

Design and synthesis of various MOFs for hydrogen storage

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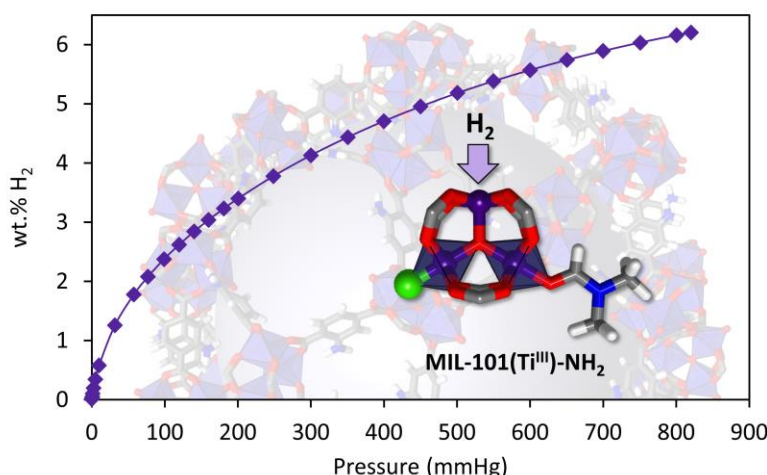
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Porous materials have emerged as highly promising candidates for hydrogen storage due to their high surface area. Metal-organic frameworks (MOFs) in particular, owing to their structural versatility, provide an ideal environment for accommodating hydrogen molecules. This presentation will showcase our latest achievements in the realm of porous hydrogen storage materials, with a primary focus on the design, synthesis, and application of MOFs. A first part of our research focusses on exploring the potential of understudied metal centers, such as Ti(III), for their interaction with hydrogen through Kubas interactions. A second part aims at investigating environmentally friendly approaches based on green chemistry procedures and sustainable biosourced linkers for discovering new efficient candidate materials for H₂ storage and separation.

One notable achievement involves the synthesis of a novel MOF, named MIL-101(Ti^{III})-NH₂, obtained from the cost-effective precursor (TiCl₃)₃·AlCl₃.¹ This MOF, featuring amine functionalities on its linkers, exhibited superior interaction with hydrogen at 77 K at pressures below 1 bar compared to the pristine MIL-101(Ti^{III}) without amine groups. Remarkably, MIL-101(Ti^{III})-NH₂ demonstrated an adsorption capacity of approximately 6 wt.% H₂ under these conditions.

Regarding green approaches, we observed exceptional interaction with H₂ in a magnesium-based MOF built from a biosourced linker, in which maximum excess adsorption at 77 K was observed at only 6 bar. In-depth studies, including in situ X-ray synchrotron diffraction experiments, revealed the activation process and the formation of active open-metal sites upon a crystalline phase transition. The H₂ sorption mechanism will be further unveiled through in situ neutron diffraction.

In summary, our findings showcase the potential of MOFs with understudied metal centers and obtained through environmentally friendly synthesis for efficient hydrogen storage applications.



References

[1] T. Steenhaut, S. Lacour, G. Barozzino-Consiglio, K. Robeyns, R. Crits, S. Hermans, Y. Filinchuk, *Inorganic Chemistry*, 61 (2022) 11084 – 11094.