to induce sufficiently large (ΔT_{PT}) (i.e., 5-10°C) 2. PCM with tunable ΔT_{PT} induced either autonomously adaptive to temperature and/or humidity or by the most suitable modes in the building settings (electrical?) 3. Identify allotropic materials with different phase transitions (e.g., α, β, γ phases) 4. Identify different phase change mechanisms (solid-solid, solid-liquid, and so on) 5. Minimize auxiliary components for T_{PT} control.	1. Since $\Delta T_{PT} = \Delta H/\Delta S$, fundamental question is how to tune and design to get desirable and tunable ΔT_{PT} 2. How narrow can be ΔT_{PT} 3. Lead to development of high-entropy alloys.	PCM with ΔT_{PT} can significantly increase the utilization of PCM across different time scales. For example, tunable PCM can be used both diurnal and seasonal (summer versus winter).
Thermal Switch	1. Lack of thermal switches with large switching ratio (5-10x) for buildings applications 2. Need for low thermal conductance at off state (for	1. All solid-state switches with low conductance at off state (air-like thermal conductivity) 2. Reliable (1,000 to 10,000 cycles),	1. Reduce the lower limit thermal conductivity in solids to yield air-like thermal conductivity	Efficient thermal switch can greatly enhance the utilization of TES and reduce the building energy load.

Major Topics	Technological Barriers	Transformational Research Topics	Potential Science Impacts	Impact on Energy Technology
	thermal insulation application in envelopes) 3. Need for high thermal conductance at on state (heat dissipation applications) 4. Need for optimization for cost, speed, efficiency (energy input for switch) 5. Building-compatible switching mechanism (electrical? mechanical? magnetic? optical?) 6. If using mechanical contacts, reliability of the contacts could be an issue. If all solid state, low conductance at off state is difficult for all-solid-state switches (amorphous limits thermal conductivity).	reversible thermal switches with high switching ratios (5-10x) with low enough conductance at off state or high enough conductance at on state; 3. Low cost thermal switching mechanism that is compatible with building environment 4. Highly reliable switches based on mechanical contacts? 5. Exploit existing materials with distinct thermal conductivities at different phases but narrower phase transition temperature range is needed with no hysteresis.	2. Highly reliable physical contact in mechanical switches mechanical contacts 3. New ways of heat transfer or engineered phase change temperature range with new structures.	
Spatial/Directional Control	1. Difficulty in defining the scale of spatial control 2. How to do spatial control for thermal services? 3. Long-range (>1 mile) transfer of heat because of being inherently entropically irreversible	1. How do you transport heat in chemical bonds? 2. How to quantify local perceived temperature? $T_{perceived} \neq T_{actual}$. 3. Multiscale solutions such as TES jacket hybrid with wall TES. Analogous in batteries	1. Materials development (high specific/latent heat, tunable k, all solid state) 2. Room temperature, transportable, directional heat distribution approaches	15%–20% energy savings already exists for localized heating in building [DELTA program in ARPA-E]. Potentially 90% energy savings if we had human space suit.

Major Topics	Technological Barriers	Transformational Research Topics	Potential Science Impacts	Impact on Energy Technology
	4. Quantification of the delivery of heat locally 5. Air as a heat-transfer fluid; energy density is the issue 6. Modularity and compactness are still challenging.	will be supercapacitor hybrid with Pb-acid 4. Transportable and noncontact heat delivery (Radiative heating/cooling and evaporative cooling for spatially controlled heating) 5. Induction for human body heating 6. Flexibility in activation and deactivation 7. Reduction of loss in the delivery of heat 8. Potential of extreme long distance (Use thermochemical materials for intercontinental heat storage and delivery, vaccine cooling).	3. Improve the effectiveness of delivery of heat/mass/photon for localized temperature control 4. Nonlinear thermal device for directional transport of heat (switch, diode, and so on).	
Hybrid Systems	1. Low-delta T electric generation efficiency 2. Need to decouple electric and thermal load/generation 3. Lack of quantifying potential 4. Lack of collaboration of materials and thermal researchers.	1. Ab-initio codesign of materials and systems 2. Equipment for heat pump and heat engine: Same or different? 3. New materials to enable low-dT high efficiency power generation	1. Need high-efficiency electric generation from low-grade sources 2. Hybrid thermal-electric improvements (not just “thermoelectric”)	1. Improve energy conversion efficiency 2. Full usage of energy. Reduce waste thermal energy.

