

An Optimal Single-Walled Carbon Nanotube Vessels for Short Term Reversible Storage of Carbon Dioxide at Ambient Temperatures

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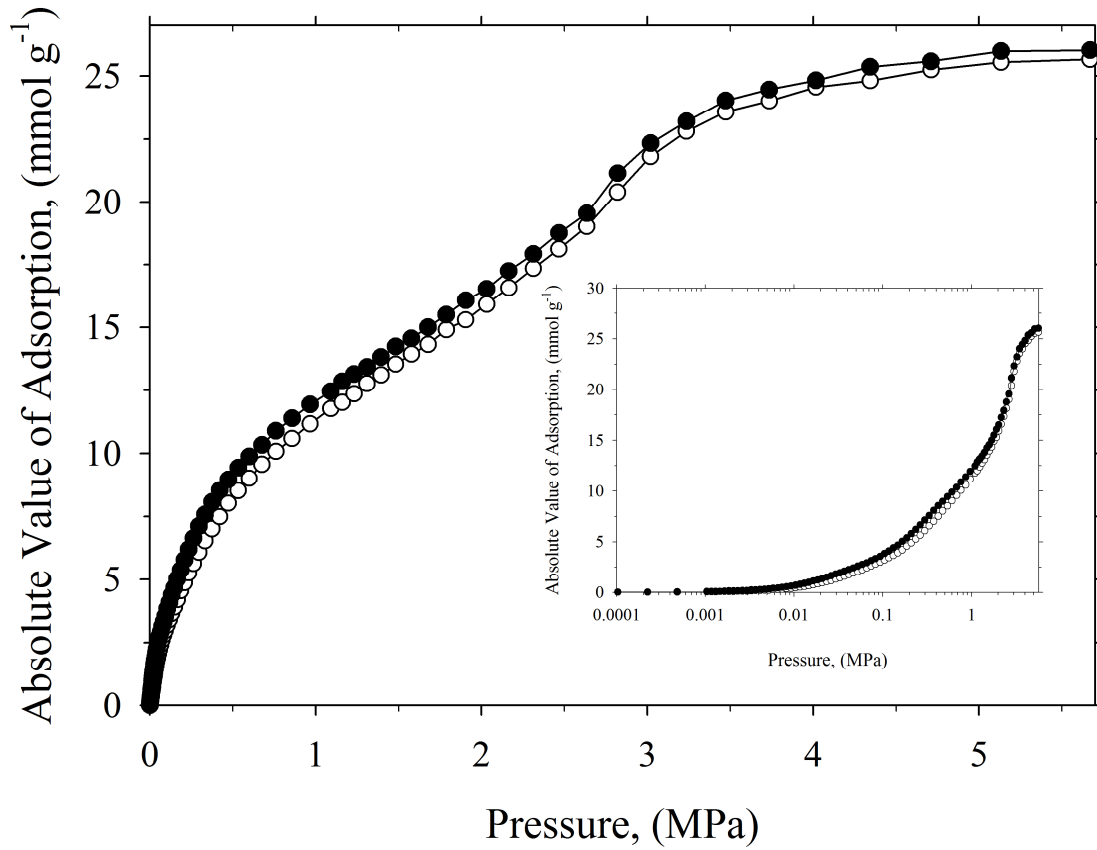


Figure 1S. Variation of the absolute value of CO₂ adsorption with the well depth of the solid-fluid Lennard-Jones potential (ϵ_{sf}) computed for the bundle of (28,28) single-walled carbon nanotubes at 298 K. Open circles correspond to well depth of solid-fluid Lennard-Jones potential computed from Lorentz-Berthelot mixing rule, ϵ_{LJ}^{LB} , whereas black circles correspond to $\epsilon_{sf} = 1.05 \cdot \epsilon_{LJ}^{LB}$. Note that an increase of ϵ_{sf} by 5 % results only slightly shifts of the absolute value of CO₂ adsorption due to altering of solid-fluid interactions. Observed increasing of adsorbed amount is within the accuracy of typical high-pressure adsorption measurements.

