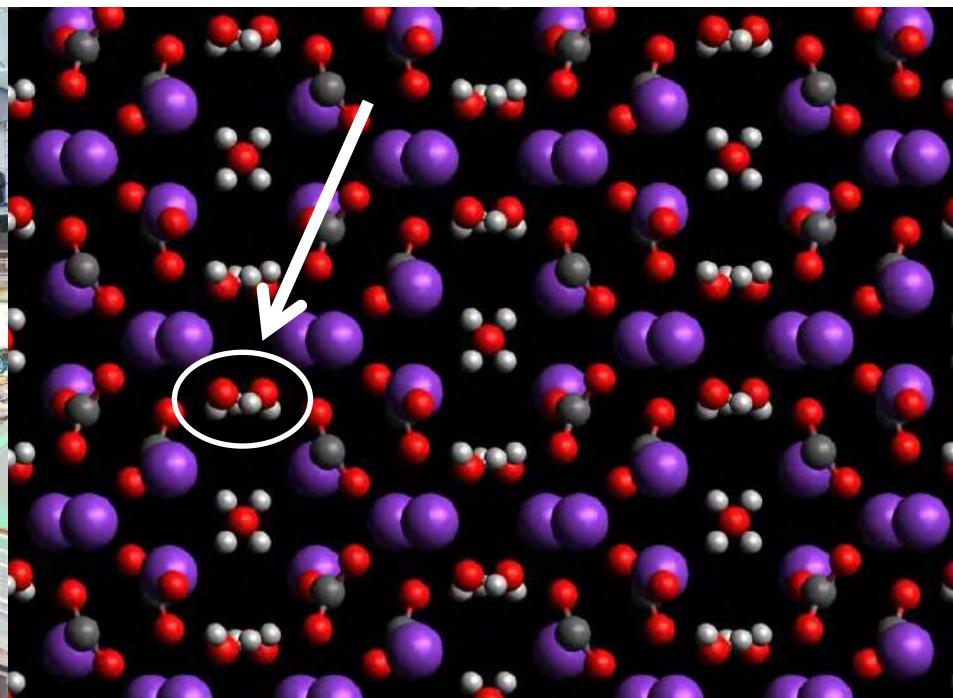


# Utilization hydration transitions of crystals

## 4 heat storage



# Storing heat/cold

Option 1: heat capacity

$$E / V \sim C_p \rho \Delta T$$

kinetic energy atoms/molecules

Sensible heat

Water

Li-ion:  
~ 1 GJ/m<sup>3</sup>

0.1 GJ/m<sup>3</sup> (50 K)

Option 2: heat of melting

$$E / V \sim \Delta H_{fus} \rho$$

PCM = Phase Change Materials

0.3 GJ/m<sup>3</sup>

Option 3: heat of “vaporization”

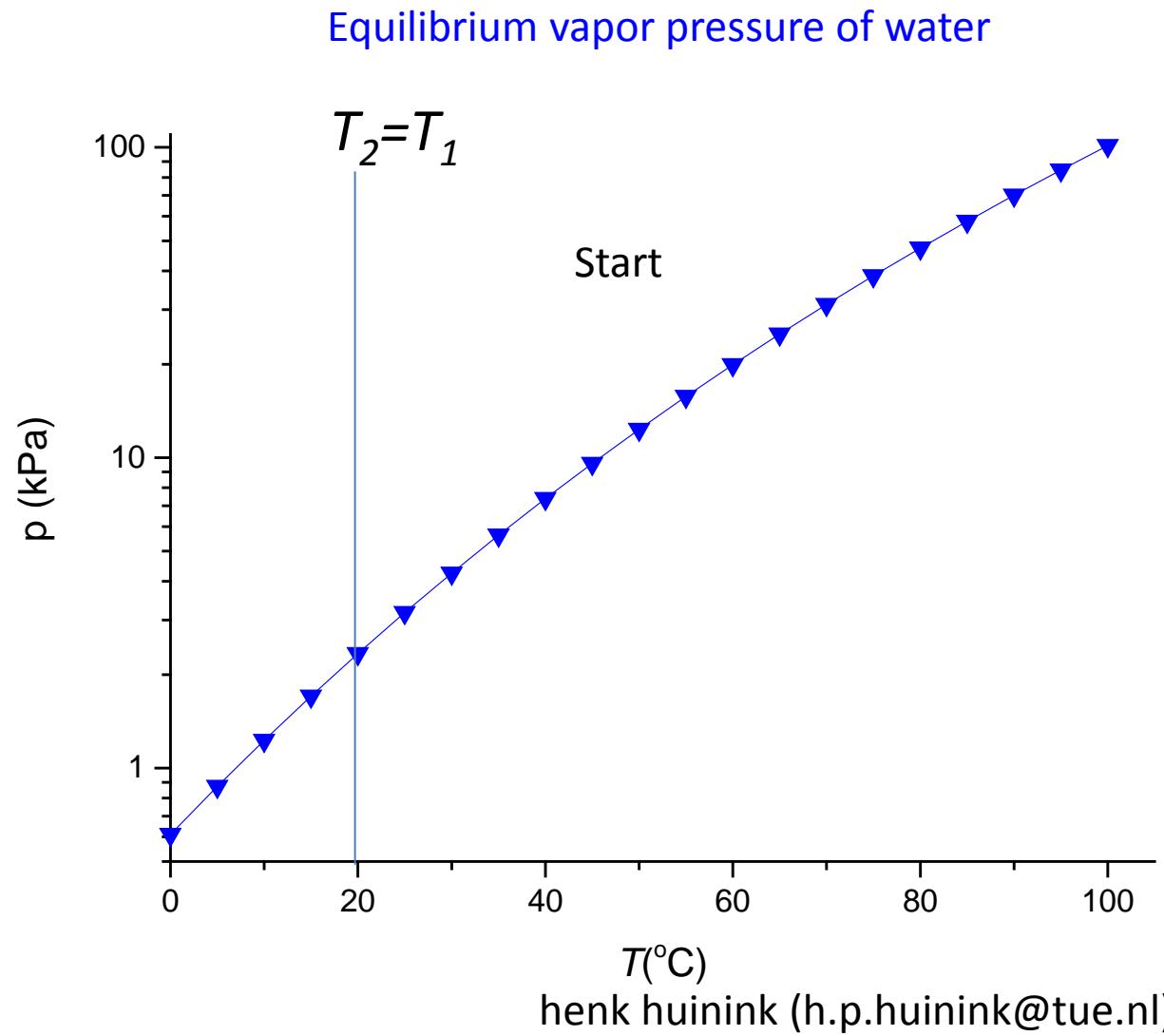
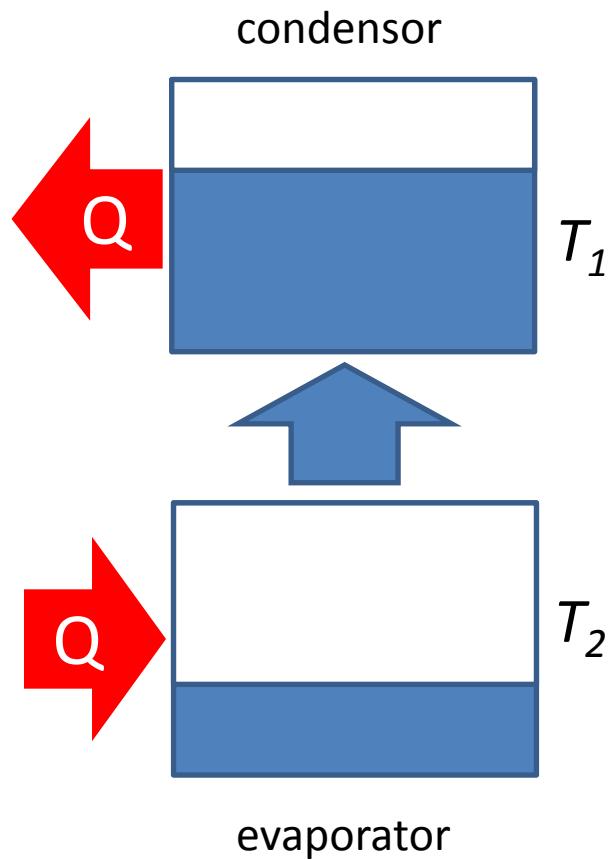
$$E / V \sim \Delta H_{vap} \rho$$

breaking physical/chemical bonds

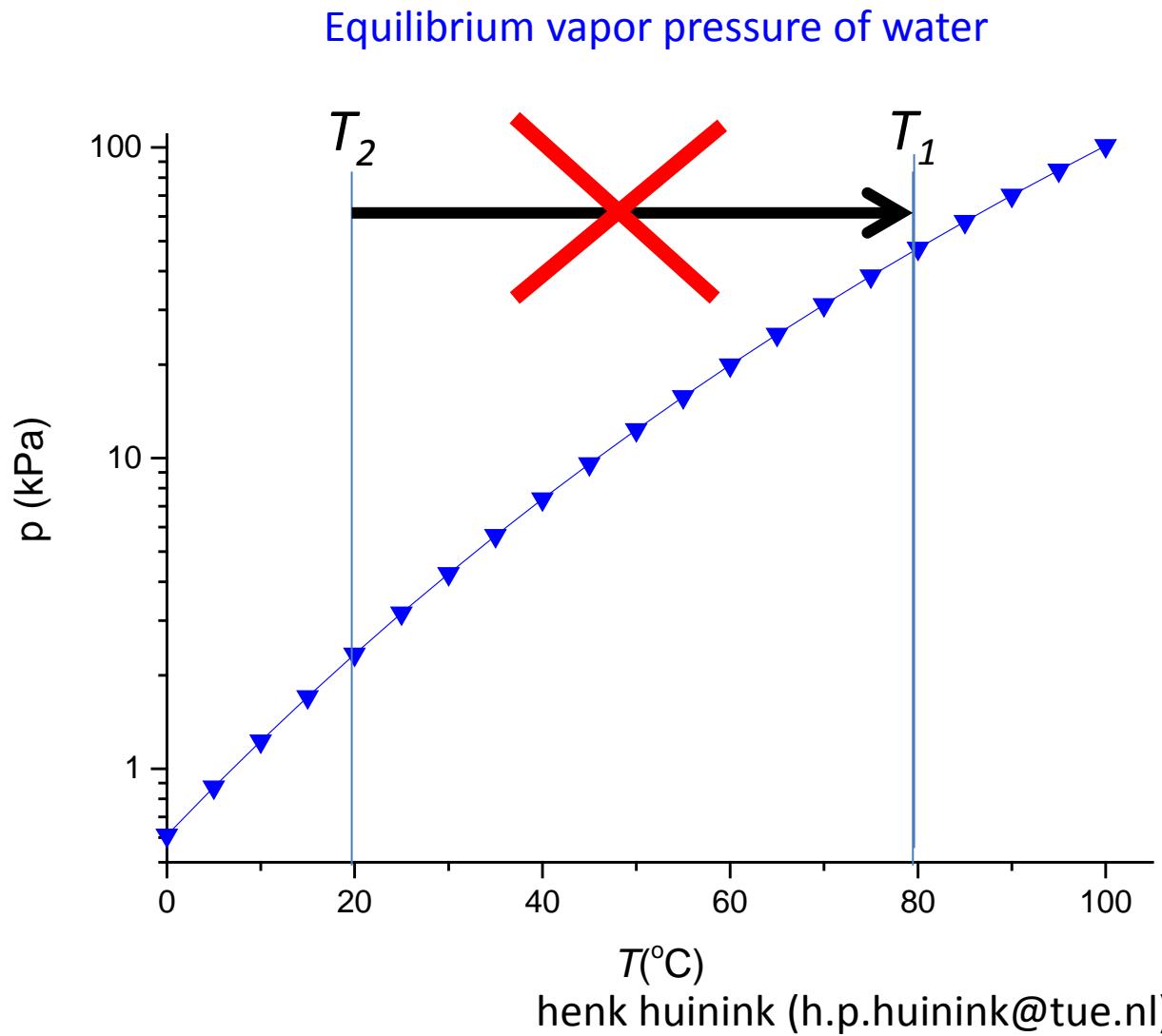
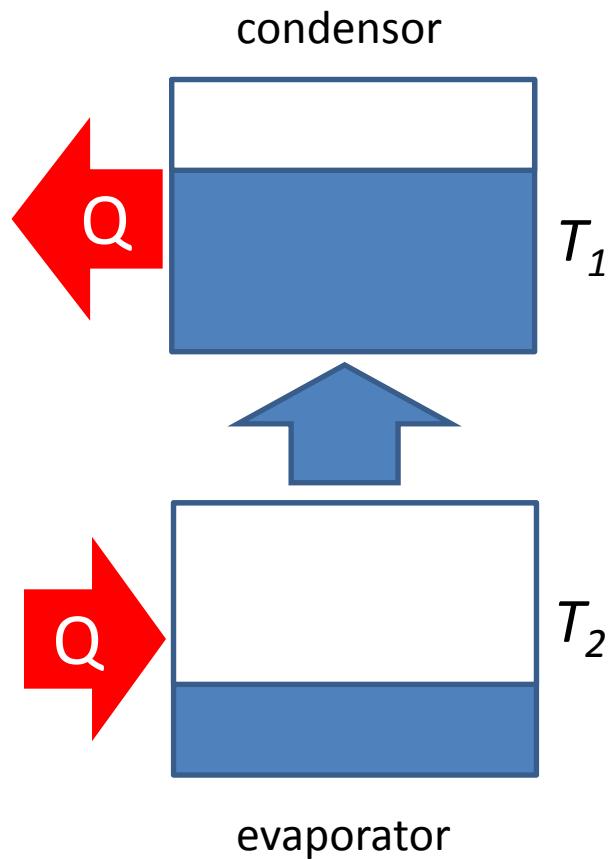
TCM = Thermo-Chemical Materials

