Electronic Supplementary Material (ESI) for Physical Chemistry Chemical Physics.

Supporting Information

Transferable Force Field for Adsorption of Small Gases in Zeolites

*A. Martin-Calvo[1], J. J. Gutiérrez-Sevillano[1], J. B. Parra[2], C.O. Ania[2], and S. Calero[1]**

[1]Department of Physical, Chemical, and Natural Systems, University Pablo de Olavide, Ctra. de Utrera, km. 1, 41013 Seville, Spain

[2] *Instituto Nacional del Carbón, INCAR-CSIC, P.O. 73, 33080 Oviedo, Spain*

[*]Correspondence should be addressed to S. Calero (scalero@upo.es)

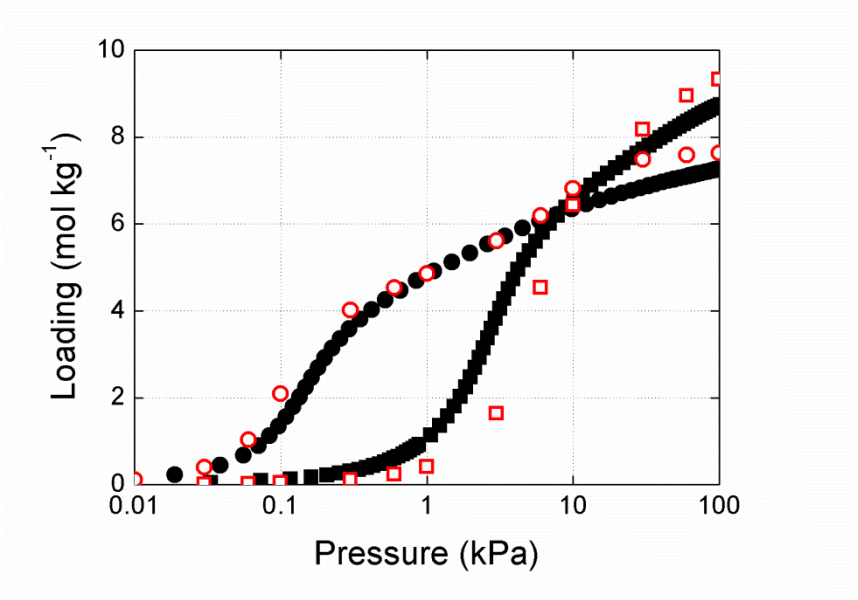

Figure S1: Experimental (full symbols) and computed (empty symbols) adsorption isotherms of argon (squares) and methane (circles) in ITQ-29 at 120 K. Computed adsorption isotherms show the excess loading for a better comparison with experiments.

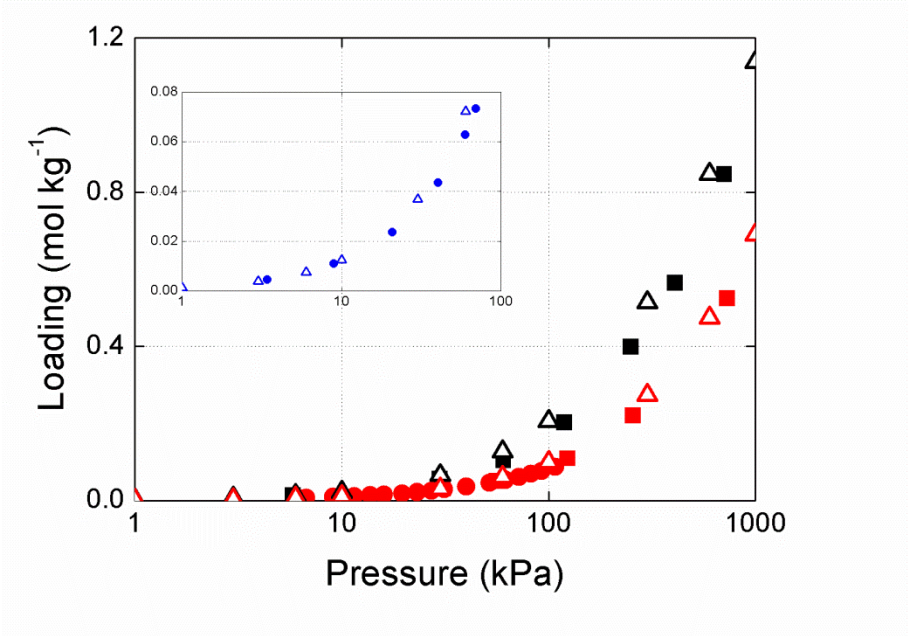

Figure S2: Experimental (full symbols) and computed (empty symbols) adsorption isotherms of nitrogen in pure silica MFI at 305K (black), 334 K (blue) and 343 K (red). Available data from Dunne *et al.*[1] (circles), and Golden and Sircar[2] (squares) are included for comparison. Computed adsorption isotherms show the excess loading for a better comparison with experiments.

