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Hydrogen storage in M(BDC)(TED)$_{0.5}$ metal-organic framework: Physical insights and capacities†

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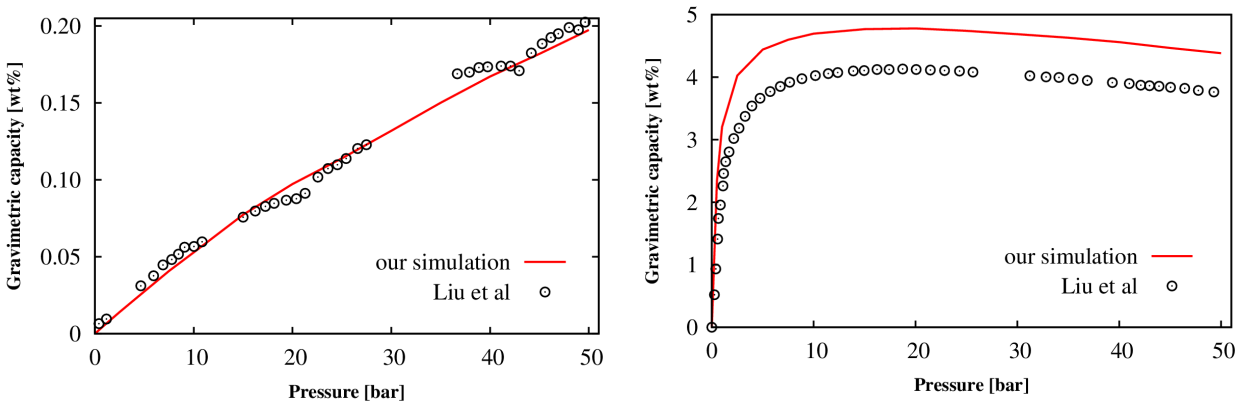

(a) At 298 K (b) At 77 K

Fig. S1 The excess H_2 uptake capacities of Zn(BDC)(TED)$_{0.5}$ at 298 K (a) and 77 K (b): our simulation and experimental data.[1]

Table S1 A comparison of gravimetric excess H_2 loadings between our simulation and available experimental data for Zn(BDC)(TED)$_{0.5}$[1]

M-MOF	Temperature, Pressure	This work (wt%)	Experimental data (wt%)	Errors
Zn(BDC)(TED)$_{0.5}$	298 K, 50 bar	0.197	ca. 0.202	ca. 0.005 wt% (2.5 %)
	77 K, 50 bar	4.380	ca. 3.760	ca. 0.620 wt% (16 %)
	77 K, the pressure at the maximum (~20 bar)	4.78	ca. 4.03	ca. 0.75 wt% (18.6 %)

1 J. Liu, J. Y. Lee, L. Pan, R. T. Obermyer, S. Simizu, B. Zande, J. Li, S. G. Sankar and J. K. Johnson, J. Phys. Chem. C, 2008, 112, 2911–2917.