Exploring Isostructural Metal-Organic Frameworks with Biosourced Linkers for Enhanced Hydrogen Sorption

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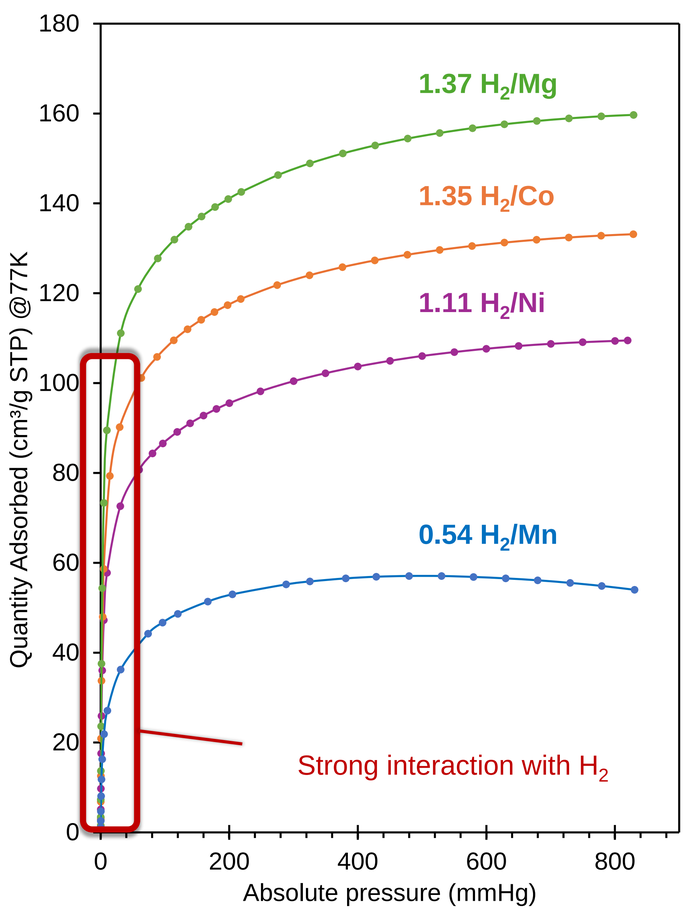
Introduction

In this work, we explore a series of isostructural M(II) gallate MOFs constructed from a biosourced linker, with metal variation influencing their hydrogen sorption behavior. Among them, MgGallate shows the highest performance. Its ultramicroporous structure enables efficient confinement-based physisorption, leading to strong H_2 uptake without the involvement of open metal sites.

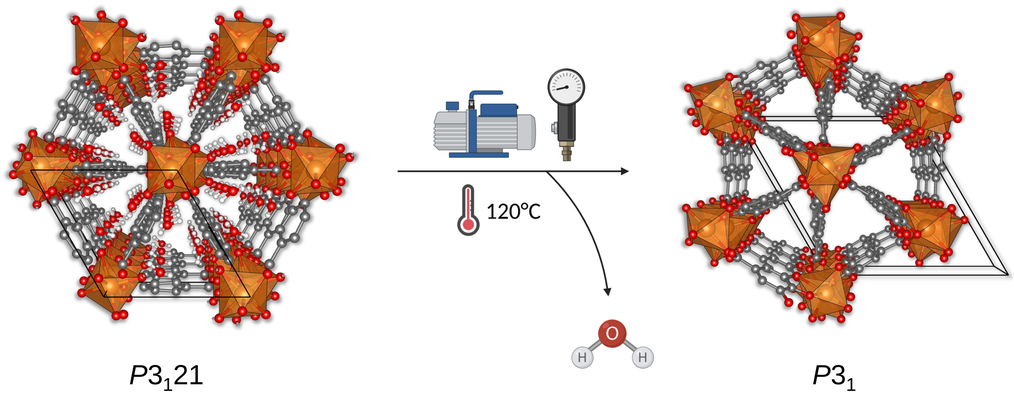
Isostructural MOFs: metal center matters



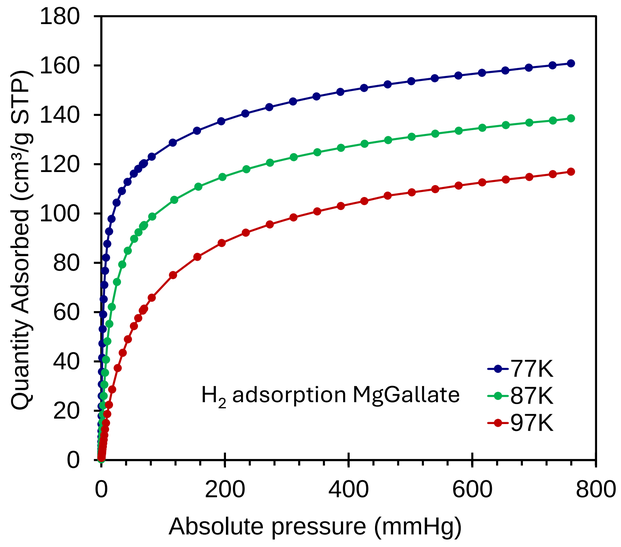
- Mg, Ni, Co & Mn gallates synthesized - all isostructural.
- H_2 uptake varies drastically by metal.
- Mg has highest uptake (1.4 wt%) - basis for further investigation.

