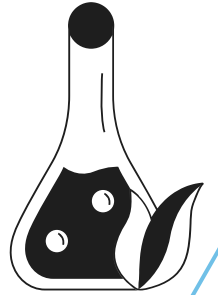
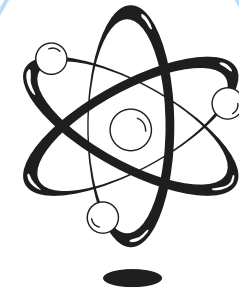
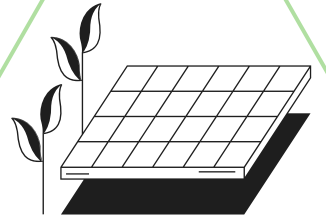


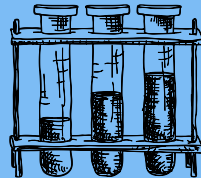
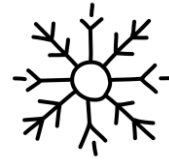
A THERMODYNAMIC JOURNEY: Unlocking Cold Thermal Energy Storage with Phase Equilibrium Studies

Maria C. M. Sequeira, Bernardo A. Nogueira, Timur Nikitin, Fernando J. P. Caetano, Hermínio A. P. Diogo, João M. N. A. Fareleira, Rui Fausto



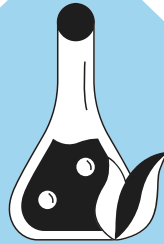
Thermal Energy Storage (TES)

- Energy Efficiency
- Supply-Demand Balance



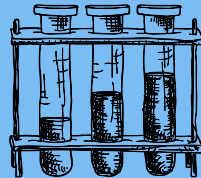
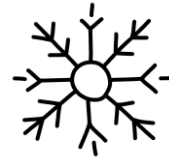
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Phase Change Materials (PCM)

- High latent heat capacity
- Reversible transitions



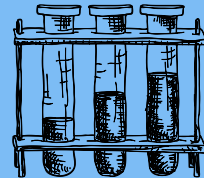
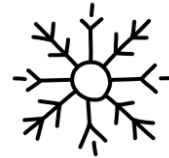
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The challenge of Designing PCM:

- Reliable and Efficient
- Environmentally Safe

Thermal Energy Storage (TES)

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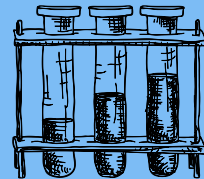
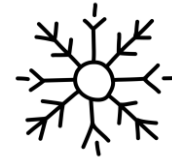


The challenge of Designing PCM:

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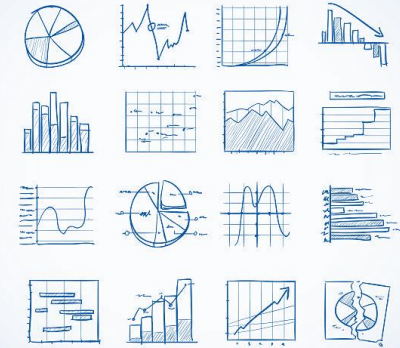
Phase Change Materials (PCM)

- High latent heat capacity
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Phase Equilibrium Studies on organic PCM for designing low-Temperature TES systems

Phase Equilibrium Studies to Unlock TES⁶



Thermal
Energy
Storage
Design

Differential Scanning Calorimetry (DSC)

Thermal Analysis

Hot Stage Microscopy (HSM)

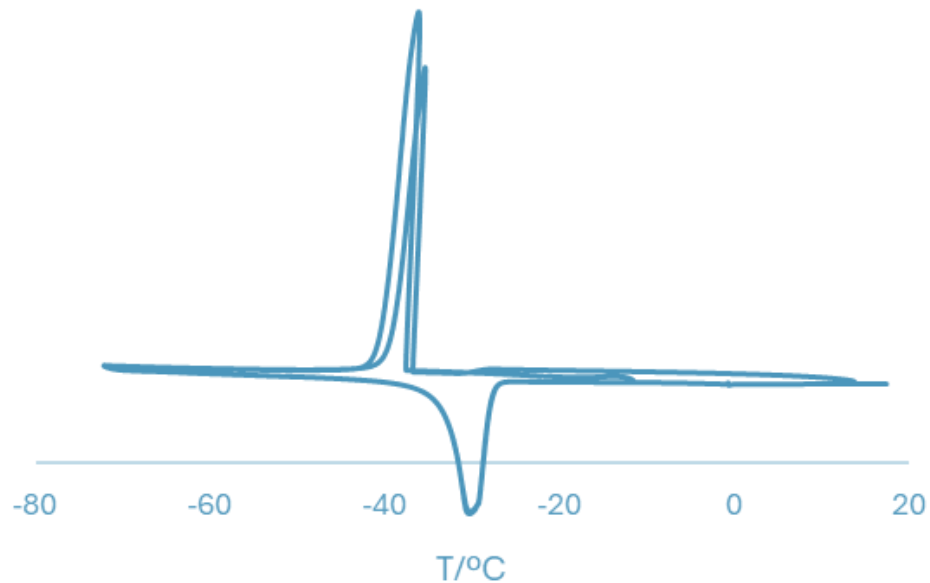
**Microscopic
Analysis**

Raman Spectroscopy

**Spectroscopic
Analysis**

Differential Scanning Calorimetry (DSC)