Major Topics	**Technological Barriers**	**Transformational Research Topics**	**Potential Science Impacts**	**Impact on Energy Technology**
		4. Ripe for seedling scoping study.	3. New more efficient thermodynamic processes for thermal to electric generation.	
Thermal Storage Power Density	1. Low thermal conductivity 2. Trade-off between power and energy 3. Larger k_{eff}, D_{eff} --> larger pen. depth --> more effectively utilize the finite-thickness TES 4. Cost for increasing k.	1. Integration of TES into envelope to enable high power density 2. Integration of TES into HVAC&R to enable high power density 3. Linking envelope and HVAC integration 4. Optimization of power and energy density through material and HX design 5. On-demand delivery of thermal energy from TES.	1. How do we independently control specific heat and thermal conductivity? 2. Fill the knowledge gap of facilitating decoupled energy transfer and storage (Cp and k) 3. Shape-stable, high-k encapsulation of solid/liquid PCM.	1. Higher power density enables access of more energy, and potentially increase efficiency 2. Improved comfort and life quality by ensuring tight temperature control.
Co-Design (TES With System-Level Optimal Design)	1. Current paradigm in building thermal management does not consider codesign of TES with heat delivery or thermal management 2. Lack of available models on this relatively disruptive concept 3. Where to strategically locate the TES and delivery components?	1. Comprehensive modeling to consider codesign of TES and heat pumping/delivery—this seems to be a high TRL topic 2. Convert heat to other useful energy forms (electrical, chemical?) at high efficiency.	Convert heat to other useful energy forms (electrical, chemical?) at high efficiency.	Codesign could increase the utilization of TES because it can meet diverse thermal loads and could also accommodate various available thermal and other energy sources.

Major Topics	Technological Barriers	Transformational Research Topics	Potential Science Impacts	Impact on Energy Technology
	4. If there is excessive thermal energy with high quality (high temperature), how to economically recover it to electrical or other useful form of energy (chemical?).			

4.3 Lifetime

Dr. Judith Vidal moderated the sessions on lifetime.

Highlights:

- TES is composed of multiple constituents integrated in a system.
- Thermal media: solid, liquid, gas, mixtures?
- Containments: mitigating damage through self-healing behavior of containments.
- For building applications, there are different operating temperatures based on requirements.
- Thermal cycling conditions, frequency, and ΔT.
- TES type: sensible, latent, thermochemical. The last two require different phases going through transformations (phase change, chemical reaction) that require nucleation and growth of the new phase or product.
- Lifetime barriers are identified as those that will impact the performance of the system. How to accurately predict lifetime? Experiments versus modeling? What parameters should be used to determine lifetime? Impact on energy density and power density?
- Journal articles, technical reports should provide details about chemistry, impurity levels, volume, surface, particle size, surface tension, wettability, cooling rate, and so on.
- Cost-effective systems are needed for envelopes for retrofits and repairs. Expected envelope lifetime could be at least around 30 years. Expected HVAC lifetime could be between 10 and 20 years.[2]
- In multicomponent system, additives could help increase required self-healing reactivity once exposed to specific environments if a small rupture occurs in the system. Examples could be reaction with oxygen from atmosphere, or requiring curing using ultraviolet light.
- Retrofit panels are needed. Panels should be easy to handle, transport, and install. If cost-effective, they could be replaced every 10 years.
- Modular subcomponents in HVAC and refrigeration systems should be easy to repair or remove for reinstallation.

Table 5 shows the summary of results of this breakout session as organized by Dr. Judith Vidal.

