Executive Summary

Contract 4000119798
Challenges related to the design of a reservoir for the transport of H_2

RDPower, UniBa, UniChi and UniEin

ESA internal report

Contents

1 Problem statement

In the present project ESA required computational expertise and experience in the field of material modelling, hydrogen physical/chemical properties, molecular dynamics and chemical kinetics in order to model and optimize the technologies to store hydrogen. Indeed, in silico simulations have been required to achieve the objectives of the project.

2 Results obtained in the project

Both physical and chemical storage of hydrogen have been investigated. Molecular dynamics simulations have been performed to reproduce the experimental data available in the context of hydrogen storage in some categories of materials, specifically clathrates hydrates, magnesium hydrate (pure and doped), sodium alanate (pure and doped) and metal-organic frameworks. The tested desorption and melting temperatures, and the absorption/desorption pressures for all of them are comparable with the experimental data. In order to overcome the computational impossibility to prove the asymptotic gravimetric densities, an interpolation has been provided for sodium alanate. Such an approach has been tested in several conditions and proved to be appropriately reproducing experimental data. For the physical storage of hydrogen, the calculation of excited states of H2 have been performed both in a steady-state and time-dependent approach; the level population and ortho-to-para ratio has been provided as a function of temperature and density. Also in this case a good agreement with experimental data have been achieved.

A GUI has been written in order to allow users to perform all these simulations.

3 Final thoughts and future possible applications

Reactive Molecular Dynamics and Grand Canonical Monte Carlo simulations demonstrated to be efficient computational tools to simulate the hydrogen storage in several kind of compounds. The same techniques are suggested to be used in other material modelling applications ESA might be interested in, for example water splitting, combustion, layer deposition to list some of them.