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Molecular simulation of copper based metal-organic framework (Cu-MOF) for hydrogen adsorption

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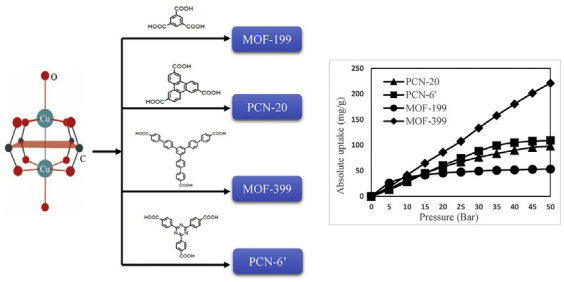
HIGHLIGHTS

- The hydrogen adsorption capacity of four copper-based Metal-organic frameworks is discussed.
- Grand Canonical Monte Carlo simulation is used to determine the adsorption capacities.
- Simulation is carried out at ambient and cryogenic temperatures for 0–50 bar pressure.
- Isosteric heat affects the adsorption at lower pressure and surface area affects the adsorption at high pressures.
- PCN-6′ is considered a viable material at 298 K and 77 K due to its high hydrogen uptake.

GRAPHICAL ABSTRACT



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ABSTRACT

Metal organic framework (MOF) are widely used in adsorption and separation due to their porous nature, high surface area, structural diversity and lower crystal density. Due to their exceptional thermal and chemical stability, Cu-based MOF are considered excellent hydrogen storage materials in the world of MOFs. Efforts to assess the effectiveness of hydrogen storage in MOFs with molecular simulation and theoretical modeling are crucial

Abbreviations: AA, Associative adsorption; BTC, Benzene-1,3,5-tricarboxylic acid; BBC, 1,3,5-Tris(4′-carboxy[1,1′-biphenyl]-4-yl)benzene; DA, Dissociative adsorption; GCMC, Grand Canonical Monte Carlo; MOF, Metal-Organic Framework; SBU, Secondary building unit; tbo, twisted boracite; TATB, 4,4′,4″-[1,3,5-triazine-2,4,6- triyltribenzoate]; TTCA, triphenylene-2,6,10-tricarboxylic acid.

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