[2] https://www.nrel.gov/docs/fy11osti/50572.pdf

Table 5. Lifetime: Major Topics, Technological Barriers, Transformational Research Topics, Potential Science Impacts, and Impact on Energy Technology

Major Topics	Technological Barriers	Transformational Research Topics	Potential Science Impacts
Subcooling[3]	1. Subcooling is unpredictable. Degree of subcooling depends on many variables (Purity of PCM, type of phase change—solid-liquid or solid-solid, and so on, system design).	1. Models predicting the max subcooling expected.	1. Reducing or eliminating subcooling will increase round-trip efficiency of the TES system. The following approaches could help in reducing the subcooling: -Similar bonds might increase effectiveness of new phase formation over available surface; -In solid-liquid phase change adjusting surface tension can increase wettability of new phase with available surface, thus enhancing nucleation probability; -Similar crystallography or lattice parameters of available surface with nucleating phase can improve nucleation, thus minimizing subcooling; and -Similarly, if surface charge helps increase attraction of elements in forming, phase nucleation can be enhanced. 2. Understanding of chemical degradation of surfactants,
	2. Makes use of inorganic salt hydrates, sugar alcohols, and pure polymer systems as TES difficult as typically the higher the purity the higher the degree of subcooling. 3. Transformation is delayed to lower temperatures, decreasing available latent heat.	2. In case of solid-liquid PCM: control and understanding of variables that are key to eliminate subcooling (i.e., wet well/low contact angle).	
	4. Observations at lab scale might be different at large scale. Determination of representative sample volume because some systems might not show it at large scale but at small scales.	3. Effect of impurities on nucleation level and chemistry 4. Can supercooling be controlled/designed for via low energy barrier metastable paths?	
	5. Subcooling degrades exergy because of presence of liquid in nonequilibrium thermal state	5. Demonstrate efficiency of: (1) hosting matrices; (2) encapsulation; (3) walls of container; and (4) nucleating agents	
	6. Lack of model to accurately predict subcooling at system level 7. Absence of understanding of nucleation parameters for multiscale modeling of PCMs 8. Lack of understanding of polymorphs and effect of cooling rate on their formation	6. Effect of surfactants on increasing available effective surface for nucleation 7. Effect of volume and system design on subcooling degree	

[3] While subcooling is usually perceived as part of utilization and efficiency, it was discussed in this breakout and the findings are also captured here.

Major Topics	Technological Barriers	Transformational Research Topics	Potential Science Impacts
	9. Absence of understanding of thermal conductivity impacting subcooling degree 10. Lack of understanding main mechanisms for nucleating agents and surface impact. Effect of chemistry, surface charge, surface morphology, crystallography, lattice parameter, surface energy, contact angle, available active area.	8. Effect of cooling rate 9. Effect and control of incomplete melting on subcooling by the presence of previous unmelted regions. Can other methods trigger nucleation?	available surfaces, or nucleating agents will help determine lifetime of system 3. If subcooling does not reduce latent heat and can be controlled, could help tune when the transition is needed.
Phase Segregation	1. Decrease of energy density due to phase segregation. Steep composition gradients, and stratification in multicomponent systems reduce thermal energy transfer. 2. Decrease in energy stored and released because of incomplete reaction (latent and thermochemical TES). Physical contact among reactants is minimized. 3. Thermal cycling can increase phase segregation. 4. Energy capacity reduction 5. If components have very different densities, slow cooling rates might increase phase segregation. 6. Phase stratification with time is highly feasible in multicomponent polymer systems having different densities and melting points.	1. Confining reactant's space (controlling volume) to minimize diffusion length. Example: host porous matrices and encapsulation. 2. Understanding nucleation and growth kinetics to determine minimum diffusion length needed for given systems. 3. Careful system design and modeling to determine and mitigate occurrence, severity, and impact of phase segregation. 4. Reliable accelerated testing emulating real operating conditions.	1. Reliable models with representative control volume can accurately predict lifetime when phase segregation is controlled. 2. Accurate data collection allows small amount of reliable data collected. 3. Controlled experiments with real operating conditions can produce accurate results. 4. Keeping main degradation mechanisms active during evaluation can help determine real degradation mechanisms. 5. Determination of synergy among degradation mechanisms can help understand impact on lifetime.

