Understanding the Effect of Confinement on the Liquid-Gas Transition: A Study of Adsorption Isotherms in a Family of Metal–Organic Frameworks

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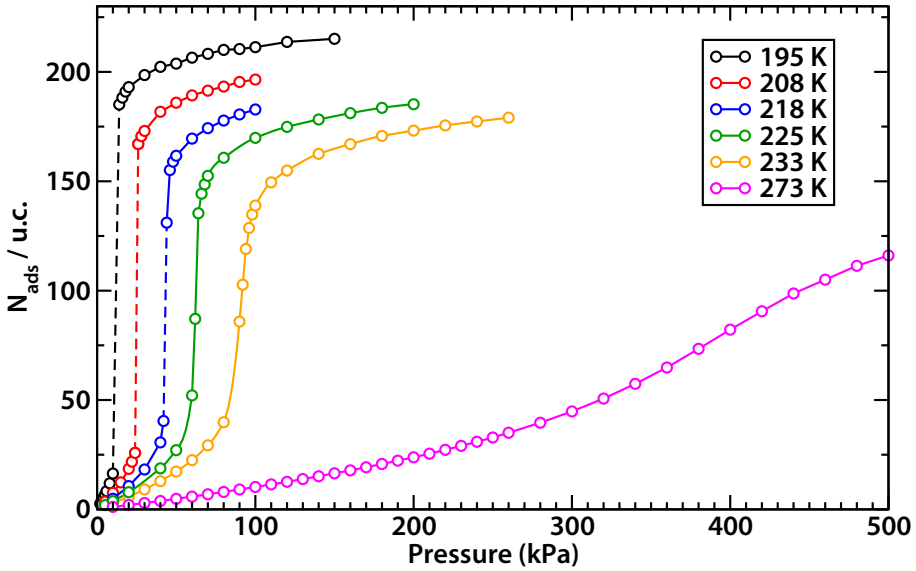

Fig. 1S: Adsorption isotherms of CO_2 in IRMOF-1 at different temperatures in the 195–273 K range, in linear pressure scale. The same data is plotted in fig. 2a with a logarithmic pressure scale.

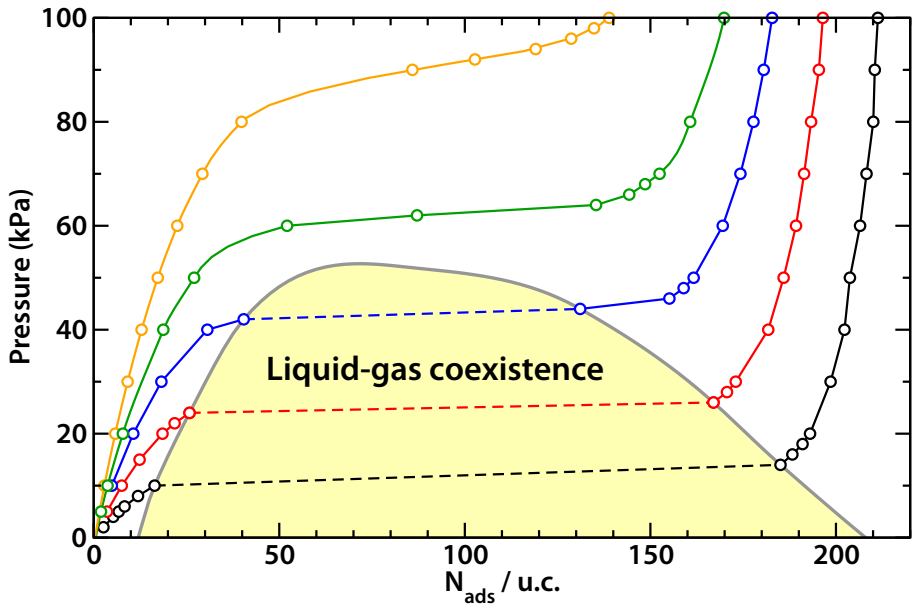

Fig. 2S: Adsorption isotherms of CO2 in IRMOF-1, plotted as P vs. N_{ads}, to highlight the similarity with classical compression isotherms in liquid–gas transitions. The liquid–gas coexistence area is highlighted in yellow.

