Multiscale modeling in search of new materials for thermochemical energy storage.

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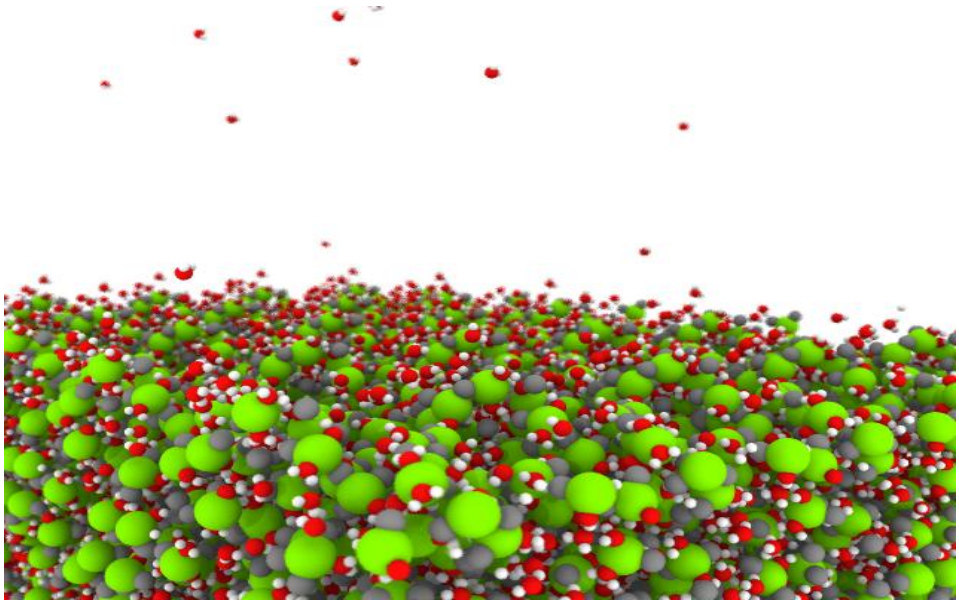
In order to improve the energy savings and promote renewable resources a reliable storage system is necessary. Among different approaches to store energy, thermochemical heat storage is a highly appealing. It is based on a reversible chemical processes, like sorption of water in hygroscopic salts. Salt-hydrates are one of the most relevant materials, because of their availability, costs, operating temperature, and energy density.

The concept of storing heat in a salt hydrate is based on the following three steps. (1) In a charging cycle (endothermic reaction) the salt hydrate adsorbs solar energy and disintegrates into a lower hydrate and water vapor. (2) The water and salt are stored separately. (3) In discharging (exothermic reaction) the dried salt hydrate is recombined with H_2O, and forms a higher hydrate again, which results in a release of heat. This allows one to store heat almost without losses over long periods of time in a compact and efficient way. However, challenges remain related to the materials stabilities and kinetics.

To overcome these challenges you have to use multiple simulation methods (Molecular Dynamics, Monte Carlo methods, machine learning USPEX) to study these salts on a nanoscale level. Firstly, to get more insights in fundamental characteristics like water and heat transport through the material. Secondly, to study nano-tailored modifications of the materials to improve their performance for the heat storage application.



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