2.5 GJ/m<sup>3</sup>

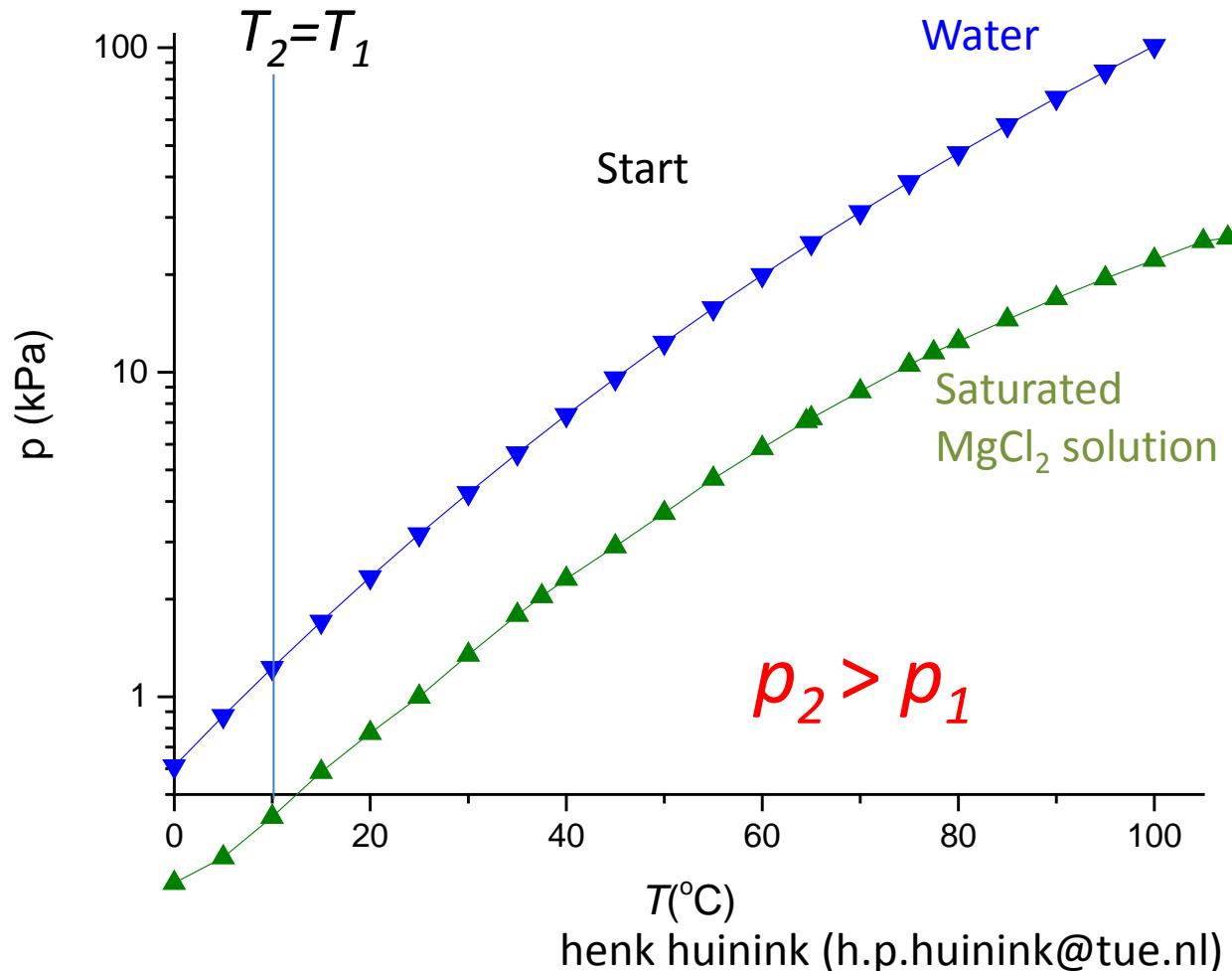
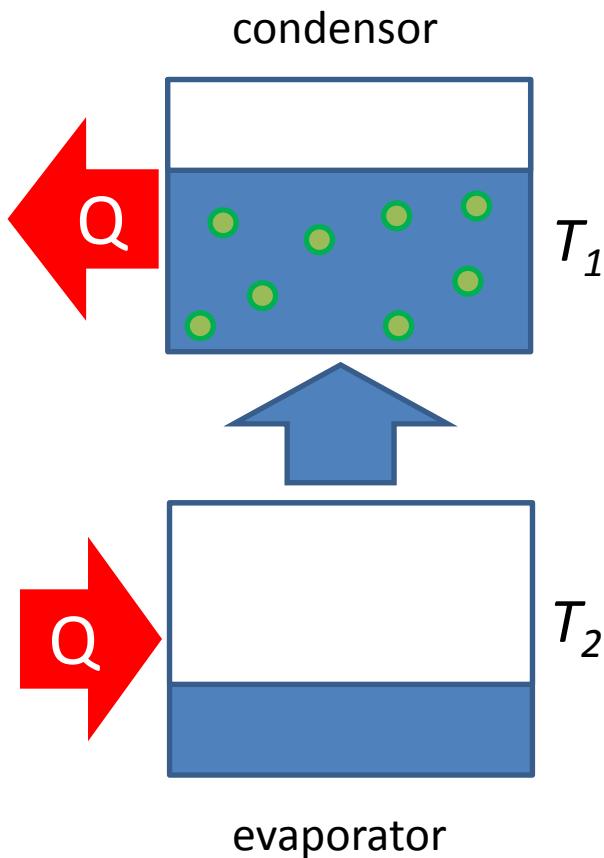
# Condensation of water



# Condensation of water

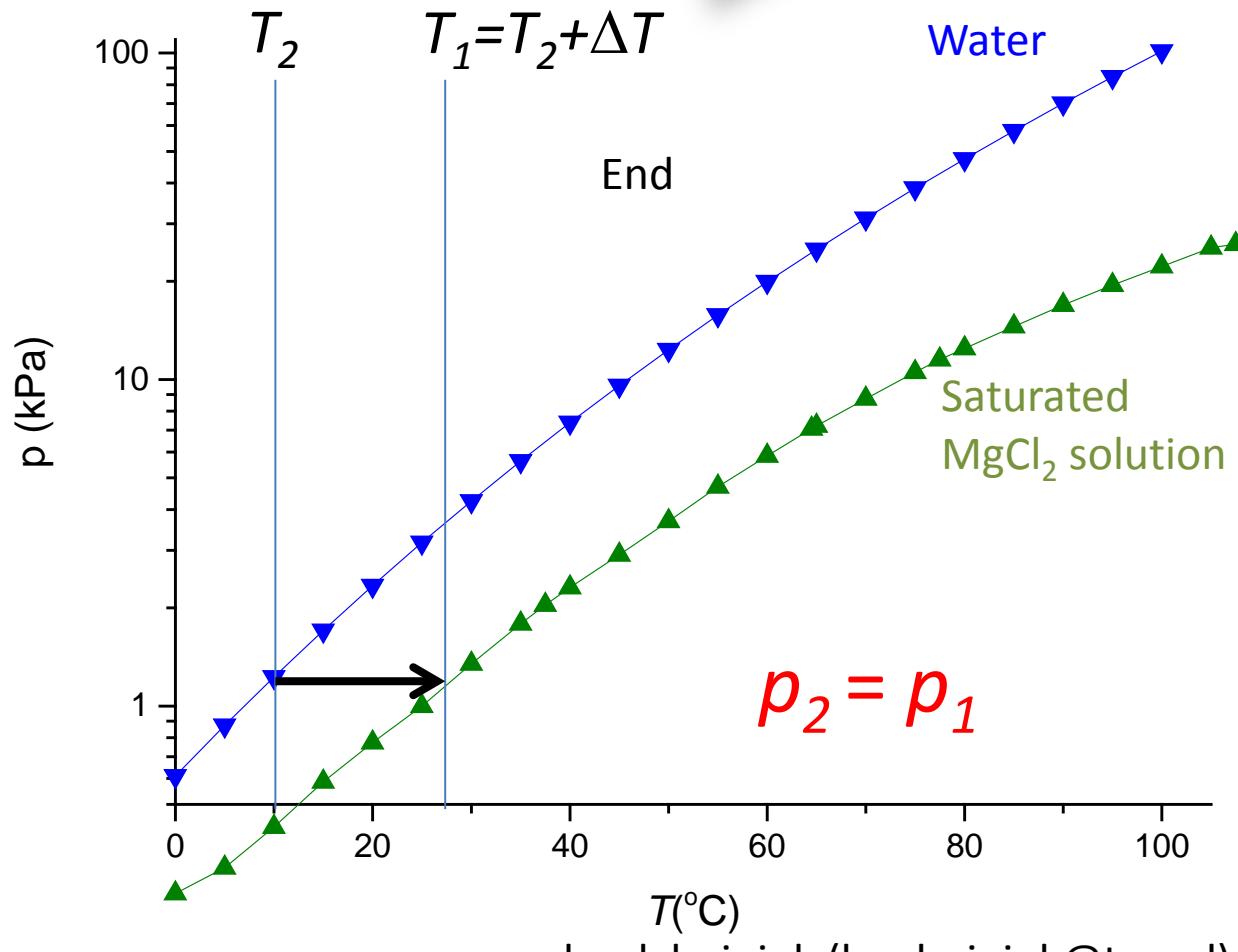
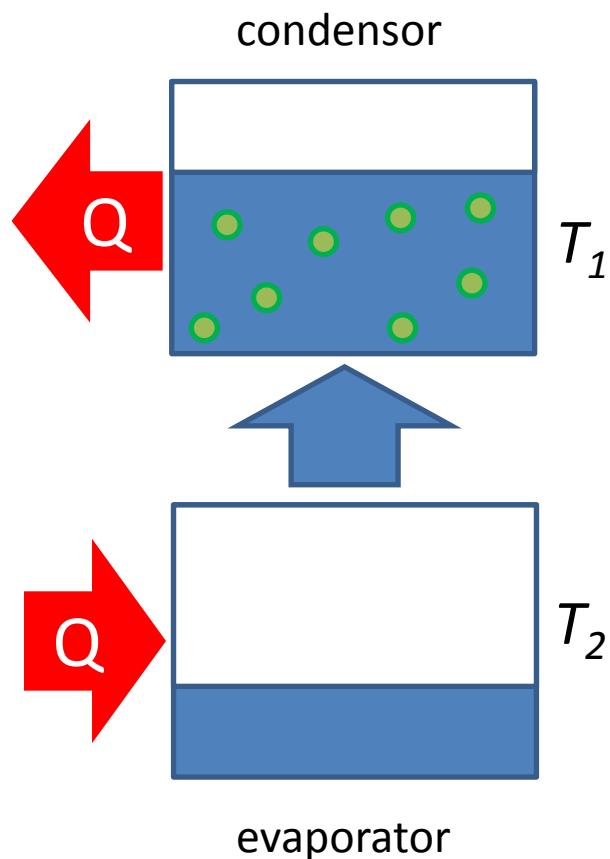


# Water++



# Water++

Increase bond strength



# Options

Energy density



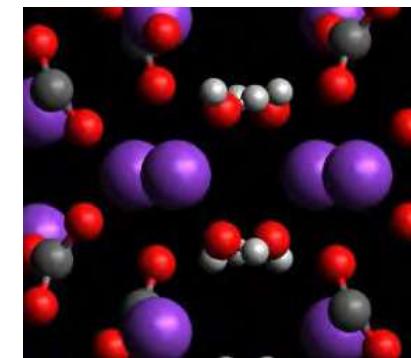
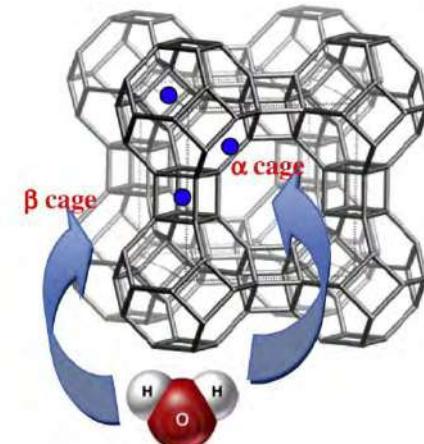
Temperature lift



How to concentrate water at low water vapor pressures?