Thermal Analysis



- **Temperature** and **enthalpy** of phase transition

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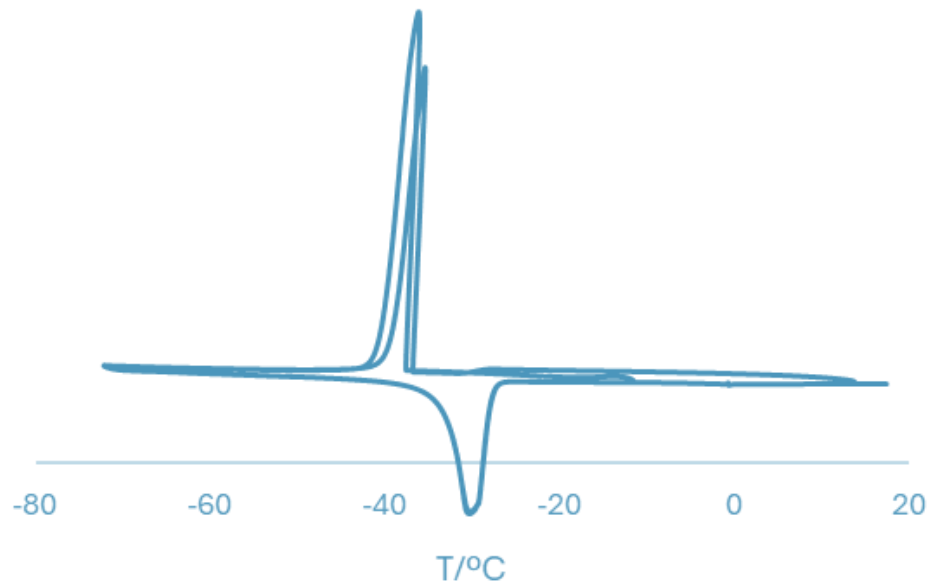
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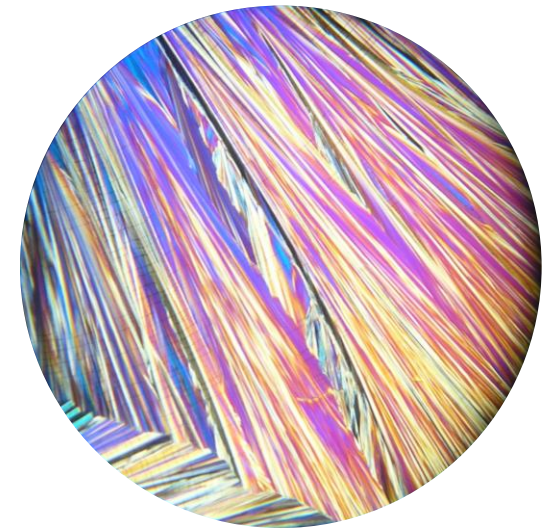
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Microscopic Analysis



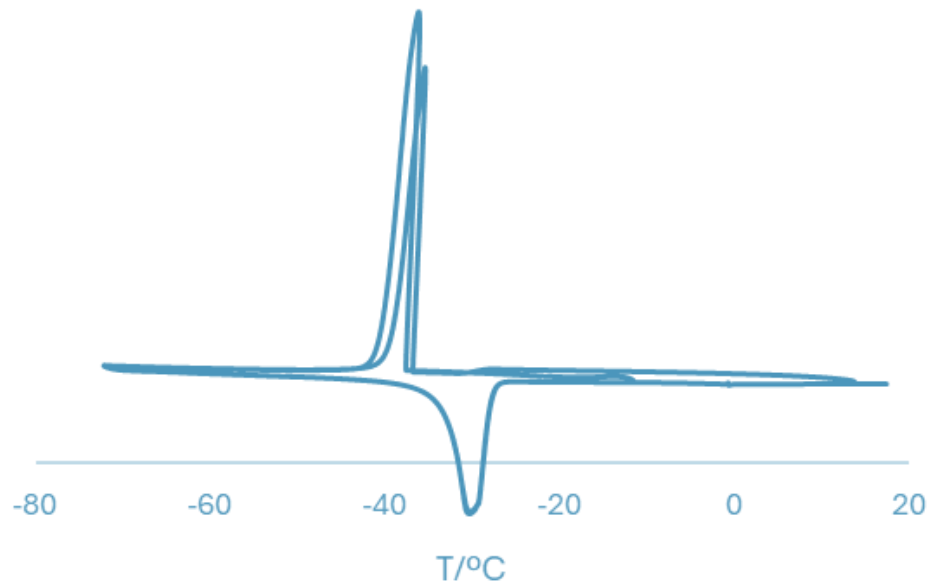
- Real-time **visual evidence** of thermal events

Raman Spectroscopy

Spectroscopic Analysis

Differential Scanning Calorimetry (DSC)