Major Topics	Technological Barriers	Transformational Research Topics	Potential Science Impacts
Mass Changes	1. Mass changes (loss/gain) degrade energy density (e.g., high vapor pressure phases). 2. Mass leakage reduce energy density by decreasing extent of reactions. 3. Phase solubility and dilution can decrease energy density.	1. Design at the material and system level to confine phases and control mass losses/gain. 2. Have excess of the reactants with high vapor pressure (e.g., addition of extra water in hydrate systems above the stoichiometric value to account for mass loss).	1. Closed systems can eliminate mass loss/gain and thus eliminate concerns of energy density decreasing. 2. In hydrate systems, water addition control can mitigate detrimental effect on energy density and thus on lifetime. 3. Volumetric control at both at material and system levels can mitigate detrimental impact of stresses on lifetime.
Volume Changes	Volume change during phase transition or reaction can generate stresses that might produce mechanical failure of hosting matrix or encapsulating material (shell).	Accommodate volumetric changes by incorporating control design of available space for TES materials.	
Phase Decomposition	Thermal decomposition of materials degrades energy density.	Selection and synthesis of stable materials	
Corrosion	Chemical degradation of containment materials (e.g., paraffin wax can react with some concrete components, and salt hydrates are very corrosive to metallic systems).	1. Materials selection 2. Control of atmosphere 3. Corrosion Inhibitors 4. Redox control to decrease corrosion rate 5. Surface passivation of corroding material 6. Coatings.	Controlling and mitigation corrosion extends lifetime of system.

4.4 Computational Aspects

Two broad computational aspect themes emerged:

1. How can improvements in materials modeling, along with parallel improvements in synthesis and characterization, be leveraged to develop and improve thermal battery materials?
2. How can we develop algorithms (e.g., machine learning) to better manage thermal storage assets and their quirks, as well as understand economic impacts of new storage technologies?

A common hurdle also emerged—the need for community data to validate computer models.

Table 6 shows the summary of results of this breakout session as organized by Dr. Anubhav Jain.

Table 6. Computational Aspects: Major Topics, Technological Barriers, Transformational Research Topics, Potential Science Impacts, and Impact on Energy Technology

Major Topics	Technological Barriers	Transformational Research Topics	Potential Science Impacts	Impact on Energy Technology
Computational Discovery/Materials Modeling	1. Need for data sets to validate methods, whether that is theoretical models or machine learning methods 2. Lack of dedicated funding for data set generation 3. "ImageNet" for thermal sciences—or "Thermal Materials Genome" 4. Lack of high-throughput synthesis opportunities 5. Use Natural Language Processing to assist? 6. Need multiscale modeling methods to integrate work from different theories all the way to building scale.	1. Ability to use computational screening to accelerate experimental work 2. What can be efficiently modeled, and what is better to simply perform experiments on (e.g., can we screen the space of salt hydrates/dehydrogenation reactions/organic PCMs computationally)? 3. Investigate the kinetics of thermal storage via a suite of computational methods.	1. Basic research into modeling surface processes/surface adsorption—important to nanofluids 2. Basic research into modeling heterogeneous catalysis to promote nucleation in PCMs 3. Modeling of reaction kinetics 4. Ability to help characterize 3D structure of thermal storage materials (e.g., as a function of cycling) 5. Predict and prevent degradation mechanisms.	1. More efficient use of research resources 2. Decouple data collection and method development/algorithm development 3. Accelerated design of novel materials solutions to thermal energy problems 4. Improved ability to diagnose and fix issues in current materials solutions.
Better Managing Thermal Technology Materials	Data sets to train and validate algorithms and models for thermal technology management (e.g., experimental data on deployed systems or prototype systems).	1. Application of machine learning to control thermal management systems 2. Prevent need for undercooling (e.g., stop before fully melt)	1. Can guide the development of what types of thermal technologies are most needed 2. Tunable phase change temperature? 3. Reduced degradation?	1. More efficient use of thermal batteries 2. More accurate economic estimates of Levelized Cost of Storage (LCOS).