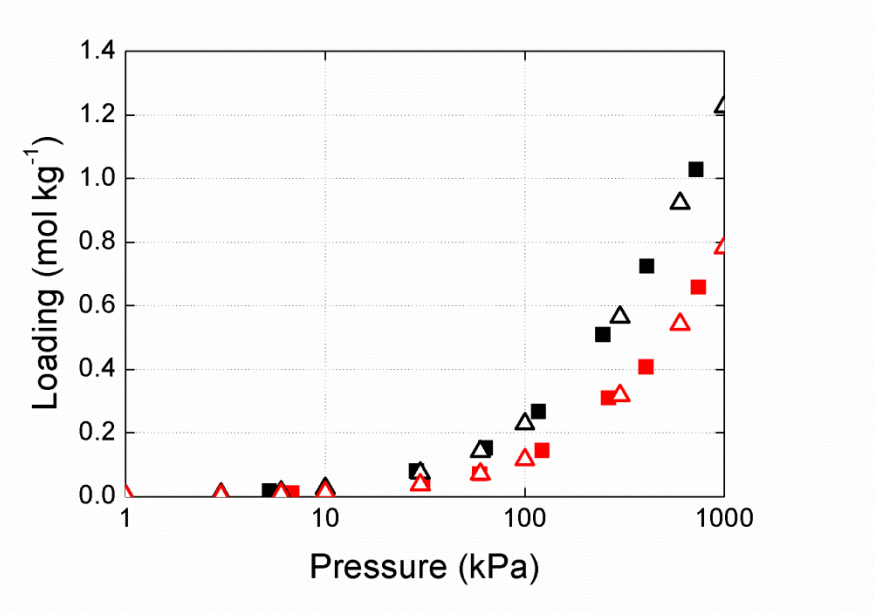

Figure S3: Experimental (full symbols) and computed (empty symbols) adsorption isotherms of carbon monoxide in MFI at 305K (black) and 341 K (red). Available data from Golden and Sircar[2] (squares) are included for comparison. Computed adsorption isotherms show the excess loading for a better comparison with experiments.

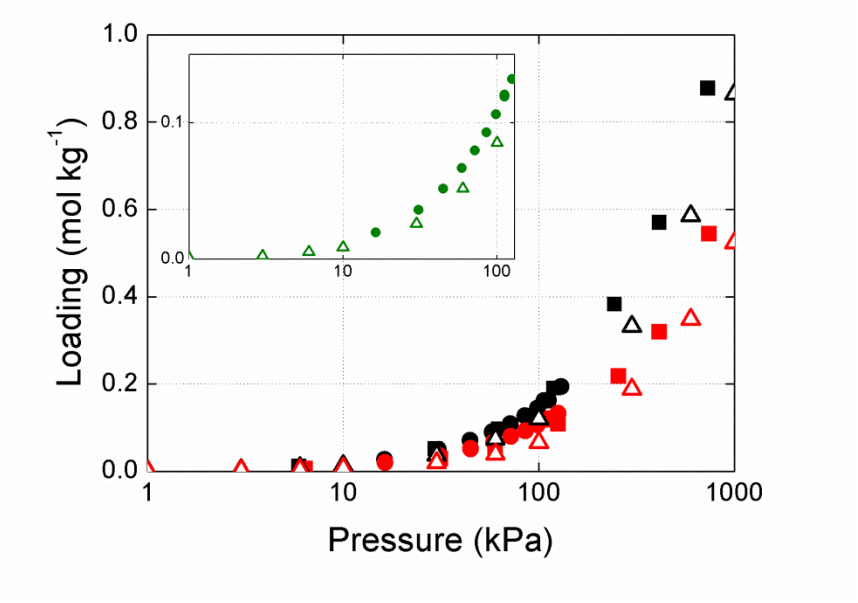

Figure S4: Experimental (full symbols) and computed (empty symbols) adsorption isotherms of argon in MFI at 305K (black), 325 K (green) and 342 K (red).Available data from Dunne *et al.*[1] (circles), and Golden and Sircar[2] (squares) are included for comparison. Computed adsorption isotherms show the excess loading for a better comparison with experiments.