Hydrogen sorption properties of MgGallate

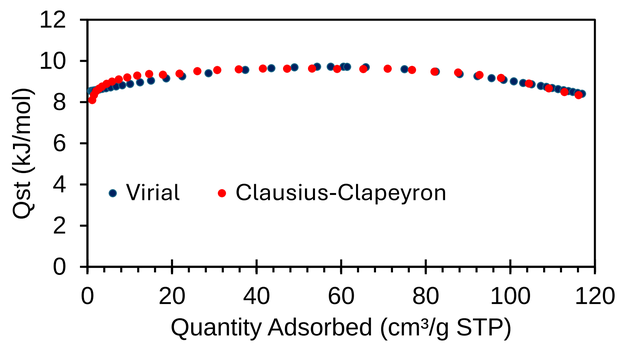
Organic linker rotation & space group change determined by PXRD



$P3_121$ $P3_1$

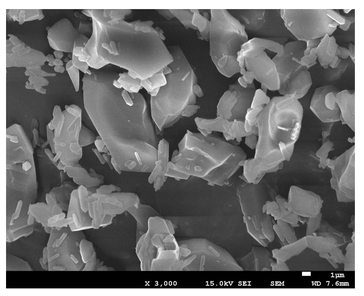


- Q_{st} = 8.6 kJ/mol, over full coverage
- Equilibrium reached in < 2 min

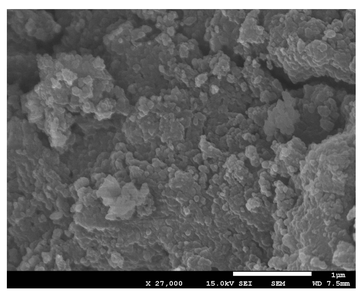


Synthesis: green & scalable production

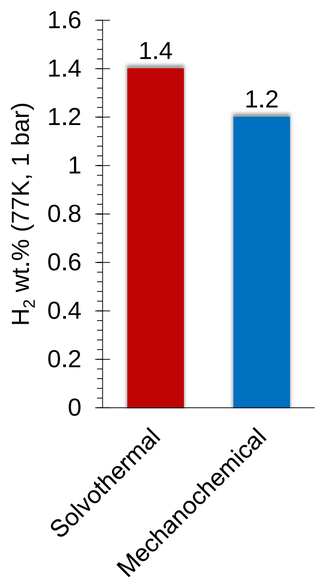
	Solvothermal	***Mechanochemical***
Reagents	$MgCl_2$ + gallic acid + KOH	$Mg(OH)_2$ + gallic acid
⏱ Time	24 h	1 h
🌡 Temperature	100 °C	RT
🔁 Yield	~62%	Quantitative
♻ Byproducts	❌ KCl	✅ None
📦 STY	30 kg/m³/day	605 kg/m³/day



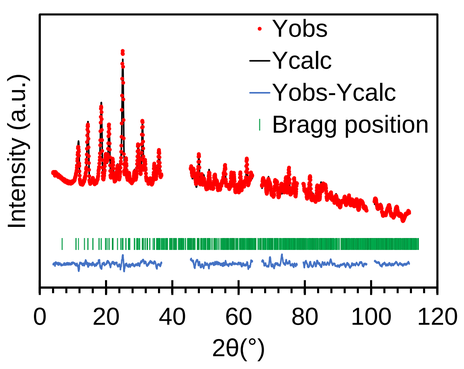
Solvothermal

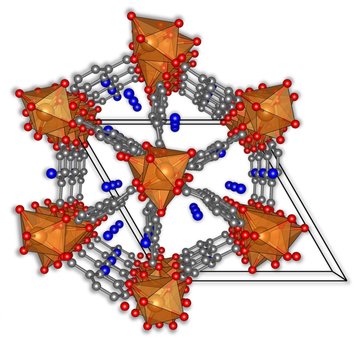


Mechanochemical



Confinement-based sorption confirmed by NPD





- D_2 adsorption sites located inside pores
- No binding to metal - purely van der Waals
- Matches bulk sorption data

Conclusions

We present a series of sustainable, ultramicroporous gallate-based MOFs. Among them, MgGallate exhibits the highest H_2 uptake (1.4 wt.% at 77 K and 1 bar) and a constant heat of adsorption (Q_{st}) of 8.6 kJ/mol. Neutron diffraction confirms that H_2 adsorbs within the pores without interacting with the metal centers. A green, scalable mechanochemical synthesis enables efficient production with high space-time yield.

Acknowledgements

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