

Supporting Information:

Evidence of Gate-Opening on Xenon Adsorption on ZIF-8: an Adsorption and Computer Simulation Study.

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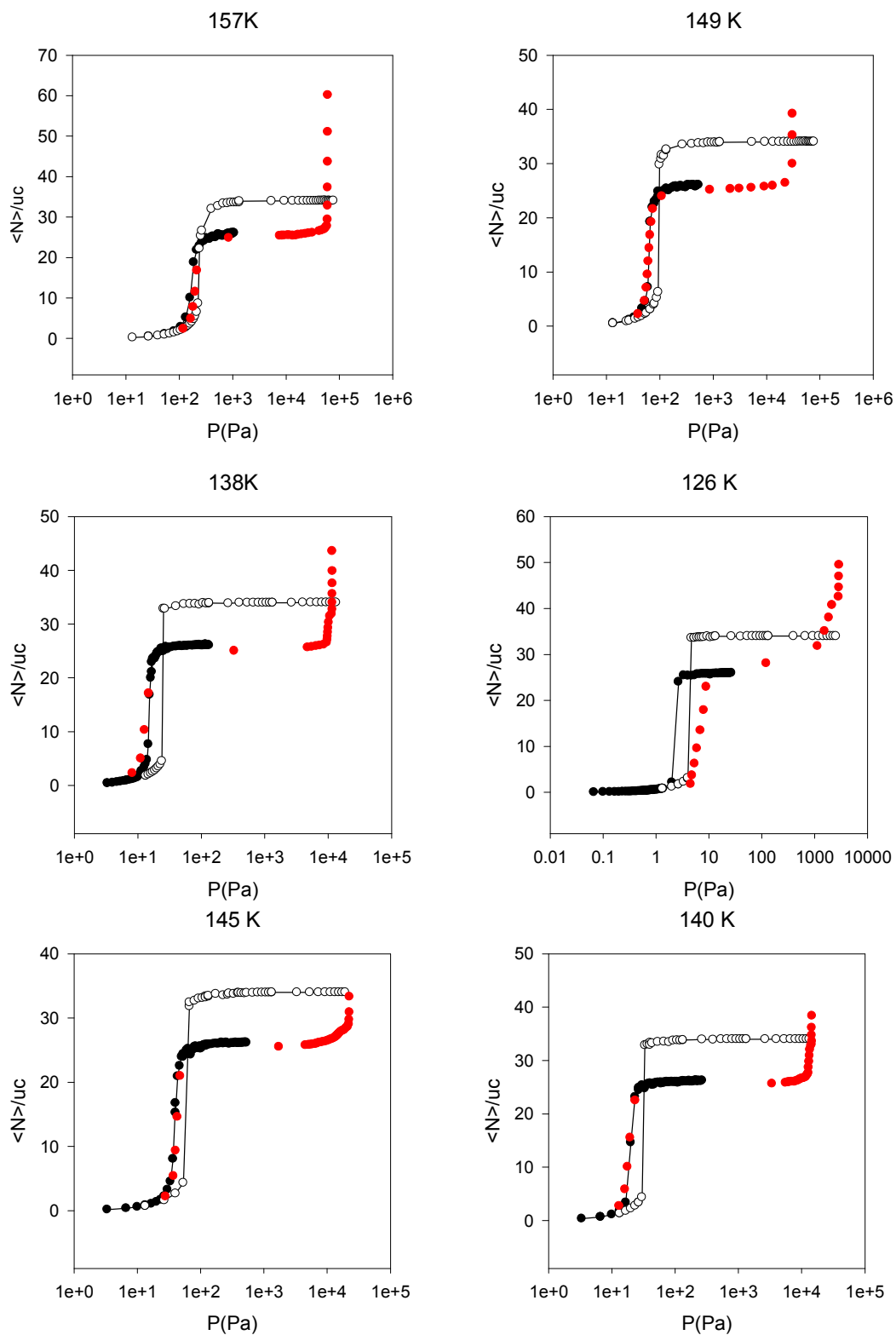


Figure S1- Experimental and simulated isotherms using the Mix Force Field at different temperatures.

