

Nanoconfinement of metal borohydrides in zeolitic imidazolate frameworks

The use of hydrogen as an energy carrier is one of the major scientific fields focused on lowering the carbon footprint of energetics. Even though the gravimetric energy density of hydrogen is very favourable, its volumetric density is low, necessitating the development of advanced storage materials and techniques.

This work presents the synthesis and characterization of hydrogen storage material ZIF-8/LiBH₄, composed of microporous zeolitic imidazolate framework ZIF-8 (the compound of zinc cations and 2-methylimidazolate anion ligands) and nanoconfined borohydride LiBH₄. The material has a relatively low dehydrogenation onset temperature of about 120 °C, binds CO₂, and is not stable in air. Based on periodic DFT calculations, we have made predictions on the behaviour of the nanoconfined species in the pores of the framework.

We have performed additional characterization of [Mg₃{(Im)BH₂(Im)}₆(ImH)₆] · CH₃CN, a trinuclear magnesium complex compound, where magnesium centres are bridged by imidazole-substituted borohydride anions, and attempted to use it as a precursor for further syntheses. We have shown that the compound is stable in air and determined the temperature of its thermal decomposition. We have explored the behaviour of CH₃CN solvate molecules by DFT methods.

Several computer programs were developed in this work to support the research process, including a program for powder pattern indexing using the Monte Carlo method and a program for crystal structure manipulation. The principles of their operations, as well as general experience with publicly sharing the programs, is presented.

Keywords: ZIF, borohydrides, hydrogen storage, computer programs