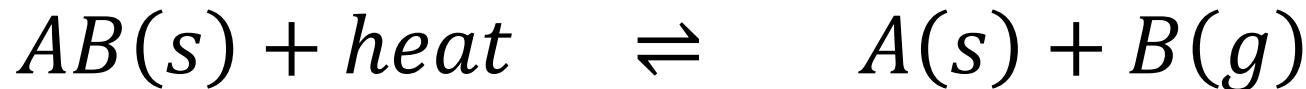
<https://doi.org/10.1016/j.micromeso.2014.10.039>

- **Solutions:** dilution
- **Zeolites/MOF's:** adsorption to ionic sites
- **Hydrates:** incorporation in crystal lattice

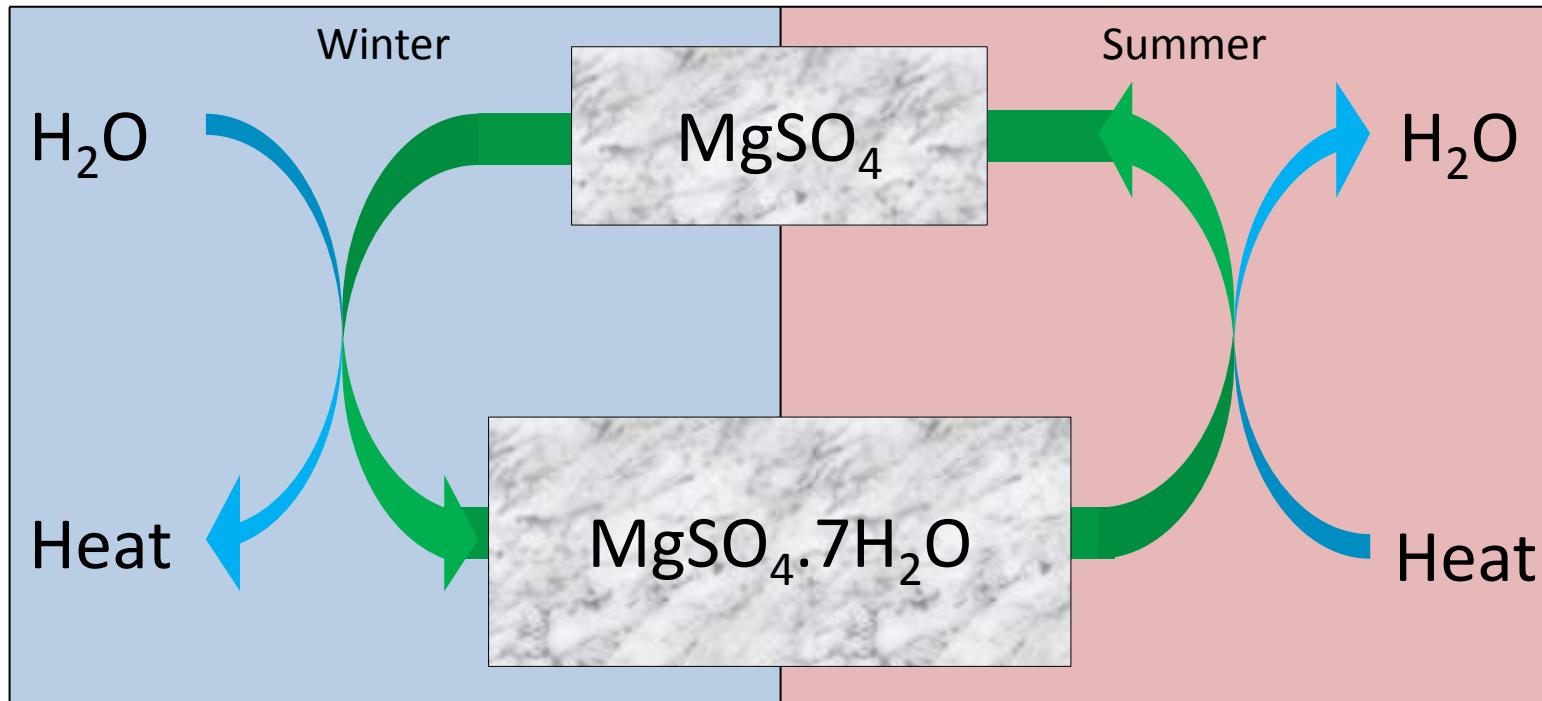


# Thermo-chemical energy

## Gas-solid reactions



Storing energy by storing components separately



# Built environment

$T > 60^\circ\text{C}$



$T > 40^\circ\text{C}$

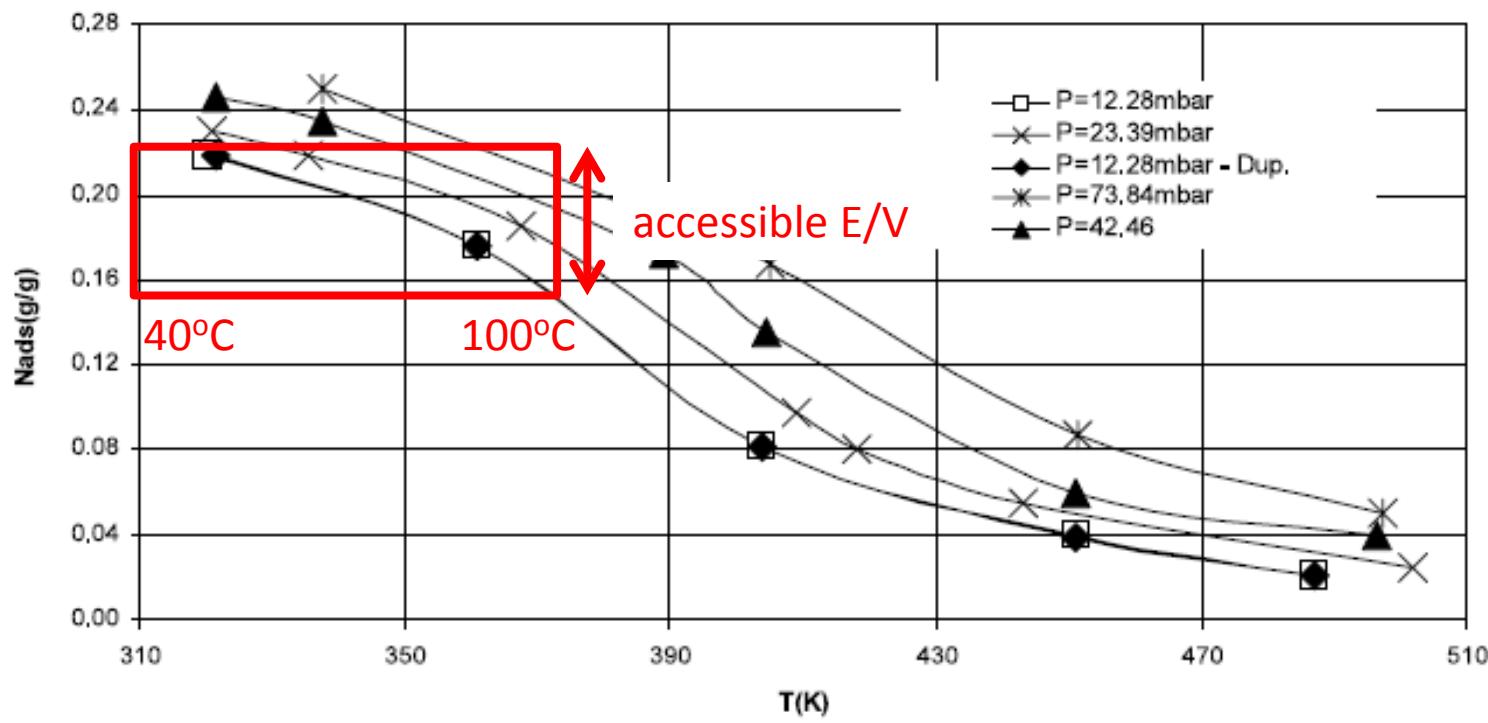


Source water vapor:  $T \sim 10^\circ\text{C}$   $p = 12 \text{ mbar}$

Dehydration temperature:  $T < 100^\circ\text{C}$

# Boundary conditions matter

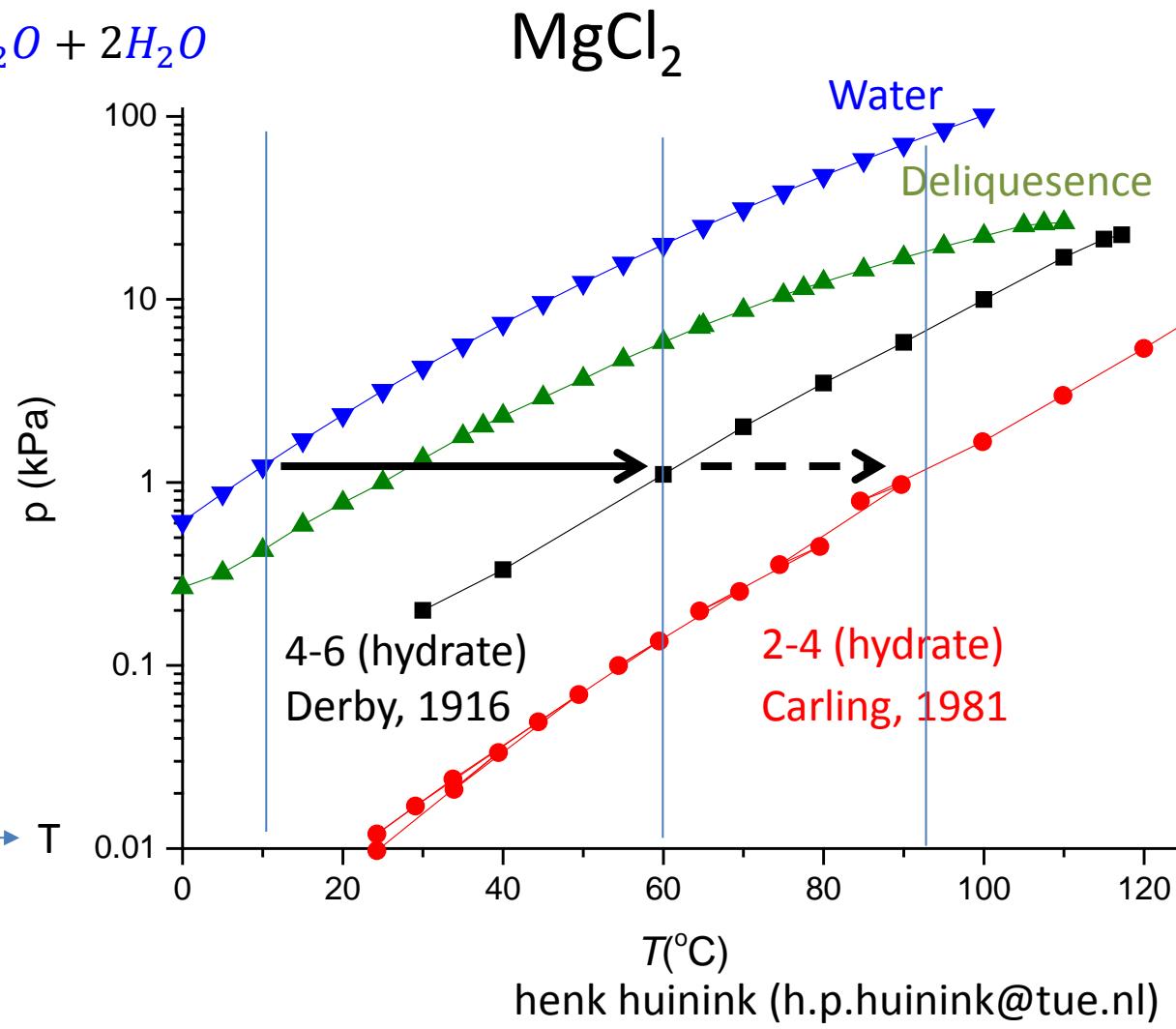
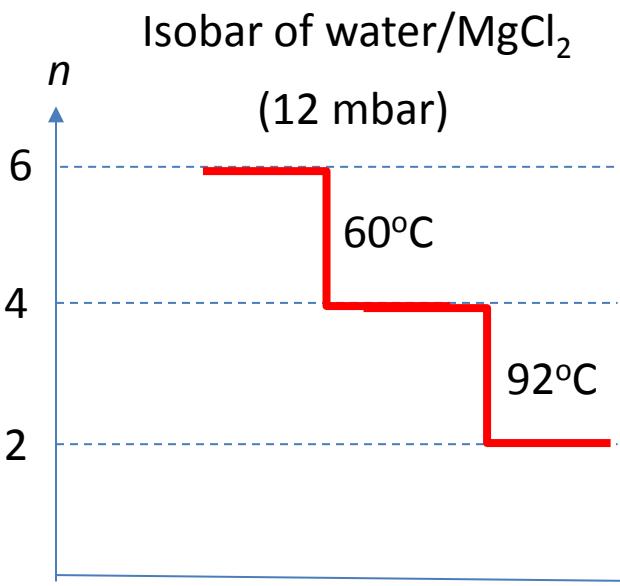
Isobars of water/zeolite 13X



