A heuristic model for H_2 physi-sorption on and in nanomaterials

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Abstract

The gravimetric and volumetric hydrogen density in porous and non-porous nanomaterials is determined with a model only based on two material parameters, the material density and the specific surface area. Materials as small particles after synthesis exhibit a much lower packing density than the crystal density, which significantly reduces the volumetric hydrogen density.

Introduction

Nanomaterials absorb empirically 0.6 monolayer [1] of liq. hydrogen at 100 K based on the surface determined by N_2 adsorption in liq. N_2 with the BET method. However, the fit of the excess hydrogen uptake vs. the BET specific surface area intercepts the axis close to 1.5 mass%H_2 ($A_{spec.}$ = 0 $m^2 \cdot g^{-1}$). The packing density of MOF's is only close to 50% of the crystal density [2].

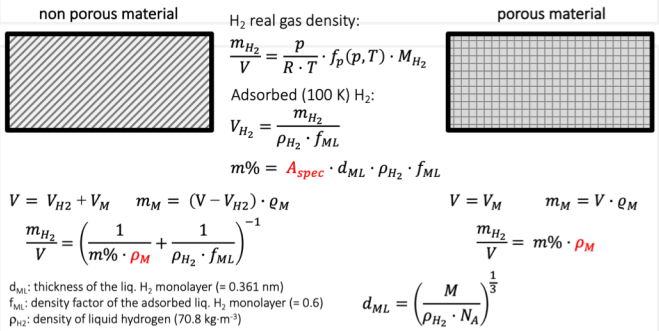
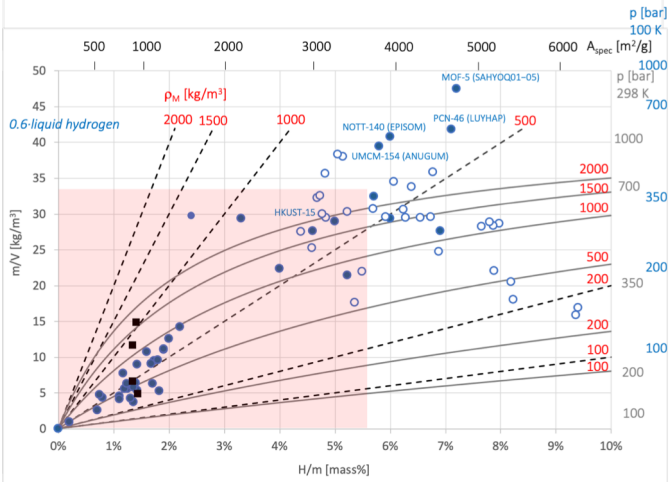


Fig. 1 (above) Model conditions and results for non porous and porous materials. Fig. 2 (right) Volumetric versus gravimetric adsorbed hydrogen density in nanomaterials. The red area indicates the rage covered by compressed hydrogen at 298 K.

Model

The model assumes the adsoption of 0.6 monolayer of liq. hydrogen at 100 K on the surface of non-porous materials and in the pores of porous materials. The gravimetric and volumetric hydrogen density is calculated with only two material parameter the packing material density ρ_M and the specific surface area A_{spec} using the density of liquid hydrogen (70.8 kg·m^{-3}) at 21 K.



Conclusion

Very few metal organic frameworks (MOFs) exceed the gravimetric and volumetric hydrogen density at 100 K of compressed H_2 at 700 bar and 298K (red area in fig. 2). However, some reported data are erroneous, the pore volume in the material is not large enough to host the reported amount of hydrogen, due to overestimation of the packing density and the excess hydrogen uptake.

References

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[3] A. Züttel, W.K. Liu, J. Ruffiner, L. Lombardo, "A heuristic model for H_2 physisorption on and in nanomaterials", to be submitted (2025).

[4] Poster presentation, GRC: Hydrogen-Metal Systems, Les Diablerets, 22. – 27. June 2025

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