440d Mechanisms of Hydrogen Adsorption in Metal Organic Frameworks

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We present the results of Grand Canonical Monte Carlo simulations of hydrogen adsorption in rigid Isoreticular Metal Organic Frameworks using the Universal Force Field. We calculate the adsorption isotherms at 77 and 298 K and compare our results with the available experiments. We find that the adsorption at 298 K does not meet either the gravimetric (6 wt%) or the volumetric (45 kg H2/m3) DOE 2010 target for use in automotive applications. The best material that we have tested, IRMOF-14, shows an excess adsorption around 10% at 77 K and 50 bar of pressure. The same material at room temperature presents an adsorption of only 0.7 wt% but, in this case, a large discrepancy between the available experiments and simulations is observed. We discuss the origin of this poor performance by an analysis of the potential energy surfaces of the hydrogen-framework interaction and give some indication on how the adsorption properties could be optimized.