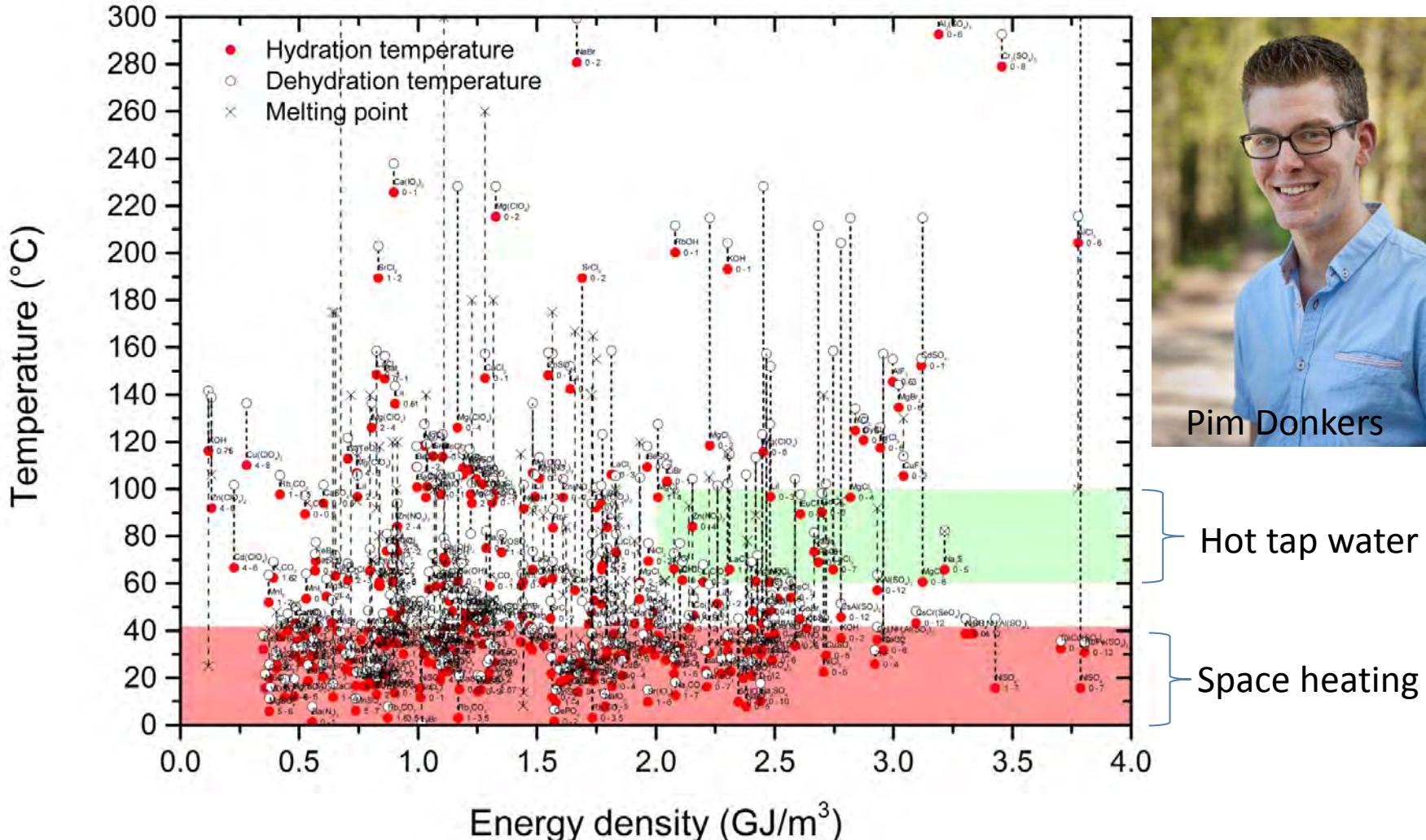
Cortes et al., Adsorption, 16:141-146 (2010)

To use zeolites, the heat for dehydration should be sufficiently high

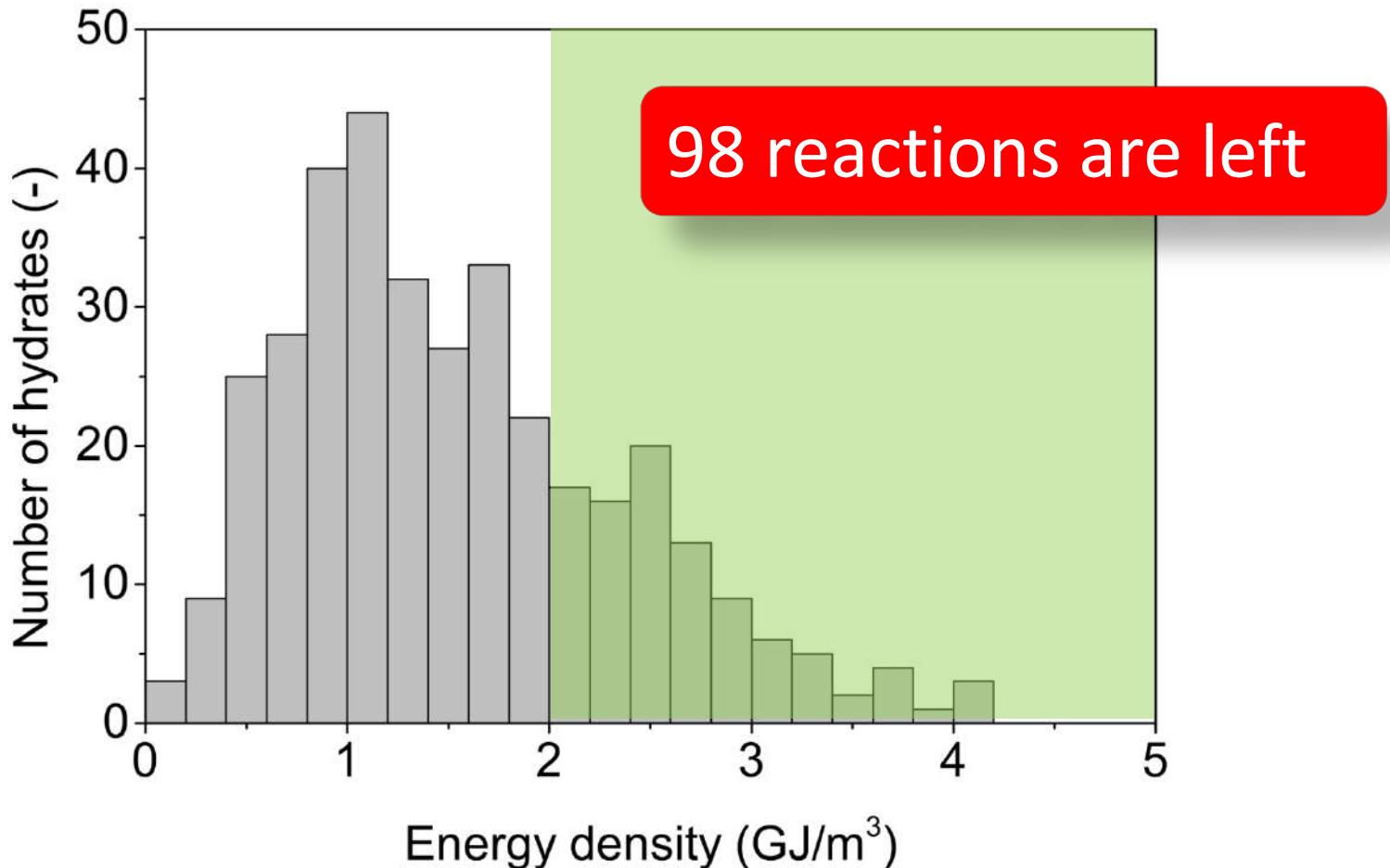
# Salt hydrates



# Overview (650 reactions)



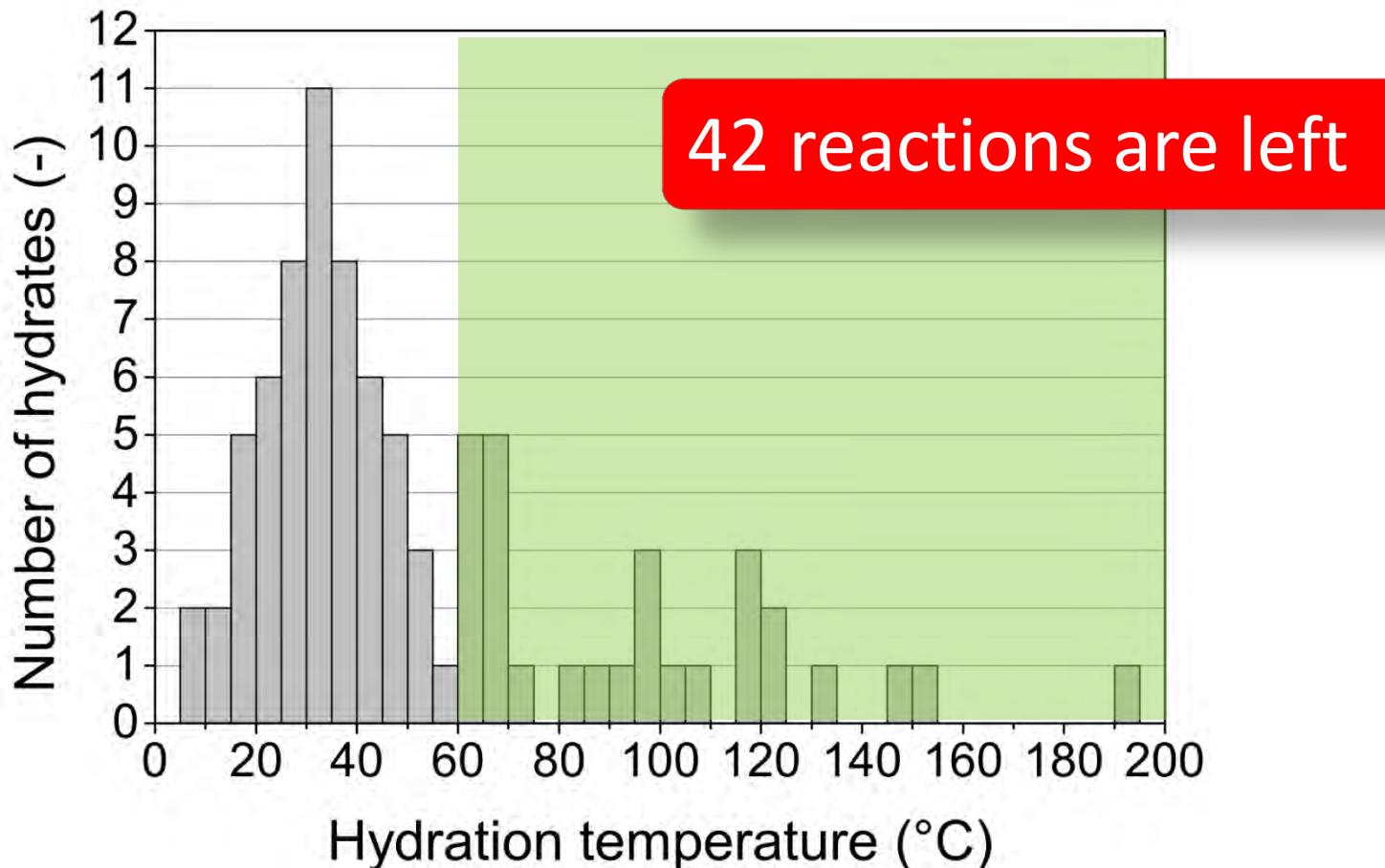
$$E/V > 2 \text{ GJ/m}^3$$



Water source at 10 °C (12 mbar)

$T_{\text{output}} > 50^\circ\text{C}$

# Hydration



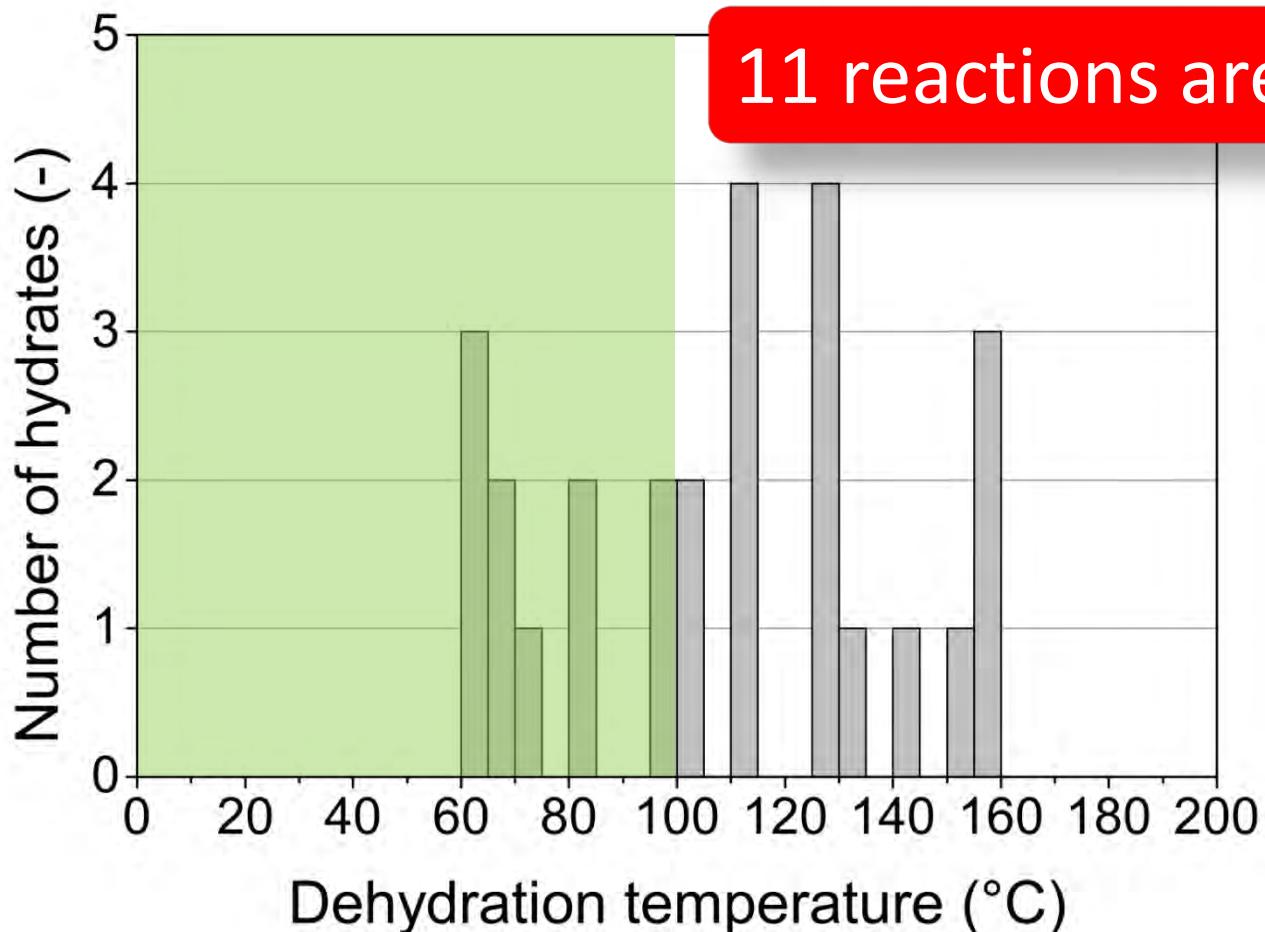
Water source at 17 °C (20 mbar)