Transferability of the potential

In order to check the transferability of the new developed potential, we have performed simulations of methane and argon adsorption. The results are in excellent agreement with the isotherms obtained by Fairen-Gimenez et alⁱⁱ for methane at 125 K and Pantatosakiⁱ for argon at 87 K

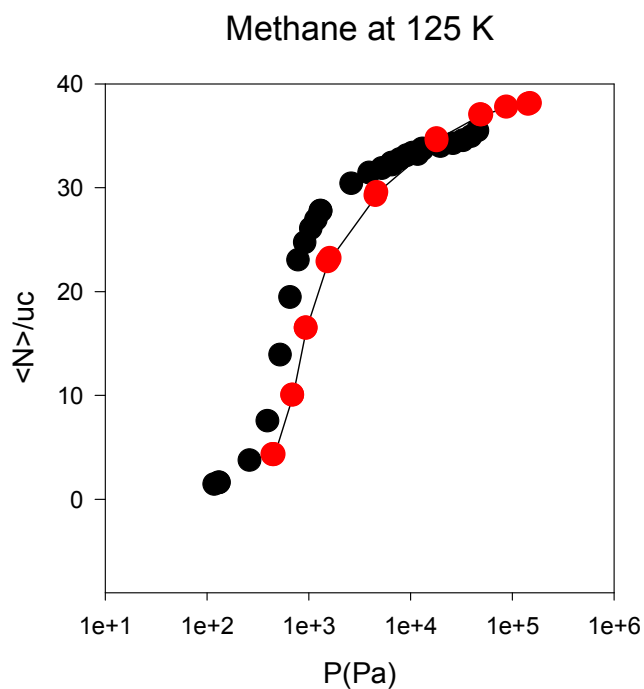


Figure S2. Methane adsorption at 125 K. The small circles are the simulation data. The big circles are the experimental data obtained by (Fairen-Jimenez, D., Galvelis, R., Torrisi, A., Gellan, A. D., Wharmby, M. T., Wright, P. A., ... & Dueren, T. (2012). Flexibility and swing effect on the adsorption of energy-related gases on ZIF-8: combined experimental and simulation study. *Dalton Transactions*, 41(35), 10752-10762).

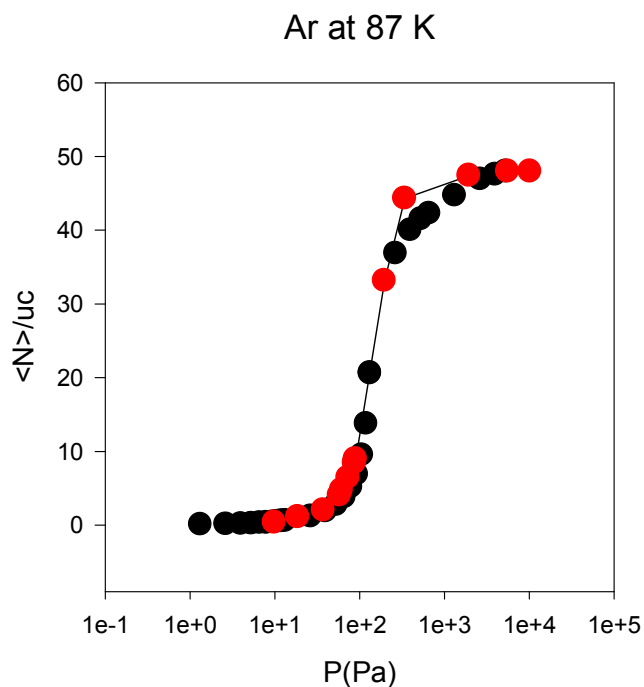


Figure S3. Argon adsorption K. The red circles are the simulation data. The big circles are the experimental data obtained by (Pantatosaki, E., Pazzona, F. G., Megariotis, G., & Papadopoulos, G. K. (2010). Atomistic simulation studies on the dynamics and thermodynamics of nonpolar molecules within the zeolite imidazolate framework-8. *The Journal of Physical Chemistry B*, 114(7), 2493-2503)

ⁱ Pantatosaki, E., Pazzona, F. G., Megariotis, G., & Papadopoulos, G. K. (2010). Atomistic simulation studies on the dynamics and thermodynamics of nonpolar molecules within the zeolite imidazolate framework-8. *The Journal of Physical Chemistry B*, 114(7), 2493-2503.