Optimization of molecular simulations for thermochemical heat storage using new composite materials

Background

A promising concept for seasonal solar heat storage in the built environment is based on the reversible sorption process of water vapor into the crystalline structure of salt hydrates. The released heat can be used for room and/or tap water heating. Their main advantages are a high energy density, a reaction temperature in the proper range for domestic applications and their low price. However, the rate of heat release of these materials is low due to the low rate of hydration under atmospheric conditions. Composite and doped materials based on salt hydrates show better performance compared to pure materials. Furthermore, it is known that the crystalline structure and composition but also the surface defects and dislocations show a huge impact on the hydration/dehydration behavior. Besides, for some of the materials overhydration or decomposition of the matrix material is observed.

A detailed study on molecular level of the involved processes is necessary in order to gain insight into the dynamics of the hydration/dehydration processes and their limiting factors. A breakthrough will be possible by using a combination of Quantum Mechanical, Molecular Dynamics and Monte Carlo methods. We propose the use of this novel method to predict the structural and dynamic properties of new composite and doped materials in order to be used in seasonal heat storage systems. This research is going to be actively supported by ECN by comparing the simulation results with their experiments. ECN is also actively involved in materials research and reactor design for thermo-chemical heat storage.

Methods

The hydration and dehydration processes take place at molecular level and they can be modeled using the MD approach. MD simulations with reactive force fields (ReaxFF, [1]) are going to be used in order to simulate dynamic bonds in addition to non-bonding long range interactions. The force fields are going to be parameterized and optimized using quantum chemical data from Density Functional Theory (DFT) calculations [2]. On this level, there are two optimization methods available (Genetic algorithms and Monte Carlo techniques-MMC). We propose to compare the results of using these two methods and to study the hydration/dehydration of MgCl2hydrates.

Work plan

1) Literature review for implementation of genetic algorithm for optimization of reactive force field.
2) Molecular ReaxFF simulations using MMC optimization
3) Molecular ReaxFF simulations using Genetic algorithms
4) Comparison of the results for hydration/dehydration of salt hydrates
5) Writing Msc thesis

This project is in a Shell/FOM framework.

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