Major Topics	Technological Barriers	Transformational Research Topics	Potential Science Impacts	Impact on Energy Technology
		3. Degradation management 4. Ability to integrate potential next-generation tech into building modeling software (thermal switches, dynamically tunable PCM, novel materials with exotic properties).	4. Reduced need for undercooling? 5. Improved kinetics? 6. Guide the science so we don't end up focusing on unneeded technologies.	

5 Recommendations

After going over the discussion points in each breakout session, we identified the following recommendations:

1. Convene a team of researchers to create a common definition of TES efficiency;
2. Determine methods to estimate TES efficiency;
3. Determine effective ways to improve the utilization of TES;
4. Develop cost-effective and reliable PCMs (solid-liquid, solid-solid) and insulation materials with dynamic properties to enable tunable storage and thermal switches;
5. Improve the effectiveness of heat and mass transport to enable improved spatial and directional control of thermal energy;
6. Investigate methods to improve nucleation of phases when PCMs are used for TES;
7. Control segregation of phases when PCMs are used for TES;
8. Explore ways to screen the space of salt hydrates/dehydrogenation reactions/organic PCMs computationally;
9. Develop algorithms (e.g., machine learning) to better manage thermal storage assets and understand economic impacts of new storage technologies;
10. Develop data sets to validate theoretical models or machine learning methods; and
11. A more general recommendation is to create a larger effort with a consortium of national laboratories, universities, and other research organizations on TES.

6 References

U.S. Energy Information Administration. 2019. Annual Energy Outlook 2019. "Reference Case Simulations." Washington, D.C. https://www.eia.gov/outlooks/aeo/.

U.S. Department of Energy. 2019. *Grid-interactive Efficient Buildings Technical Report Series: Heating, Ventilation, and Air Conditioning (HVAC); Water Heating; Appliances; and Refrigeration.* Washington, D.C. https://www1.eere.energy.gov/buildings/pdfs/75473.pdf.

Appendix A—Agenda

Workshop on Fundamental Needs for Dynamic and Interactive Thermal Storage Solutions for Buildings

LBNL, Berkeley, California

November 19–20, 2019

Bld. 50 Auditorium

Table A-1. November 19: 8 a.m.–5:30 p.m.

8:00 a.m.	**Registration** One Cyclotron Road, 50 Auditorium, Berkeley, CA 94720	
8:30 a.m.	**Welcome (LBNL)**	Mike Witherell, Lab Director, LBNL
8:40 a.m.	**Invited Talk: Scientific and Technological Challenges in Thermal Storage (DOE)** *Why are we here? Review of goals/objectives, challenges, R&D needs, and opportunities*	Karma Sawyer, Program Manager for Emerging Technologies, DOE
9:10 a.m.	**Invited Talk: Role of Thermal Storage in Zero Net Energy Buildings (CEC)**	Robin Goodhand, CEC
9:30 a.m.	**Invited Talk: History of Electrochemical Storage**	Robert Kostecki, Scientific Division Director, Energy Storage Group, LBNL
9:50 a.m.	**Networking Break**	
10:40 a.m.	**Invited Talk: Evolution, Progress, and Challenges of Thermal Storage in Concentrated Solar Power**	Judith Vidal, Group Manager, Building Energy Science, NREL
11:00 a.m.	**Invited Talk: Computational Material Discovery**	Anubhav Jain, Staff Scientist, LBNL
11:20 a.m.	**Invited Talk: Challenges with Current Characterization Techniques for Thermal Energy Storage Materials**	Kyle Gluesenkamp and Navin Kumar, ORNL
11:40 a.m.	**Invited Talk: New Characterization Techniques for Thermal Storage Material**	Eli Rotenberg, LBNL
12:00 p.m.	**Framing Discussion for Breakout Sessions** *Discuss the flow of the day.* *Expected outcomes*	Organizers (Suman and Marcus)

