

Hydrogen storage in novel Zn(II) and Cd(II) MRT MOFs: A study using grand canonical Monte Carlo simulations

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— Author & Article Information

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The development of advanced hydrogen storage materials is essential for the adoption of hydrogen-powered vehicles as a sustainable alternative to fossil fuels. Metal–organic frameworks (MOFs) have emerged as promising candidates for meeting the Department Of Energy (DOE) storage targets. This study employs grand canonical Monte Carlo simulations to evaluate the usable gravimetric and volumetric storage capacities of hydrogen in newly synthesized Zn- or Cd-based MRT (Moldova Research Team) MOFs. These results are systematically compared to those of carefully selected MOFs that share either similar metal compositions or analogous pore structures and densities. Among the four MRT MOFs examined, MRT2 and MRT4 stand out as the most promising, exhibiting remarkable hydrogen storage capacities at ambient and low temperature and moderate pressures (25–35 MPa). In particular, the total volumetric and gravimetric storage capacities of MRT2 and MRT4 exceed the DOE targets at 77 K and ~5 MPa. Their hydrogen storage performance at room temperature proves highly competitive when assessed against MOFs with comparable metal compositions or porosity-density characteristics. The autonomy range of a hydrogen vehicle using MRT2 or MRT4 has been assessed, revealing that it can match that of a compressed hydrogen

revealing that it can match that of a compressed hydrogen system while operating at lower pressures, but requiring a larger tank volume.

Topics

[Fossil fuels](#), [Hydrogen energy](#), [Hydrogen storage](#), [Porous media](#), [Monte Carlo methods](#)

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