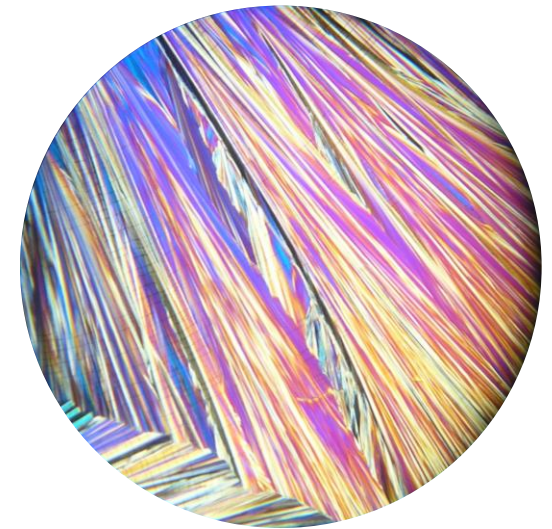
Thermal Analysis



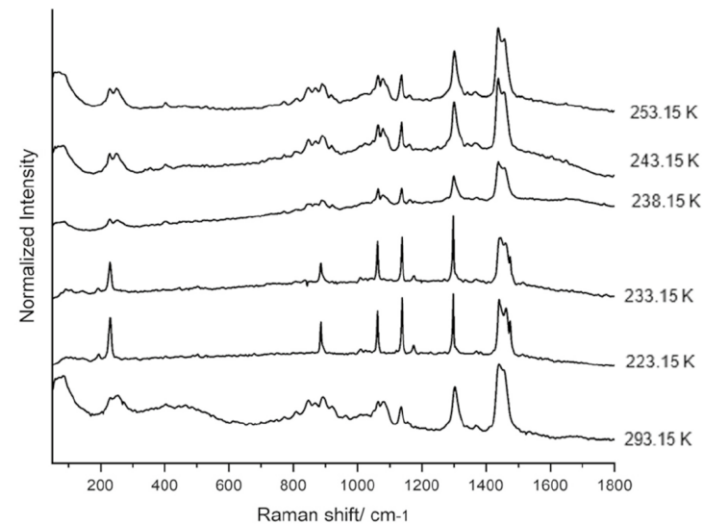
- **Temperature** and **enthalpy** of phase transition

Hot Stage Microscopy (HSM)

Microscopic Analysis



- Real-time **visual evidence** of **thermal events**



Raman Spectroscopy

Spectroscopic Analysis

- **Identification** and **characterization** of the **thermal events**

S-L Phase Diagrams

Enhancing Material Stability

Ensures that PCMs maintain consistent performance over many thermal cycles, avoiding degradation or phase separation

Designing Efficient Systems

Helps in designing TES systems with optimal heat transfer characteristics, reducing energy losses and improving overall efficiency.

Optimizing Energy Storage

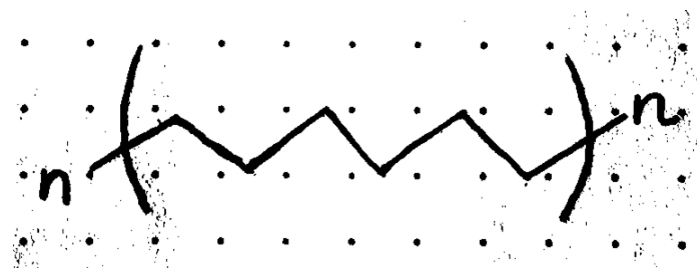
By understanding the temperatures and enthalpies associated with phase changes, materials can be selected and engineered to store and release thermal energy efficiently at desired operating temperatures

Economic and Environmental Benefits

Development of cost-effective and environmentally friendly energy storage solutions by optimizing material usage and reducing waste.