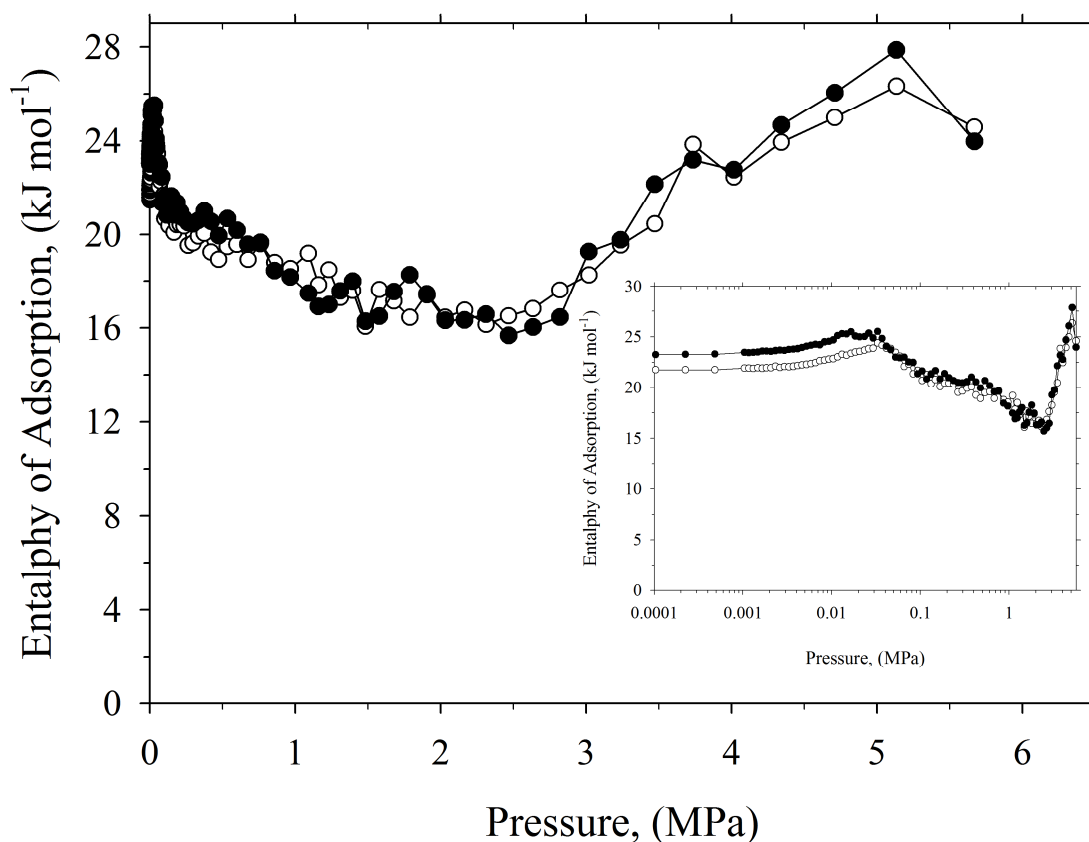


Figure 2S. Variation of the enthalpy of CO₂ adsorption with the well depth of solid-fluid Lennard-Jones potential (ϵ_{sf}) computed for the bundle of (28,28) single-walled carbon nanotubes at 298 K. Open circles correspond to well depth of solid-fluid Lennard-Jones potential computed from Lorentz-Berthelot mixing rule, ϵ_{LJ}^{LB} , whereas black circles correspond to $\epsilon_{sf} = 1.05 \cdot \epsilon_{LJ}^{LB}$. Note that an increasing of ϵ_{sf} by 5 % results only in slight shift of the enthalpy of CO₂ adsorption at low coverage due to altering of solid-fluid interactions. Observed increasing of the enthalpy of CO₂ adsorption is within the accuracy of typical calorimetric measurements.