 $T_{\text{input}} < 100^\circ\text{C}$ 

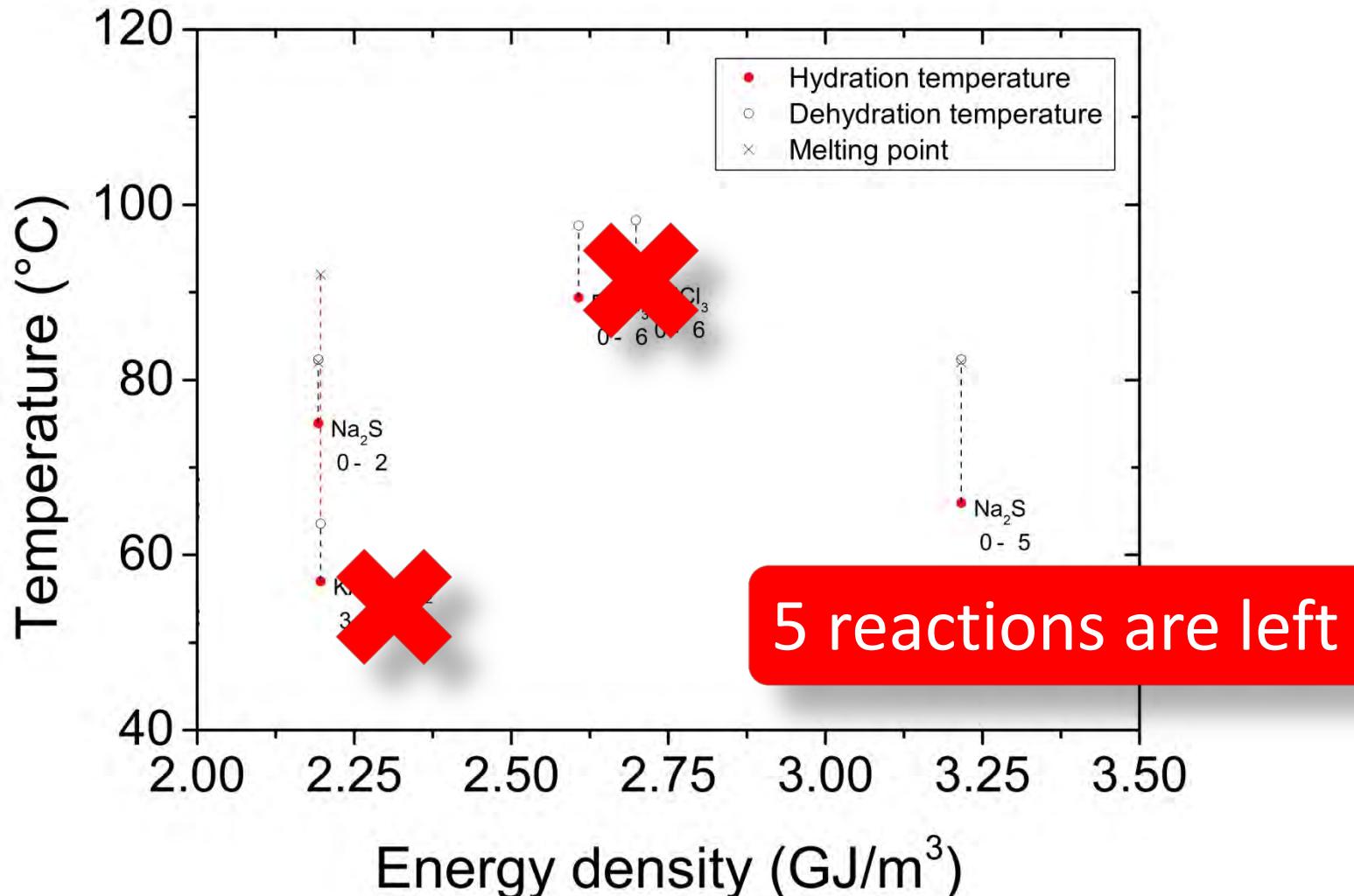
## Dehydration

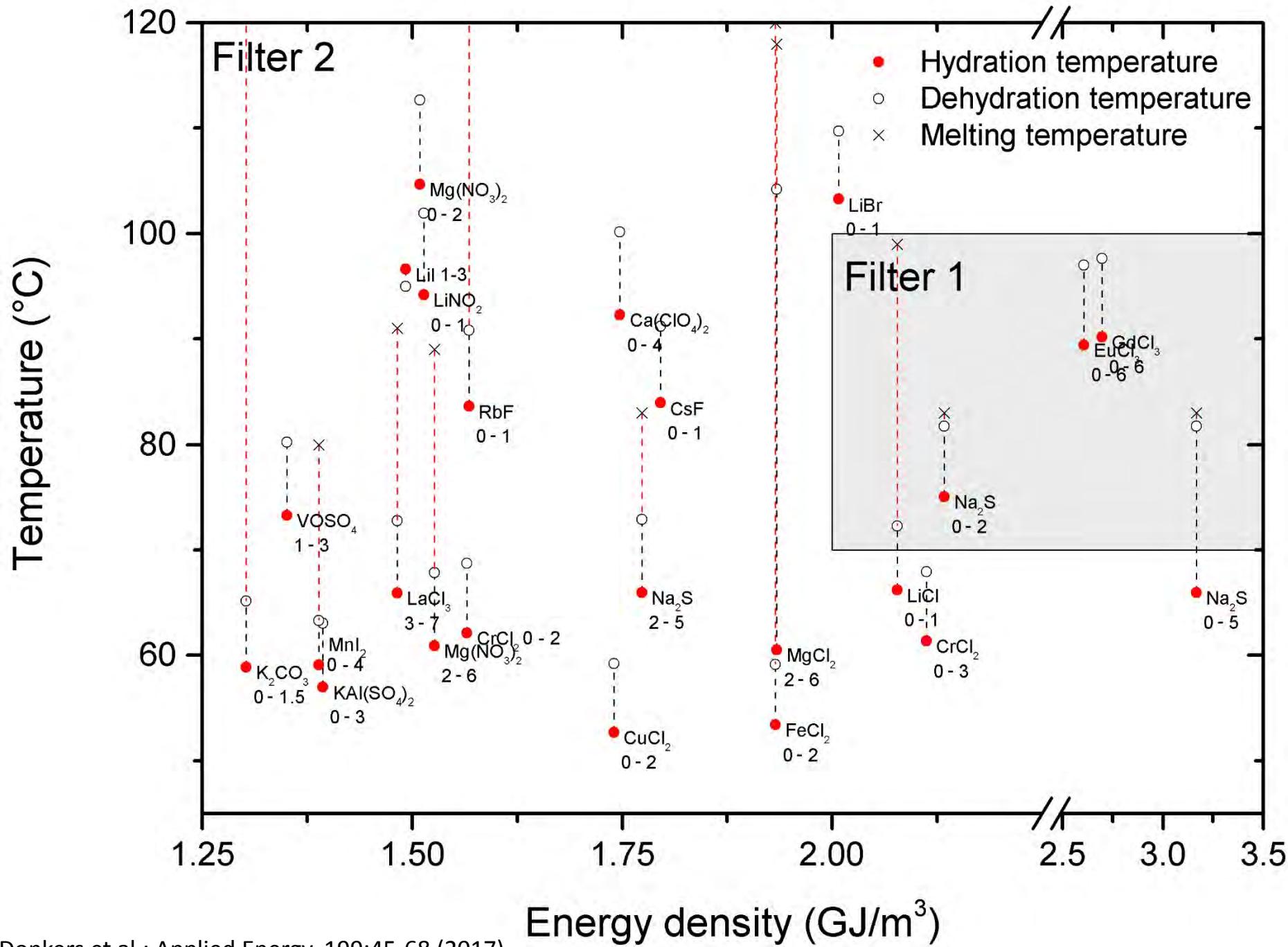


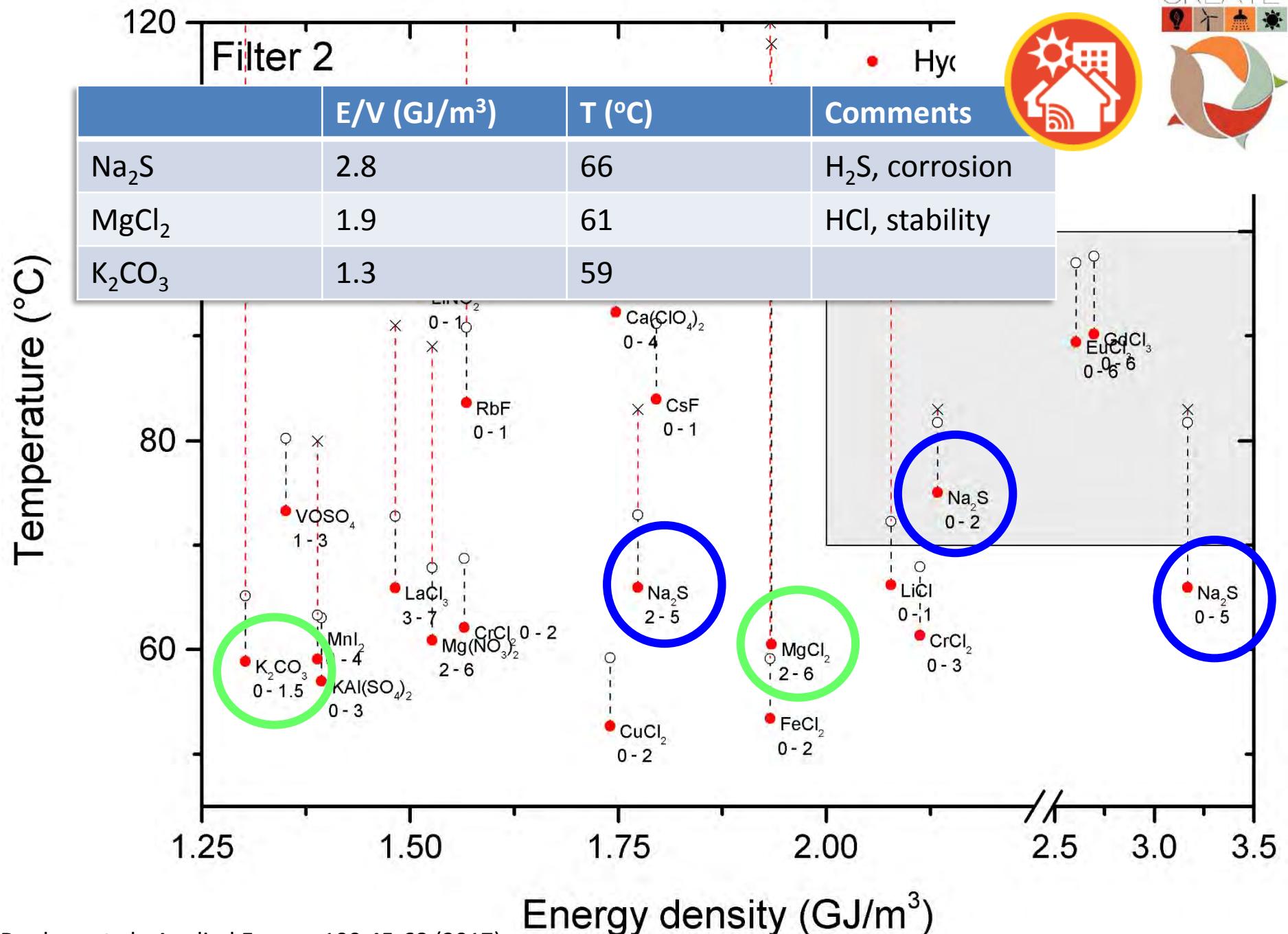
11 reactions are left



$T_{\text{melting}} > T_{\text{dehydration}}$

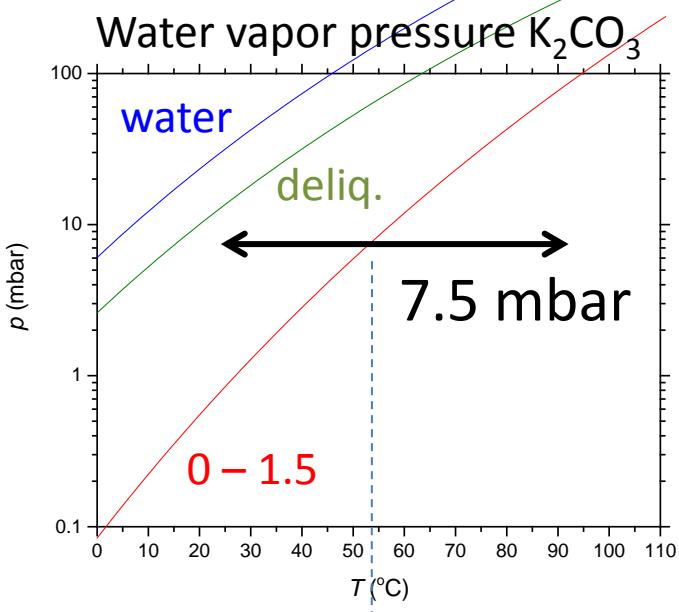
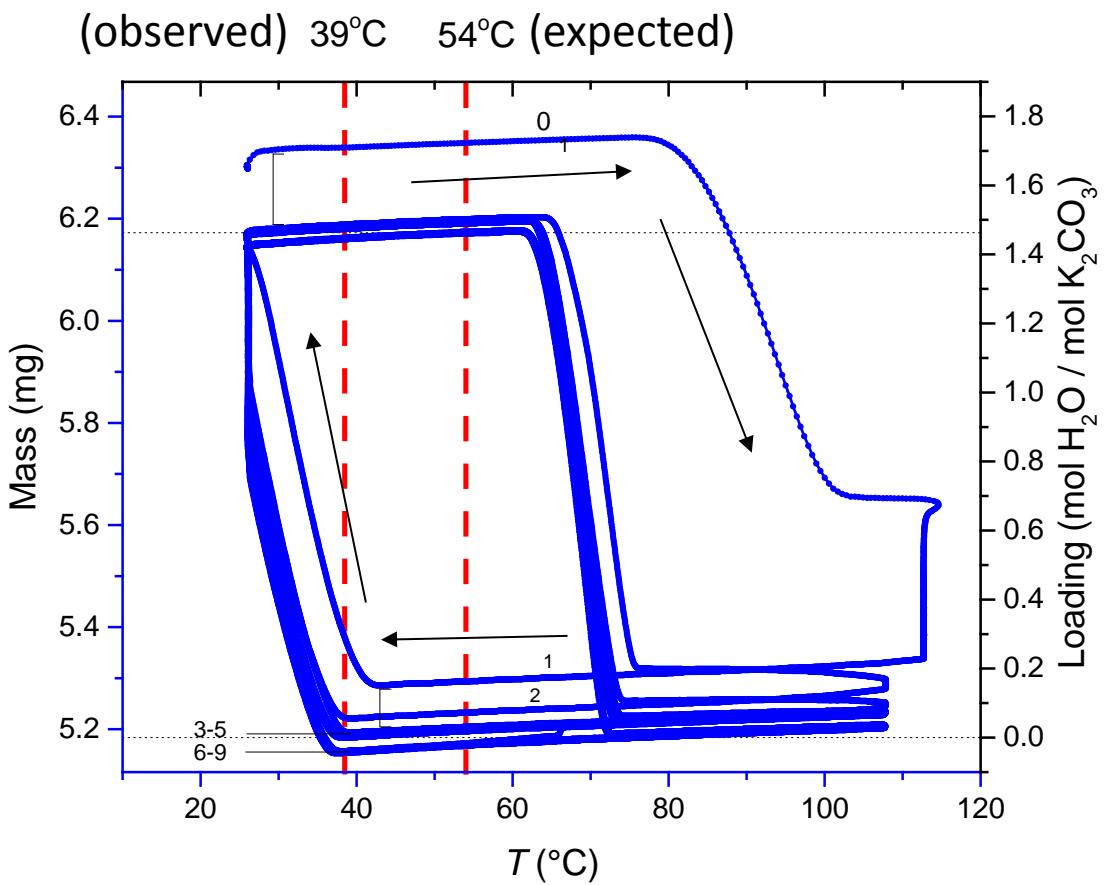