The Journey

Alkanes



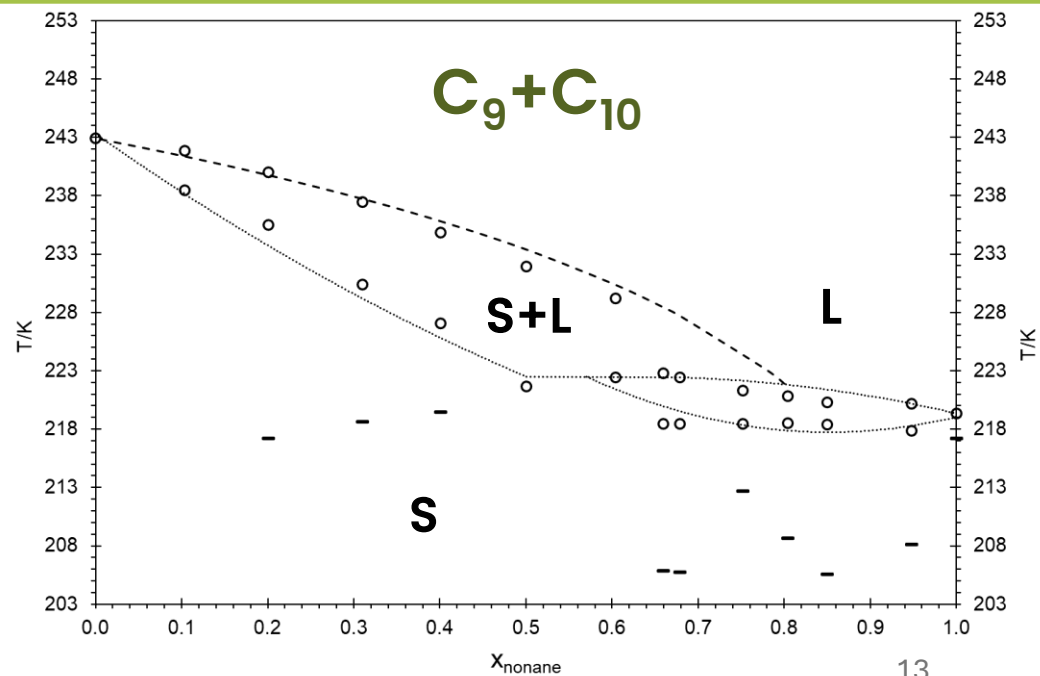
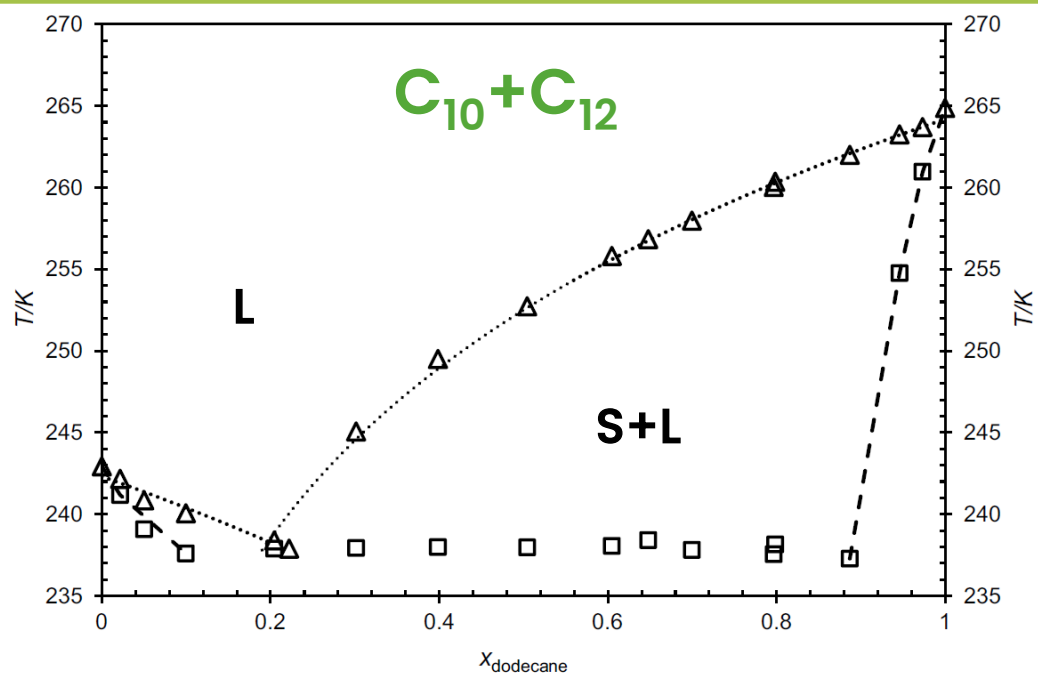
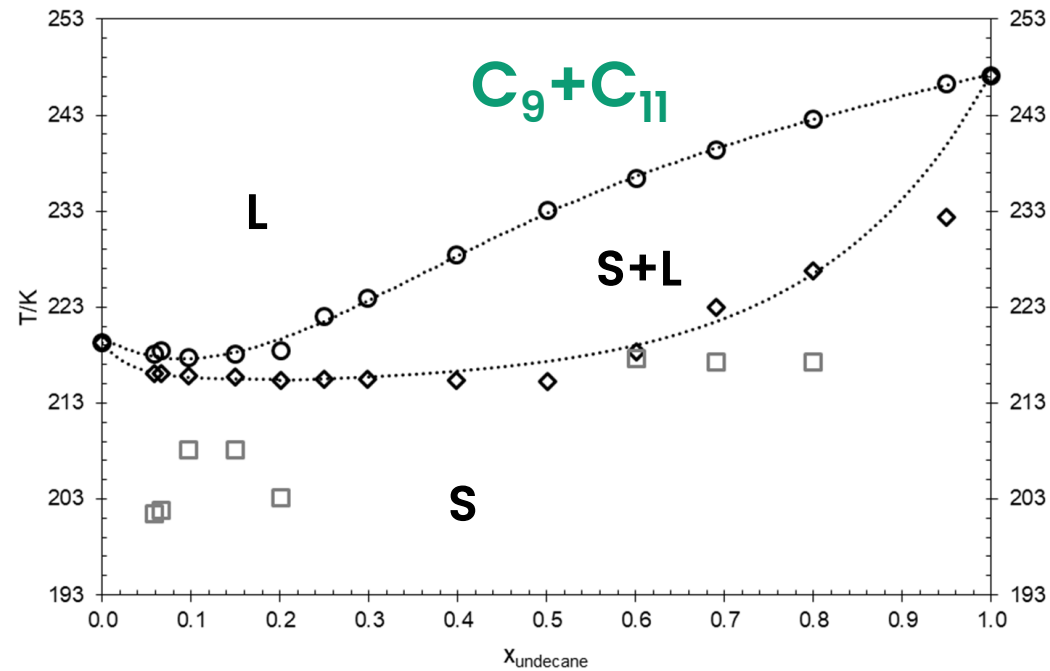
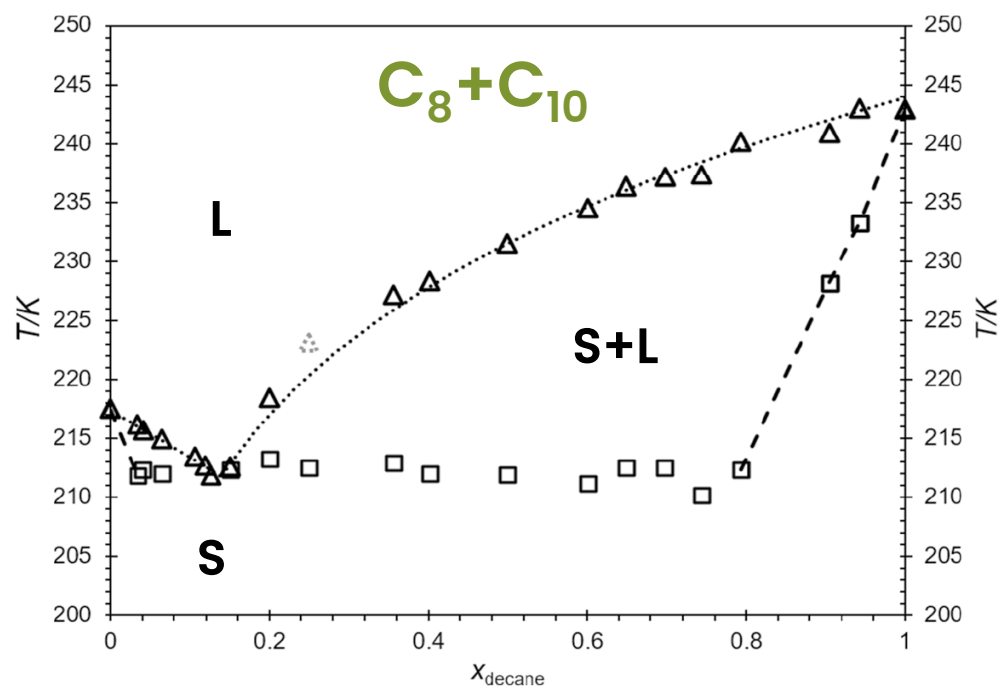