12:10-1:00 p.m.	**Innovation Approach and the Intersection of Materials Science, Measuring Science, and Integration Science** Working Lunch	Discussions with Ravi Prasher (Associate Lab Director, LBNL) and Roderick Jackson (Lab Program Manager, NREL*)*
1:00-3:00 p.m.	**Breakout A: Efficiency** *Location: 50-Auditorium*	Moderator: Judith Vidal
	Breakout B: Utilization *Location: 50A-5132*	Moderator: Chris Dames, Prof. of Mech Engineering, UC Berkeley
	Breakout C: Lifetime *Location: 70A-3377*	Moderator: Gao Liu, Group Leader for Applied Energy Material
	Breakout D: Computational Discovery of Thermal Storage Materials *Location: 70-191*	Moderator: Anubhav Jain
3:00 p.m.	**Networking Break** *Location: 50-Auditorium*	
4:00-5:30 p.m.	**Continuation of Breakout Sessions**	
5:30 p.m.	**Wrap Up/Adjourn**	
5:45 p.m.	**Travel to No-Host Dinner**	

Table A-2. November 20: 8 a.m.–12:30 p.m.

Bld. 50 Auditorium

8:00 a.m.	**Overview of Day 1** *Location: 50-Auditorium*	
8:10 a.m.	**Invited Talk: NSF Perspective on Thermal Energy Storage**	Ying Sun, Program Director, Thermal Transport Processes (ENG/CBET), NSF
8:30-9:30 a.m.	**Breakout A: Efficiency** *Location: 50-Auditorium (Left Corner)*	Moderator: Judith Vidal
	Breakout B: Utilization *Location: 50B-2222*	Moderator: Chris Dames, Prof. of Mech Engineering, UC Berkeley
	Breakout C: Lifetime *Location: 50-Auditorium (Right Corner)*	Moderator: Gao Liu, Group Leader for Applied Energy Material
	Breakout D: Computational Discovery of Thermal Storage Materials *Location: 70-191*	Moderator: Anubhav Jain
9:30-10:00 a.m.	**Break**	
10:00 a.m.	**Main Technical Findings, Roadmap from Breakout A** *Location: 50-Auditorium*	
10:35 a.m.	**Main Technical Findings, Roadmap from Breakout B** *Location: 50-Auditorium*	
11:10 a.m.	**Main Technical Findings, Roadmap from Breakout C** *Location: 50-Auditorium*	
11:45 p.m.	**Main Technical Findings, Roadmap from Breakout D** *Location: 50-Auditorium*	
12:20 p.m.	**Closing Remarks**	
12:30 p.m.	**Adjourn**	

Appendix B—Participants

Table B-1. List of Participants Who Attended the Workshop

Participant	Affiliation	Participant	Affiliation
Terry Andrews	CALMAC Corporation	Anubhav Jain	LBNL
Nick AuYeung	Oregon State University	Nelson James	DOE
Rohini Bala Chandra	University of Michigan	Sumanjeet Kaur	LBNL
Debjyoti Banerjee	Texas A&M University	Robert Kostecki	LBNL
Marcus Bianchi	NREL	Navin Kumar	ORNL
Kaushik Biswas	ORNL	Jaeho Lee	UC Irvine
Van Carey	UC Berkeley	Like Li	Mississippi State University
Dhanesh Chandra	University of Nevada, Reno	Gao Liu	LBNL
Chien-Hua Chen	Advanced Cooling Technologies, Inc.	Sven Mumme	DOE
Renkun Chen	UC San Diego	Wale Odukomaiya	NREL
Jinxing Chen	UC Riverside	Mary Ann Piette	LBNL
Chris Church	Applied Research Associates	Ravi Prasher	LBNL
Jun Cui	Ames Laboratory	Vi Rapp	LBNL
Chris Dames	UC Berkeley	Eli Rotenberg	LBNL
Spencer Dutton	LBNL	Thomas Russell	LBNL
Nicola Ferralis	MIT	Karma Sawyer	DOE
Srinivas Garimella	Georgia Tech	Som Shrestha	ORNL
David Ginley	NREL	Ying Sun	NSF
Adam Gladen	North Dakota State University	Rajeev Surendran Assary	Argonne National Laboratory
Kyle Gluesenkamp	ORNL	Paulo Cesar Tabares Velasco	Colorado School of Mines
Robin Goodhand	CEC	Judith Vidal	NREL
Shan Hu	Iowa State University	Jialai Wang	The University of Alabama
Yongjie Hu	UCLA	Jason Woods	NREL
Roderick Jackson	NREL		