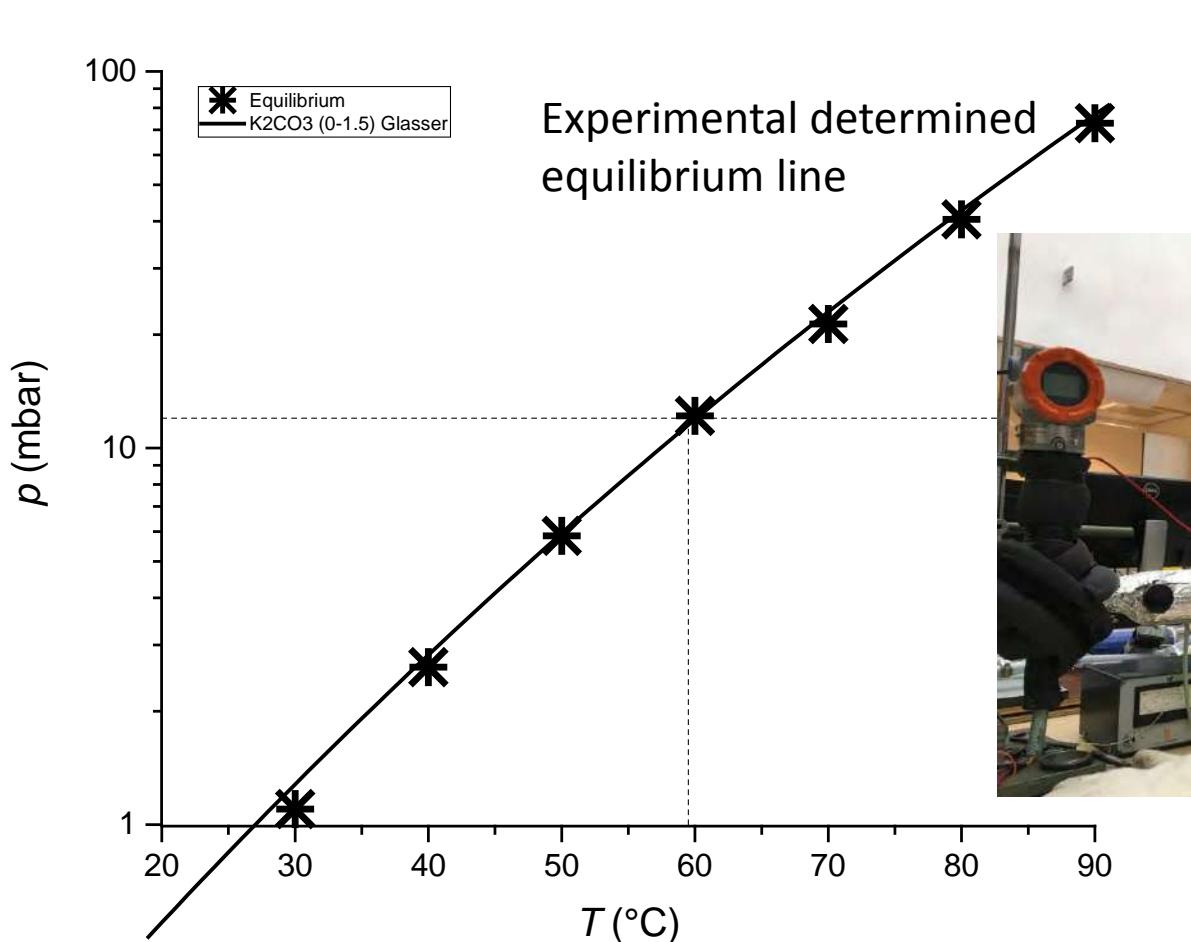
# Isobaric cycling $\text{K}_2\text{CO}_3$

7.5 mbar



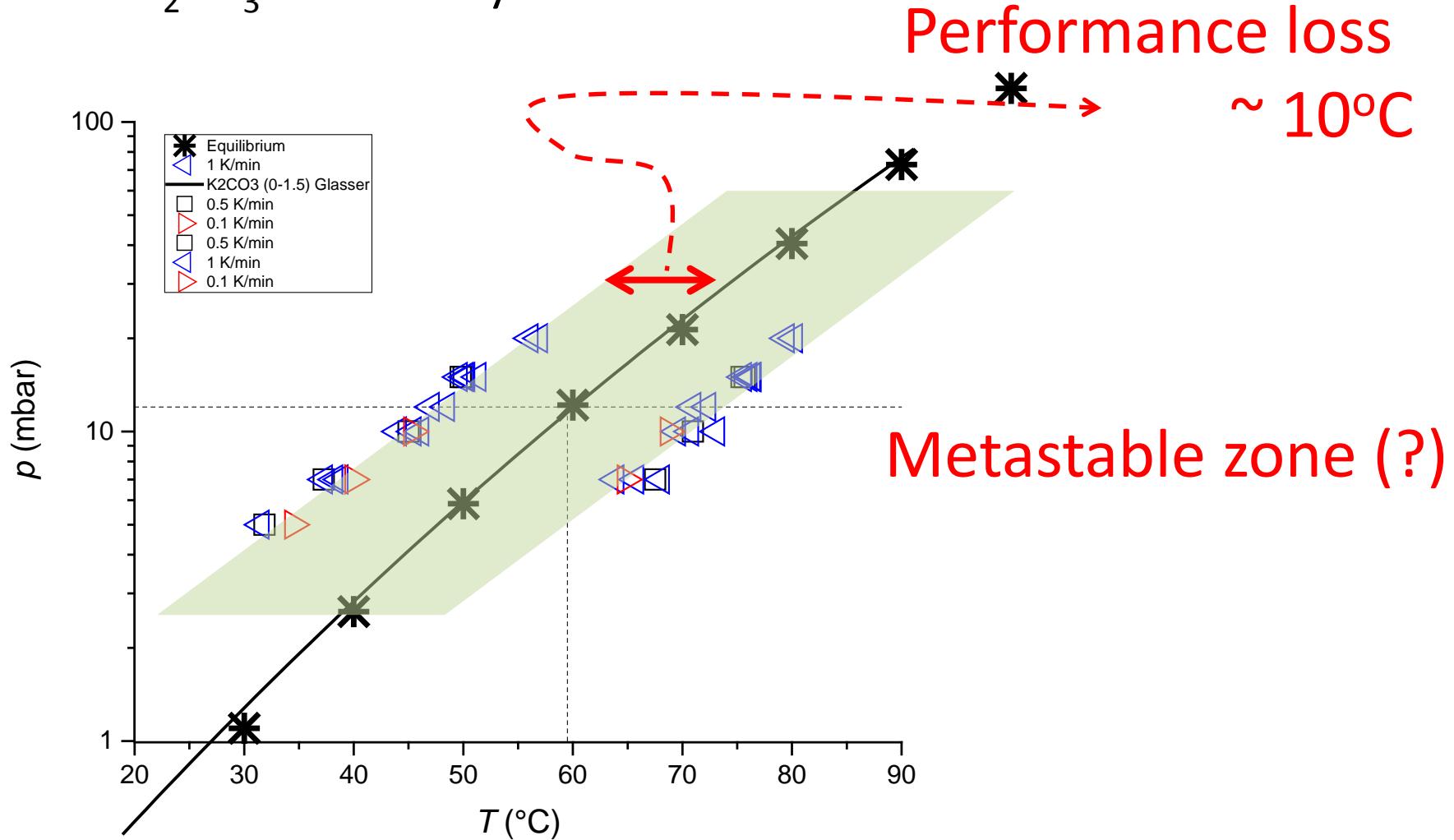
# Overshoot problem?

$\text{K}_2\text{CO}_3$ : isobaric cyclic at 12 mbar

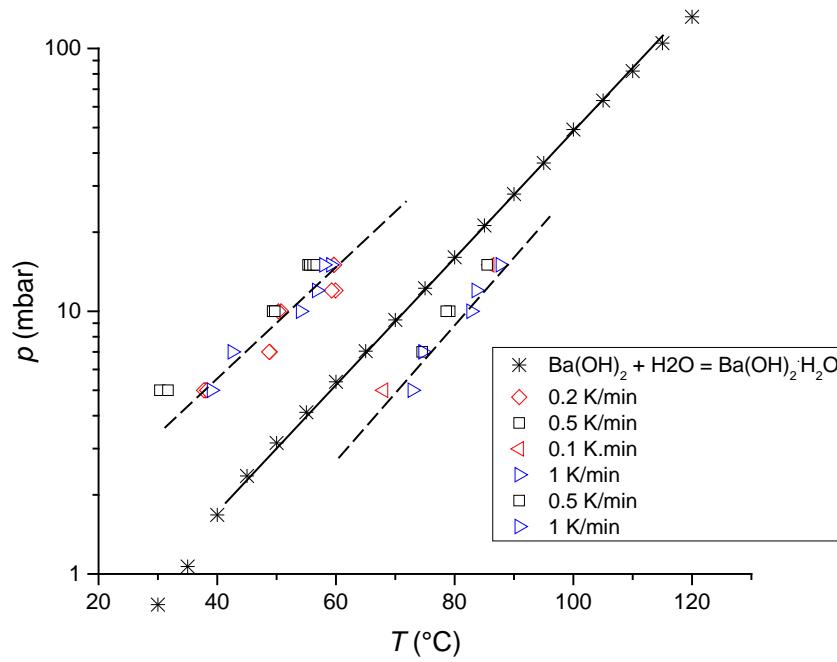
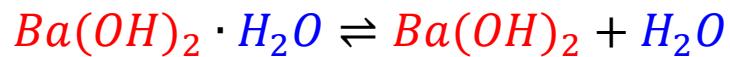
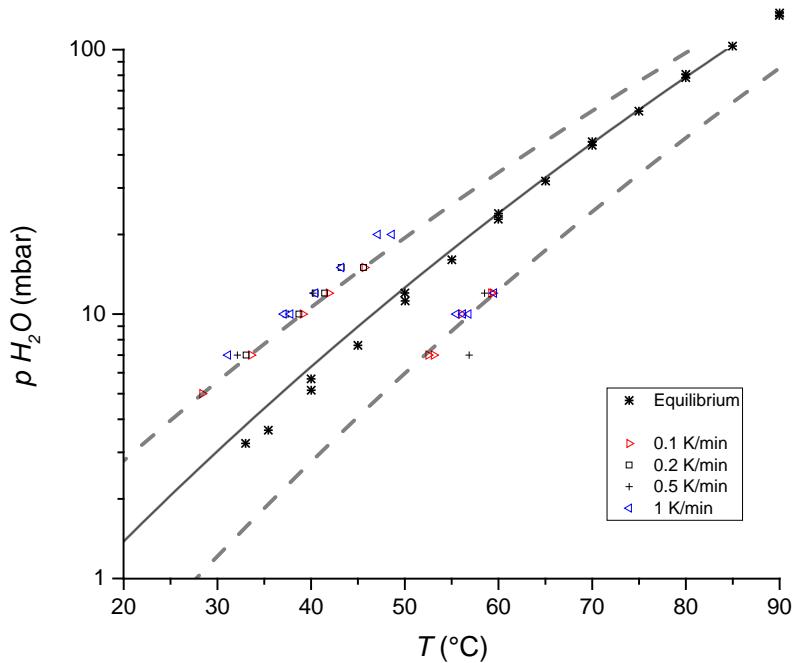
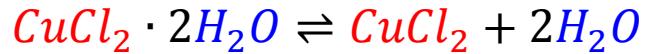