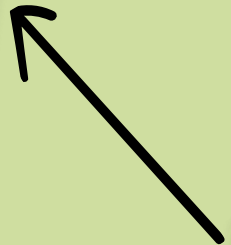
Fig. 1 Binary phase diagrams for the binary alkane systems C_8+C_{10} ; C_9+C_{11} ; $C_{10}+C_{12}$; C_9+C_{10} . Published in the International Journal of Thermophysics (IJT).



***n*-Alkanes**



**Odd-even
effects**



***n*-Alkanes**

**Odd-even
effects**

Even+Even



Eutectics

***n*- Alkanes**

**Odd-even
effects**

Even+Even

↓
Eutectics

Odd+Odd

↓
**Congruent
Melting**

***n*- Alkanes**

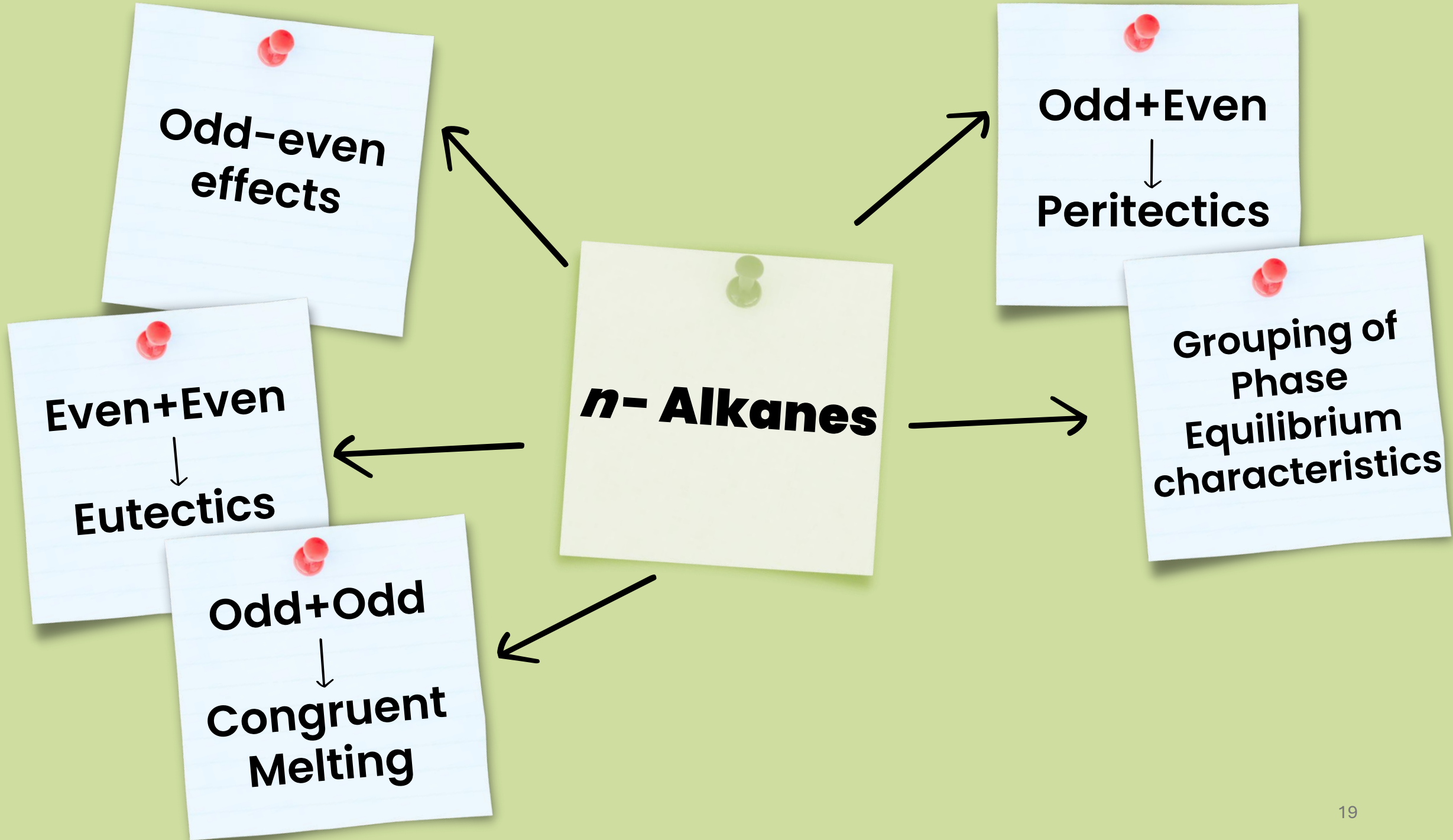
Odd-even effects

Even+Even
↓
Eutectics

Odd+Odd
↓
Congruent Melting

***n*- Alkanes**

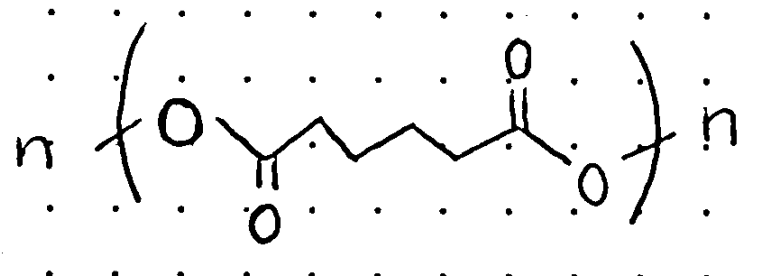
Odd+Even
↓
Peritectics





The Journey

