

## **Thermodynamic database development for phase change materials**

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The PCM-Screening project aims at identifying suitable energy storage materials by exploring the enhanced heat storage potential of Phase Change Materials. One of the target groups concerns domestic applications, such as air conditioning, heat pumps and small cogeneration units, with temperatures between 0 and 100°C. Consequently, low temperature eutectic mixtures of salts and hydrated salts look particularly promising and a corresponding thermodynamic database is under development.

However, a successful thermodynamic description of the liquid phase needs to perform well for both dilute and concentrated salt contents – up to the pure salt to describe its melting point. Such requirement is yet to be fulfilled by the classical aqueous solution models. Therefore, we turn to an approach that applies the Non-Ideal Associate Species Model to model the aqueous-salt liquid within its full composition range. Aqueous ionic species are introduced in order to reasonably reproduce the aqueous properties around dilute concentrations, while the classical associate species are resorted in order to reproduce possible short-range-ordering effects on the properties of the salt-rich liquid.