# Overshoot problem?

$\text{K}_2\text{CO}_3$ : isobaric cyclic at 12 mbar



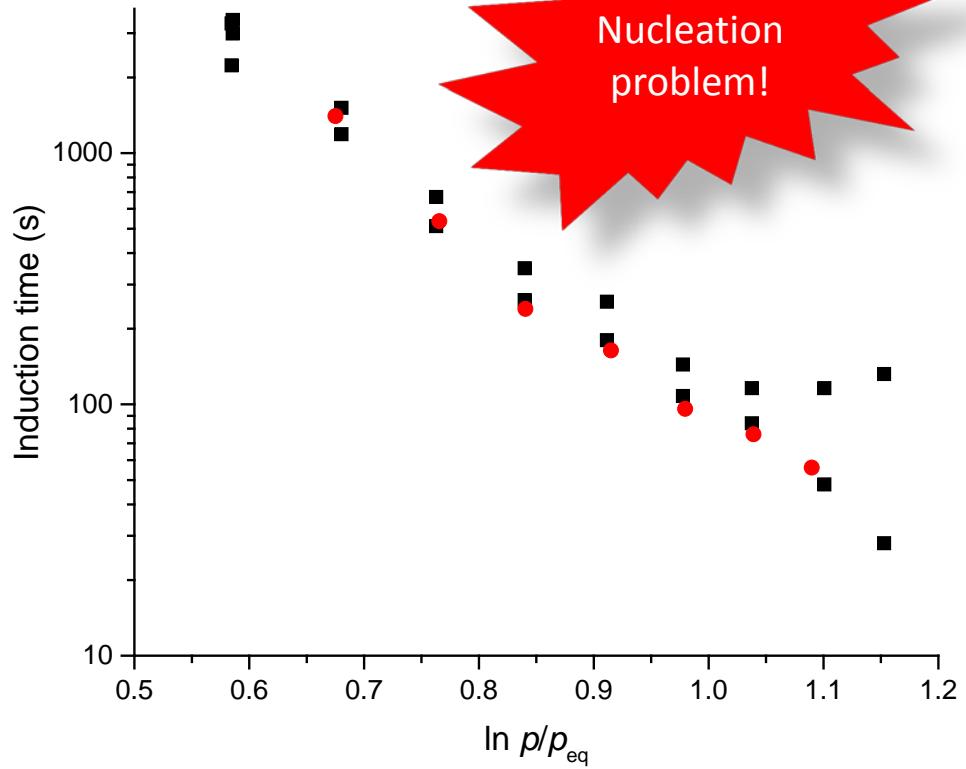
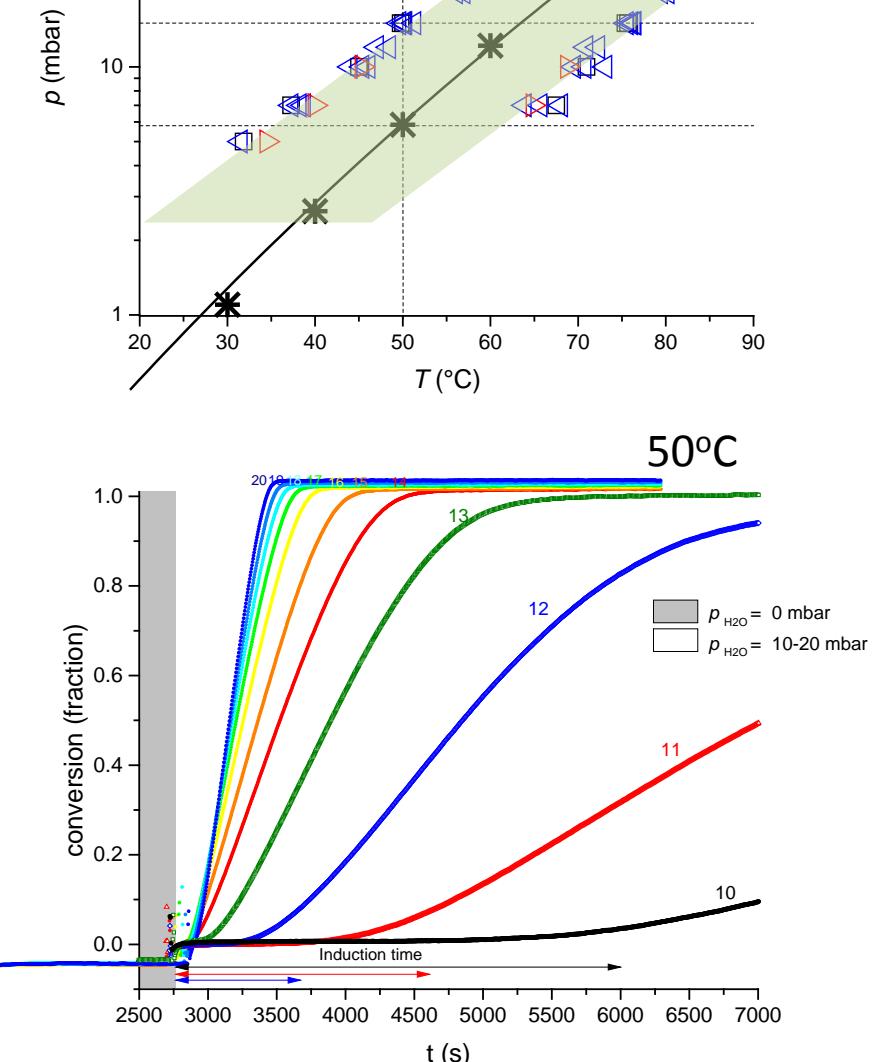
# Other hydrates



\*

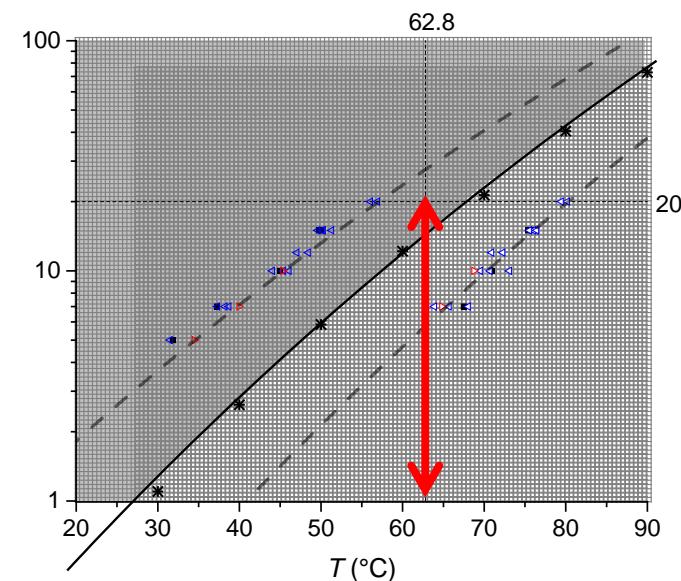
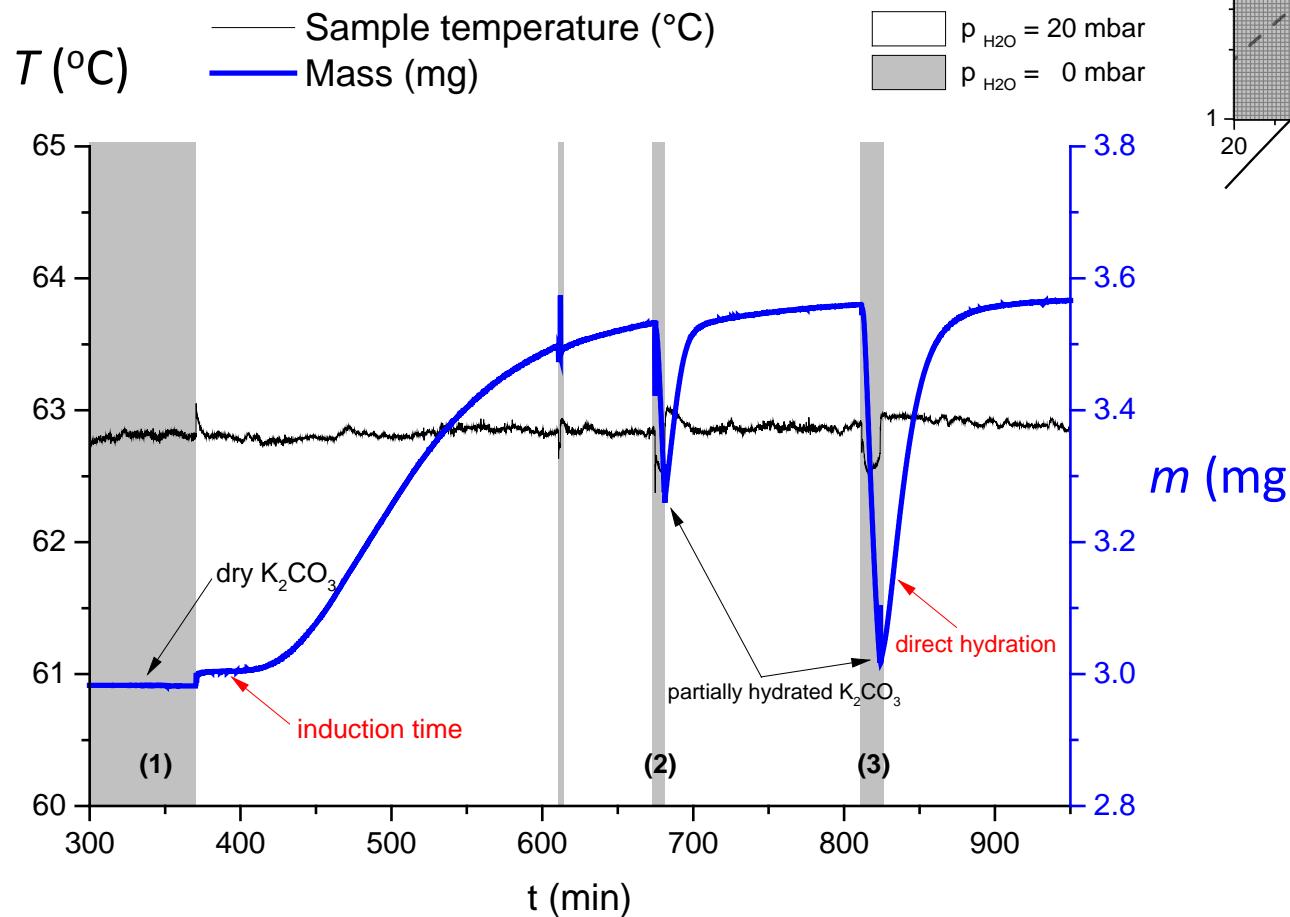
# Nucleation problem

$K_2CO_3: 50^\circ C$



# Nucleation problem

$\text{K}_2\text{CO}_3$  in the metastable zone



Solution?

# Classical Nucleation Theory (CNT)

Gibbs free energy nucleation of 3D object

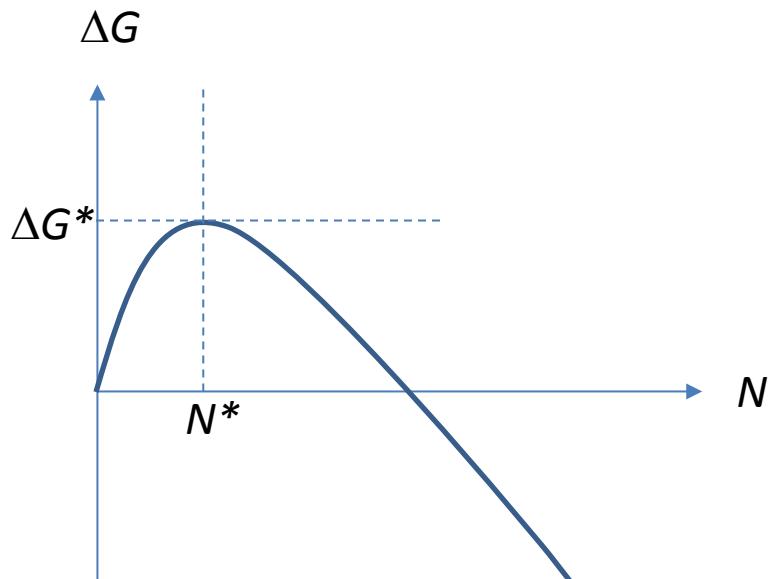
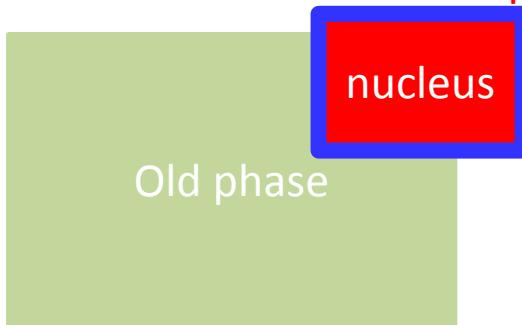
$$\Delta G = \sigma N^{2/3} - N k_B T \ln S$$