Adipates



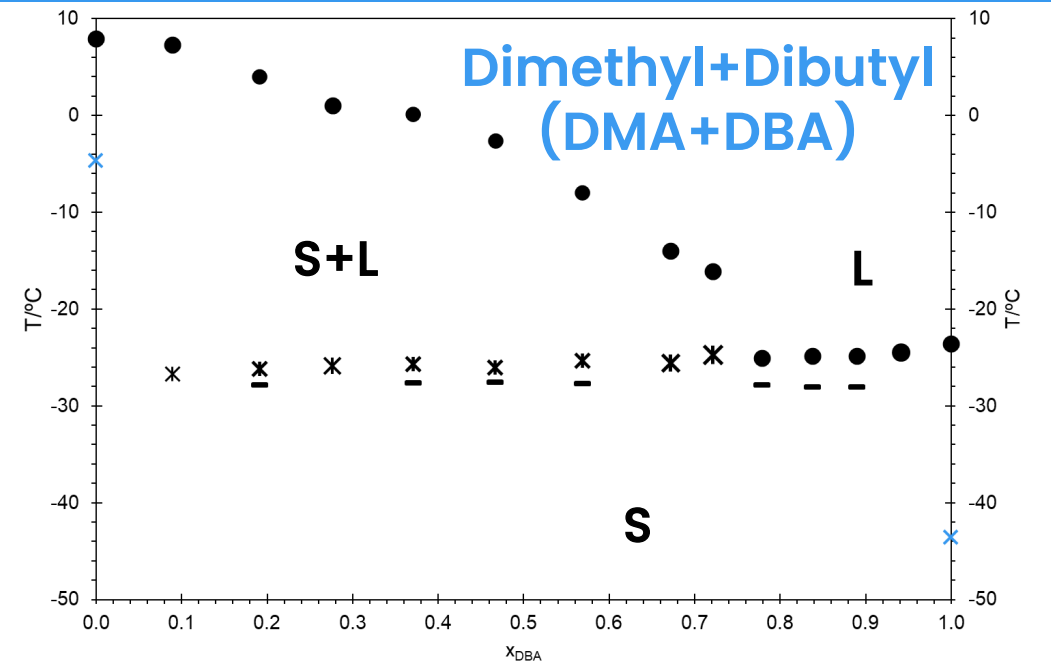
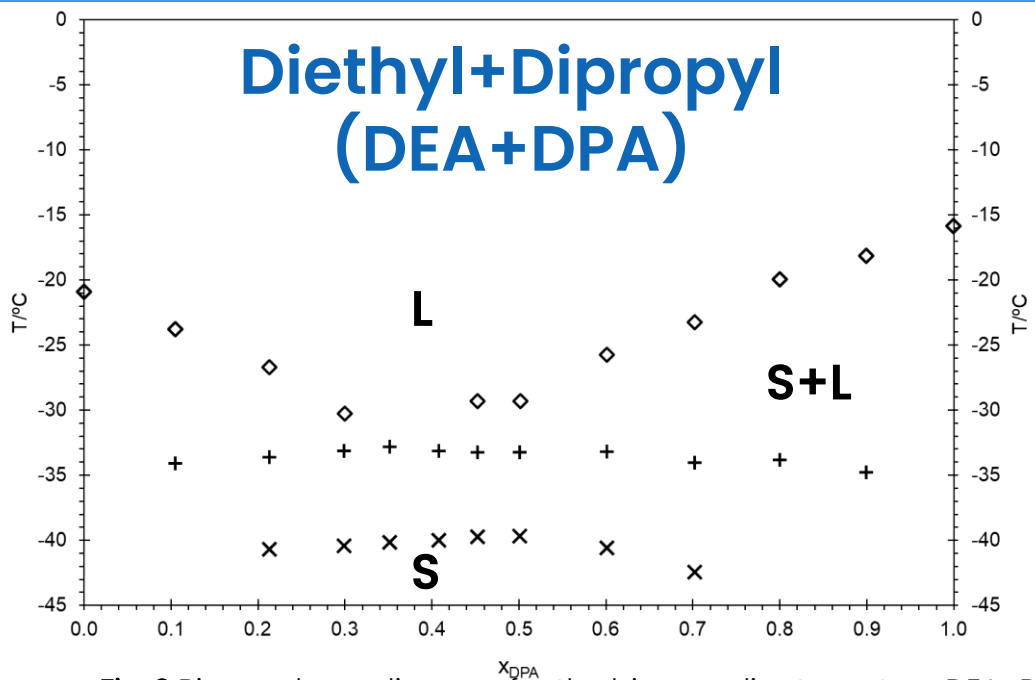
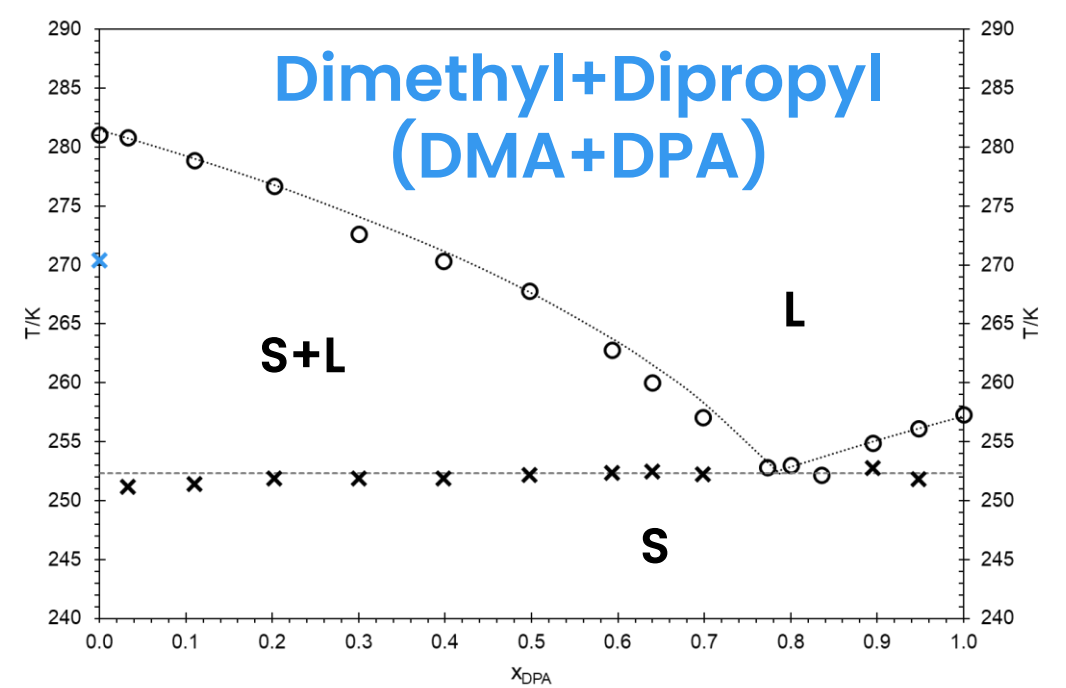
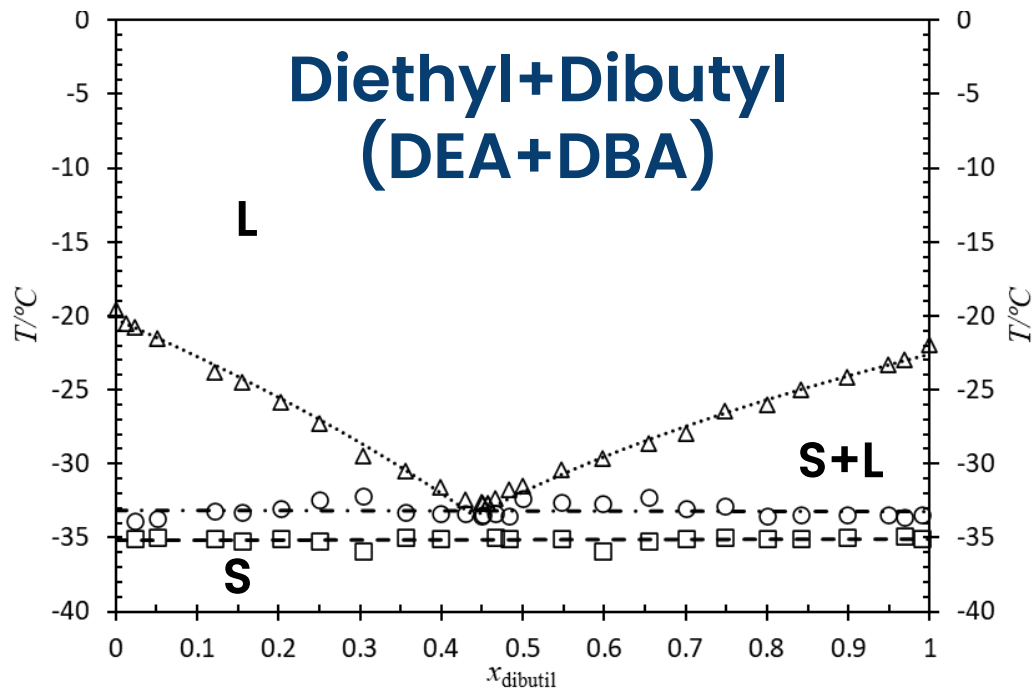


Fig. 2 Binary phase diagram for the binary adipate system DEA+DBA (Published in the IJT); and preliminary ones for DMA+DPA; DEA+DPA; DMA+DBA.