Appendix C—Invitation Sent to Prospective Participants

We prepared and sent the following message to prospective participants starting in August 2019.

Dear Invitee:

We are pleased to invite you to the Workshop on Fundamental Needs for Dynamic and Interactive Thermal Storage Solutions for Buildings, jointly organized by Lawrence Berkeley National Laboratory (LBNL) and the National Renewable Energy Laboratory (NREL), to take place on Nov 19-20 in Berkeley, CA. Details are provided below.

As space is limited, your confirmation of attendance will be greatly appreciated. Please complete the online registration for the workshop at https://sites.google.com/lbl.gov/buildingsworkshop/. Please contact us if you have any questions. We look forward to hearing from you and hope that you will be available to participate in the event.

Best Regards,

Sumanjeet Kaur (LBNL) and Marcus Bianchi (NREL)

Workshop on Fundamental Needs for Dynamic and Interactive Thermal Storage Solutions for Buildings

Driven by the deployment of variable renewable energy capacity at a large scale, energy storage systems have turned into an important element to supply on-demand electricity. Most existing energy storage solutions are electrochemical (batteries) or electromechanical (flywheels, pumped storage). In buildings, since 50% of the energy consumed is for thermal end uses, TES can also play an important role in facilitating a balanced energy system that is efficient, resilient, and affordable. While readily available, deployment of traditional latent energy thermal storage in buildings is still limited primarily because it charges and discharges passively in response to ambient temperatures and it can only shift to off-peak hours either in heating or cooling modes, not both. Additionally, most PCMs suffer from issues such as supercooling, broad transition temperatures, low energy density, poor heat transfer, degradation with cycling, and high prices. All these problems collectively make existing TES inefficient and expensive. ***Therefore, it is imperative to develop truly disruptive thermal storage solutions that enable control of charging and discharging and address the major shortcomings of existing technologies.***

Lawrence Berkeley National Laboratory and the National Renewable Energy Laboratory are inviting a group of researchers with backgrounds in materials science, thermal science, building science, electrochemistry, and organic chemistry to discuss and investigate dynamic and interactive TES solutions and its adjacent systems for building applications. Program managers from DOE and CEC will participate in the workshop.

The aim of the workshop is to revisit recent breakthroughs and identify future research opportunities in scientific areas related to:

1. **Dynamically tunable thermal storage materials** that can modify their switching temperature or characteristics to operate optimally in both summer and winter
2. **Thermal circuits elements** (analogous to electrical circuits) diodes, switches, and transistors, which could control directional heat and mass transfer and thus provide management over the timing of charging or discharging
3. **Characterization tools and techniques** to understand fundamental issues such as supercooling, non-equilibrium phases, slow kinetics, and poor cyclability in TES materials
4. **Expedite discovery of new materials** using computational materials design for thermal energy solutions, combinatorial synthesis, and high throughput characterization.

Additional details will follow as we finalize the agenda of the workshop.

Sincerely,

Organizers

Lead: Sumanjeet "Suman" Kaur (LBNL) and Marcus Bianchi (NREL)

Support: Ravi Prasher (LBNL), Roderick Jackson (NREL) and Judith Vidal (NREL)