Novel Hydrogen-rich Crystalline Compounds for Hydrogen Storage

Maaike C. Kroon,1,2 Hugh Docherty,3 Peter T. Cummings,3,4 Cor J. Peters,1,5 Geert-Jan Witkamp1 and Wendy L. Mao2,6

1Department of Process & Energy, Delft University of Technology, Delft, Netherlands
2Deparment of Geological & Environmental Sciences, Stanford University, Stanford (CA), USA
3Department of Chemical Engineering, Vanderbilt University, Nashville (TN), USA
4Nanomaterials Theory Institute, Center for Nanophase Materials Sciences, Oak Ridge National Laboratory, Oak Ridge, (TN), USA
5Chemical Engineering Program, Petroleum Institute, Abu Dhabi, United Arab Emirates
6Department of Photon Science, SLAC National Accelerator Laboratory, Menlo Park (CA), USA

Increasing world energy requirements, combined with the decreasing availability of fossil fuels, increasing environmental pollution and global climate change, has prompted an international search for more sustainable energy sources and storage media. A particularly promising alternative to fossil fuels is hydrogen. Unfortunately, due to the difficulty in finding a practical storage medium, its use as a fuel, for instance for application in the automotive sector, is currently limited. In order to be considered practical, a hydrogen storage material should satisfy a number of requirements, including a high storage capacity (high hydrogen content by mass and volume), ambient storage temperature and pressure, a fast uptake of hydrogen, and reversible hydrogen release. So far, a material that meets these requirements is does not exist. In this work, we develop a novel hydrogen storage material that fulfills the above-mentioned requirements. The idea is to store hydrogen in the hydrogen-rich crystalline molecular compound tetrahydrogenmethane ($CH_4(H_2)_4$), which contains as much as 33.4 wt% molecular hydrogen. Not much is known about how this material stores such a remarkable amount of molecular hydrogen: Even something as basic as its structure has not yet been identified. Motivated by this, we investigate the structure of tetrahydrogenmethane, as well as the interaction of hydrogen with this material, using a combined experimental – molecular simulation approach. We also identify promoters that may be added to this material to decrease the necessary storage pressure. Results will be presented at the conference.