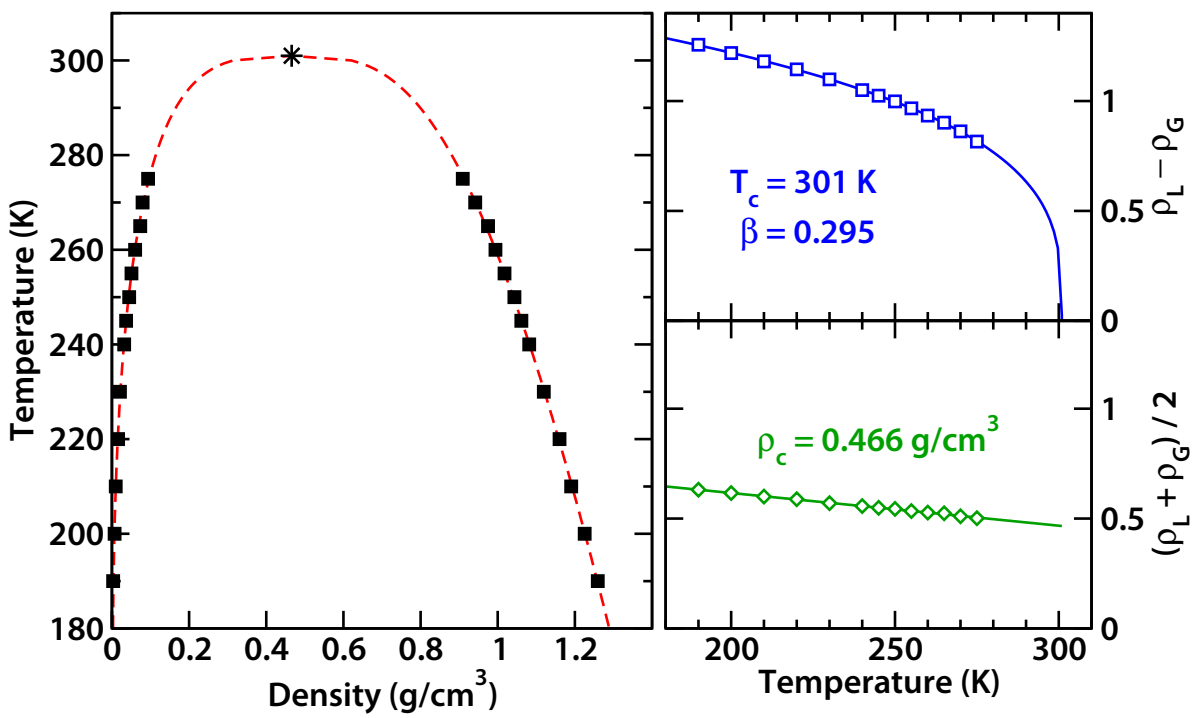

Fig. 3S: Left panel: liquid and gas densities for CO_2 phase coexistence, as a function of temperature, from Gibbs Ensemble Monte Carlo simulations. Right panels: fits of $(\varrho_L - \varrho_G)$ and $(\varrho_L + \varrho_G)/2$, determining the critical temperature and density. See text for details.

IRMOF–CO_2 interactions scaling factor λ	Adsorption enthalpy ΔH_{ads} at T = 208 K
1	13.2 kJ/mol
1.2	15.4 kJ/mol
1.5	18.6 kJ/mol
1.6	19.7 kJ/mol

Table 1S. Evolution of the adsorption enthalpy of CO_2 in IRMOF-1 (in the limit of zero loading), at 208 K, when IRMOF–CO_2 interactions are artificially scaled by a factor λ.