Application 2064

MOFs as dihydrogen containers

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Regarding potential energy sources to replace fossil fuels, green H2 represents a clean alternative fuel choice since it can be used in fuel cells. However, the high-capacity storage of H2 is a difficult problem that has to be tackled for a successful use of this gas as sustainable energy source. MOFs are materials that generally exhibit exceptionally high specific surface areas. For instance, 1 m3 of MIL-101 can absorb the equivalent quantity of 400 m3 of CO2. Hence, such highly porous materials find applications in gas storage and separation, and important progresses in the areas of H2 storage are regularly reported in the literature. However, most of this research is done at the lab scale and more investigations are still required to further improve the absorption capacities and material properties, for practical (industrial) applications.

Our objective is to design and develop porous MOFs that can selectively adsorb large quantities of H2, in a selective manner. To date, we have prepared 5 different MOFs for which the investigation of the gas-sorption properties is now required. For the accurate characterisation of the hydrogen storage properties of these materials it is thus necessary to perform a systematic series of H2 adsorption/desorption measurements at least at cryogenic temperatures and pressures ranging between 1-120 bar. In addition a comparative study of their sorption capacity with respect to other technologically relevant gases (e.g. CO2, CH4, N2) also needs to be carried out. The HYSORB facility of NCSR "Demokritos" with its specialised infrastructure for volumetric and gravimetric gas sorption studies is well-suited for these critical measurements.

It is thus proposed to carry out in HYSORB the following experiments on the five different MOF samples:

(a) TGA measurements on all samples to verify complete removal of solvents
(b) N2 adsorption/desorption measurements at 77K for the determination of the pore properties (specific surface area, pore size/volume etc.) of all samples

(c) low pressure (up to 1 bar) volumetric H2 sorption measurements at 77 K
(d) high pressure (up to 120 bar) volumetric H2 sorption measurements at 77 K
(e) depending on the time available high pressure (up to 120 bar) sorption measurements of other gases (e.g. CO2, CH4, N2) at different temperatures.

Given that prior to each sorption measurement it is necessary to appropriately pretreat

(outgass) the samples by heating under high vacuum for at least 12 hours, it is estimated that the above set of measurements will require approximately 5 x 9 days/sample = 45 days.