Interfacial free  
energy



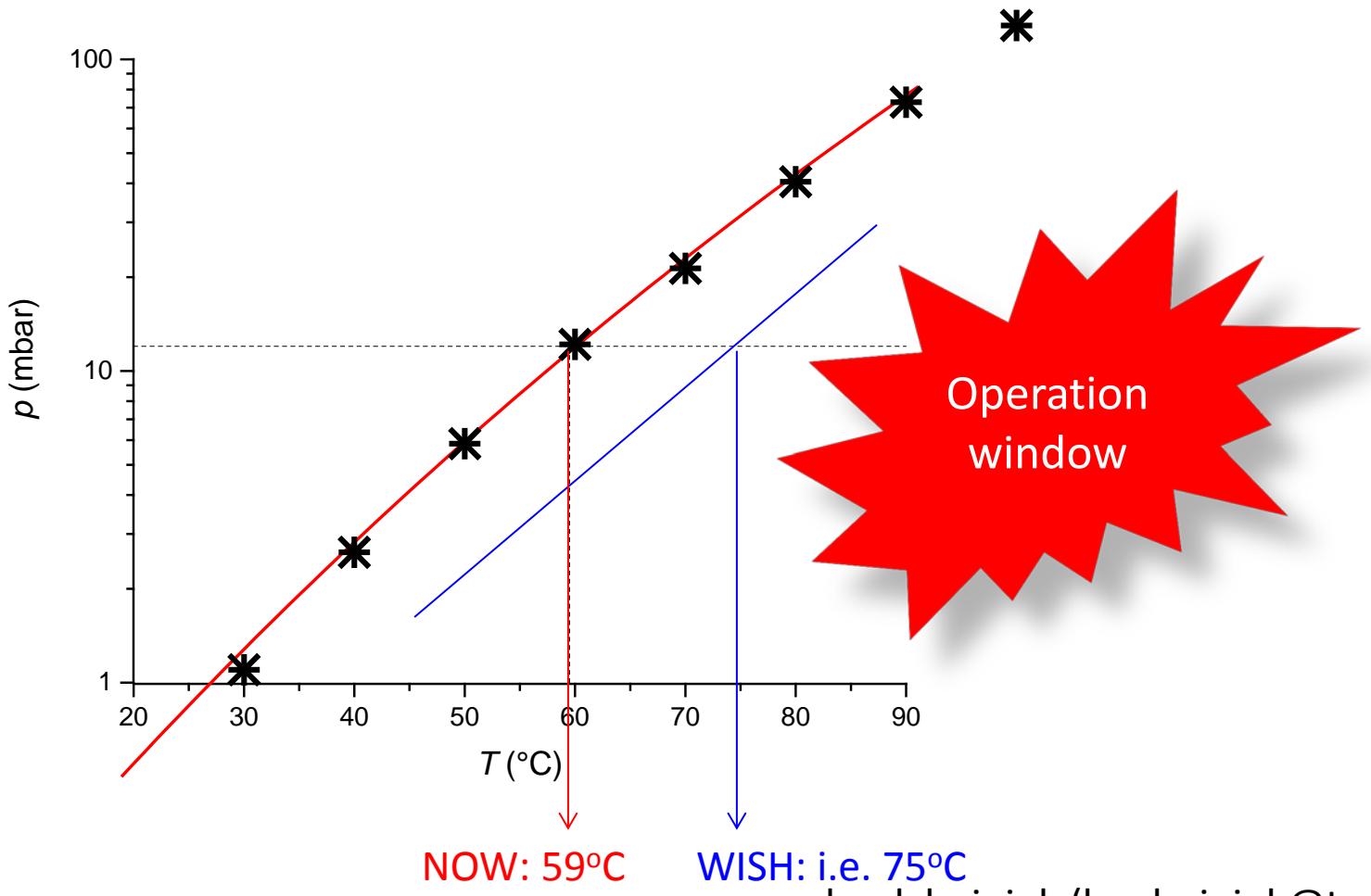
Difference between  
initial and final bulk  
phases



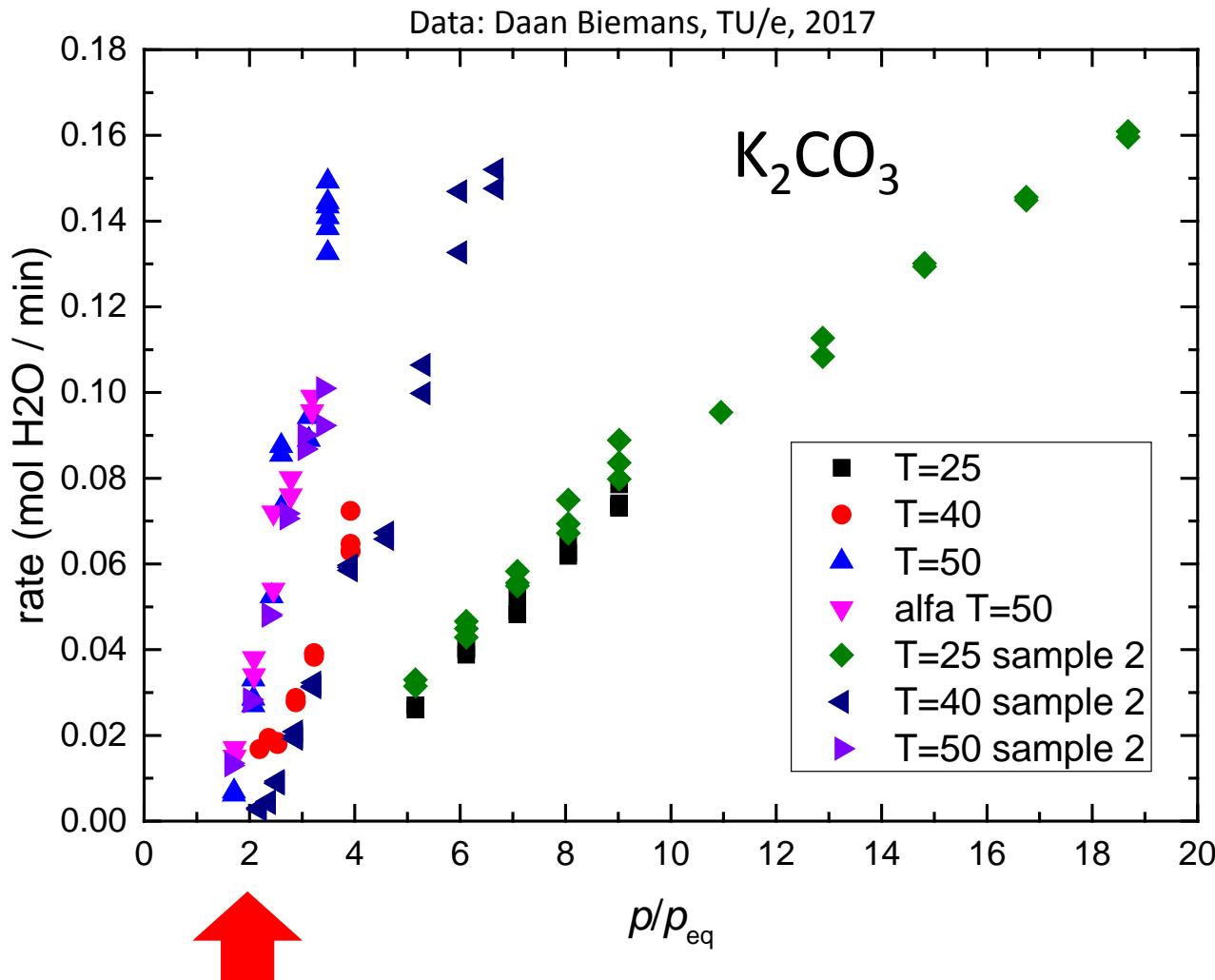
Nucleation rate

$$I \propto \exp(-\Delta G^*/k_B T)$$

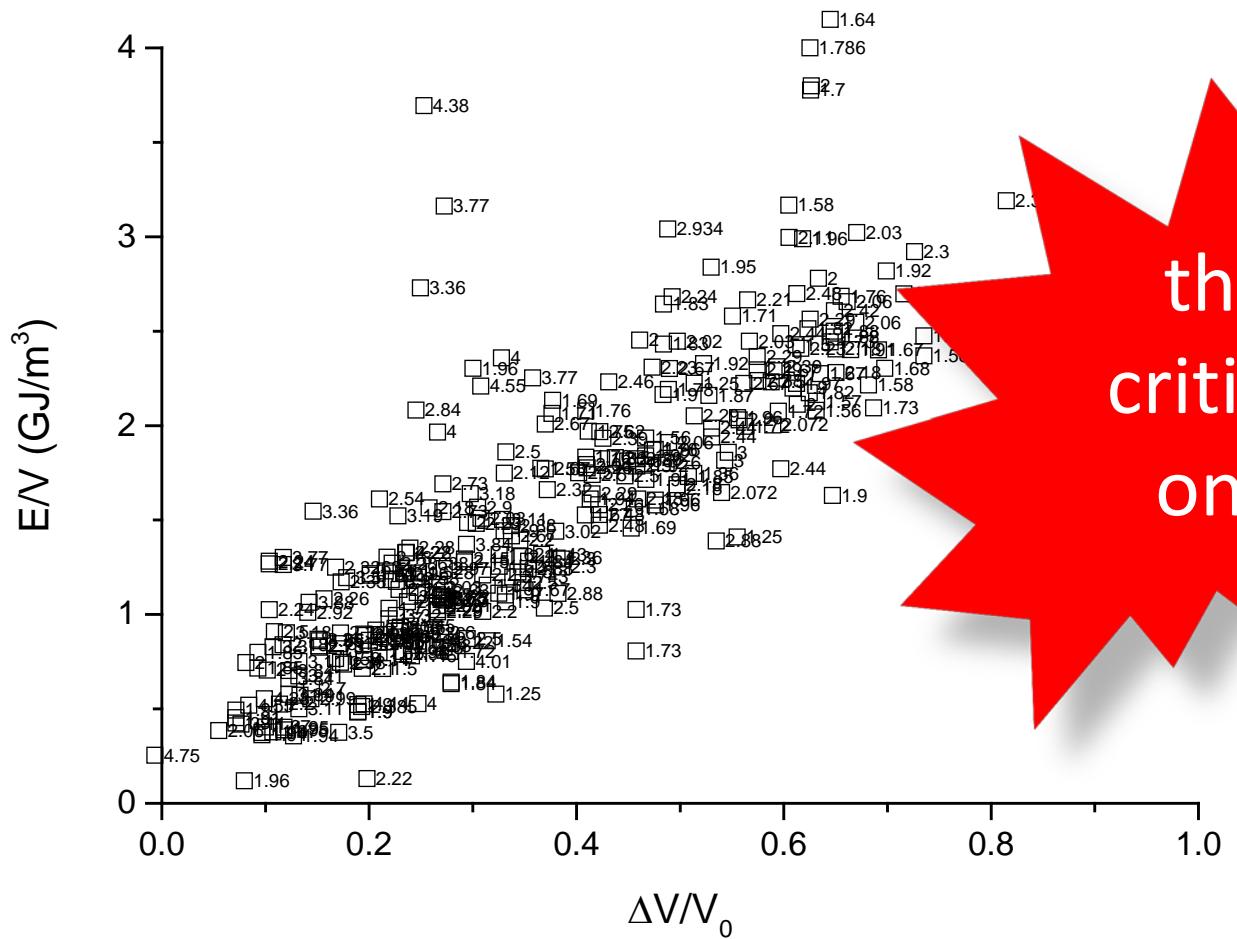
# Challenge 1: shift phase lines



# Challenge 2: accelerate kinetics

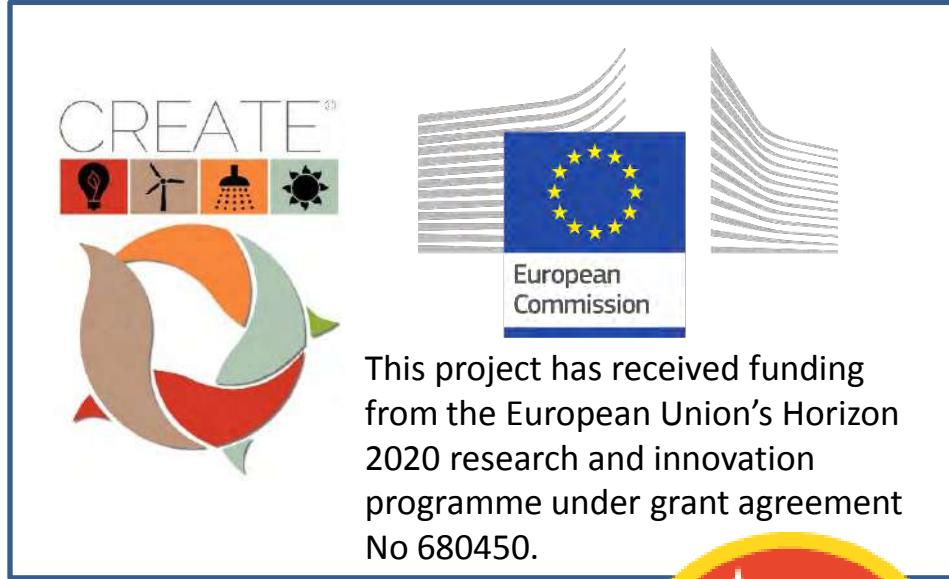


# Challenge 3: cyclic stability



# Acknowledgments

## Funding



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Hartmut Fischer  
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Leyla Sögütoglu  
Jelle Houben  
Hans Dalderop  
Daan Biemans  
Maarten Mackaij

TKI Urban Energy



CALDIC

# Challenged?

## 3 PhD positions open

Big NWO project: Mat4Heat

