1er Simposio Argentino de Redes Metal-Orgánicas (MOFs)
1st Argentinian Symposium on Metal-Organic Frameworks
ArMOF2021
7, 13-15 Octubre 2021

Design and Synthesis of Metal–Organic Frameworks for Hydrogen Storage Applications

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Hydrogen is a promising alternative fuel offering a means of storing renewable electricity and lowering greenhouse gas emissions, such as in the transportation sector. To enable the more widespread adoption of hydrogen as a fuel, adsorptive storage of high densities of H_2 at moderate temperatures and pressures has received significant attention as an alternative to high pressure or cryogenic storage. Microporous metal–organic frameworks (MOFs) are considered to be some of the best candidates for both on-board and stationary H_2 storage systems because of their high surface areas and highly tunable structures and pore chemistries. We have demonstrated that certain MOFs exhibit excellent storage properties, albeit at cryogenic temperatures. To further increase the hydrogen storage capacity of select MOFs, we pursue a promising strategy to introduce structural coordinatively-unsaturated metal centers that can bind H_2 with an enthalpy within the optimal range of −15 to −25 kJ.mol^{-1} for ambient-temperature hydrogen storage. The effectiveness of this approach is demonstrated using powder neutron diffraction and high-pressure hydrogen adsorption studies. *In situ* infrared spectroscopy is also discussed as an excellent experimental probe that affords site-specific information for hydrogen adsorption.

References

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