Unlocking Cold Thermal Energy Storage

Alkanes



Adipates



Unlocking Cold Thermal Energy Storage

Alkanes

-30 °C

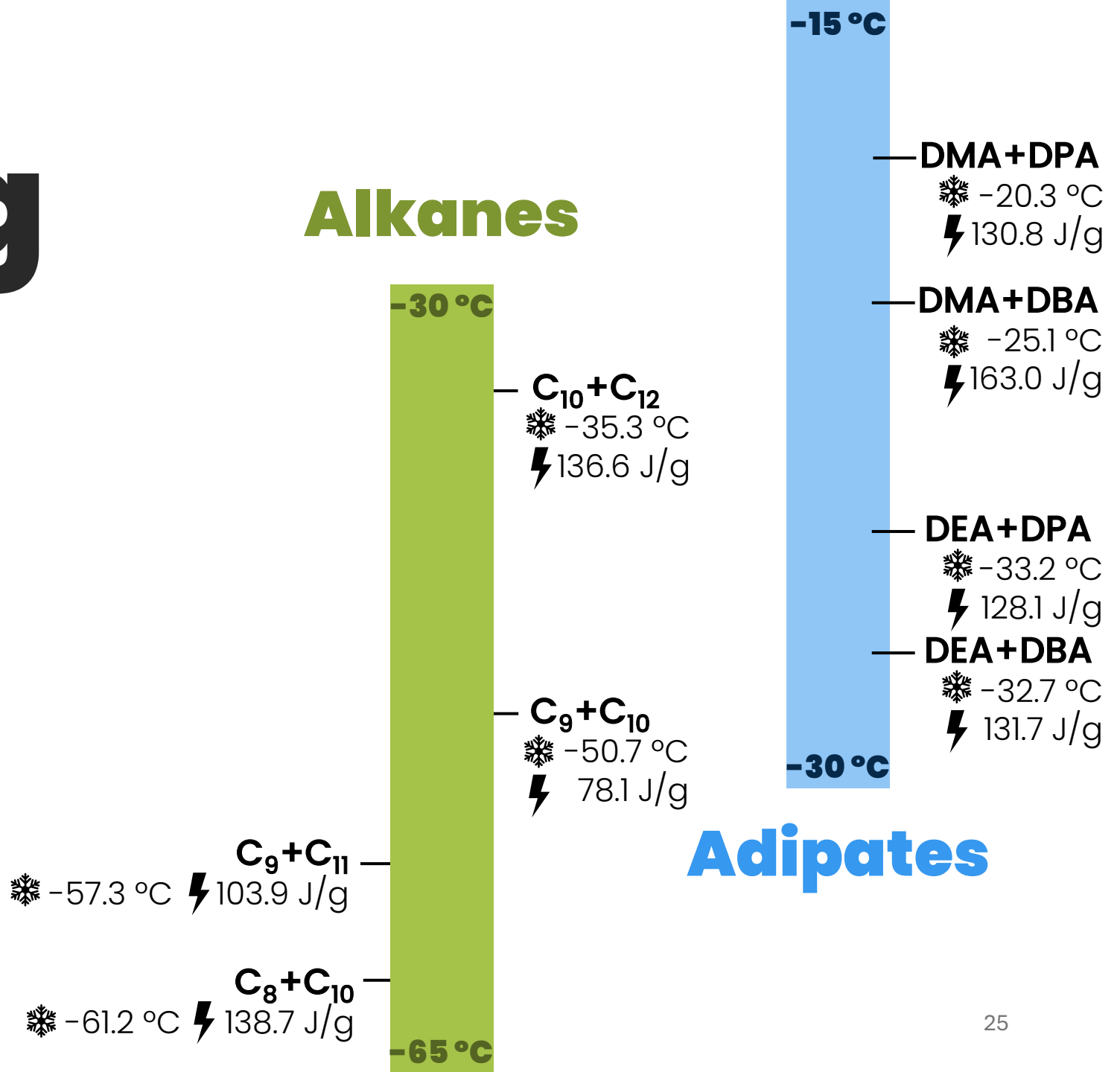
-65 °C

-15 °C

-30 °C

Adipates

Unlocking Cold Thermal Energy Storage



Unlocking Cold Thermal Energy Storage

8 different
PCM
candidates

Unlocking Cold Thermal Energy Storage

8 different
PCM
candidates

Different
applications

Unlocking Cold Thermal Energy Storage

8 different
PCM
candidates

Different
applications

Similar
performance

Unlocking Cold Thermal Energy Storage

8 different
PCM
candidates

Different
applications

Similar
performance

Fulfill the
lack of
available
data on low T
PCM systems

AKNOWLEDGEMENTS

- Centro de Química Estrutural is a Research Unit funded by Fundação para a Ciência e a Tecnologia through projects UIDB/00100/2020 (<https://doi.org/10.54499/UIDB/00100/2020>), UIDP/00100/2020 (<https://doi.org/10.54499/UIDP/00100/2020>), UIDB/00313/2025 (<https://doi.org/10.54499/UIDB/00313/2025>) and UIDP/00313/2025 (<https://doi.org/10.54499/UIDP/00313/2025>). Institute of Molecular Sciences is an Associate Laboratory funded by Fundação para a Ciência e a Tecnologia through project LA/P/0056/2020 (<https://doi.org/10.54499/LA/P/0056/2020>).
- M.C.M. Sequeira acknowledges the PhD grant funded by FCT ref. UI/BD/152239/2021 (<https://doi.org/10.54499/UI/BD/152239/2021>).
- The ERA-Chair Spectroscopy@IKU - Manipulating and Characterizing Molecular Architectures: From Isolated Molecules to Molecular Crystals (Project number: 101184899) is funded by the European Research Agency under the HORIZON-WIDERA-2023-TALENTS-01-01 Program.