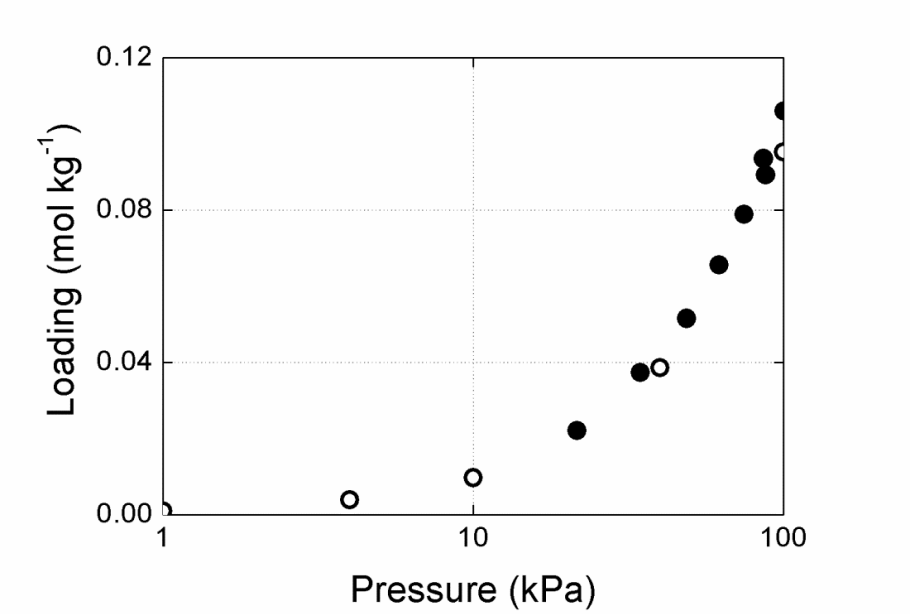

Figure S5: Experimental (full symbols) and computed (empty symbols) adsorption isotherms of oxygen in NaX Si/Al ratio=1.23 at 305 K (circles). Available data from Dunne *et al.*[3] are included for comparison. Computed adsorption isotherms show the excess loading for a better comparison with experiments.

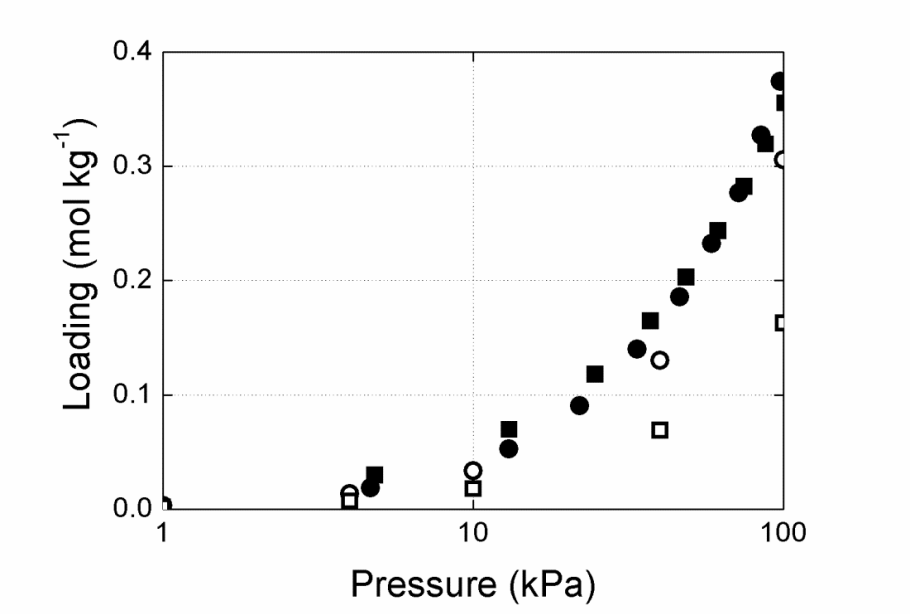

Figure S6: Experimental (full symbols) and computed (empty symbols) adsorption isotherms of nitrogen in NaX Si/Al ratio=1.23 at 305 K (circles), and Na-MFI Si/Al ration=30 at 295 K. (squares) Available data from Dunne *et al.*[3] are included for comparison. Computed adsorption isotherms show the excess loading for a better comparison with experiments.

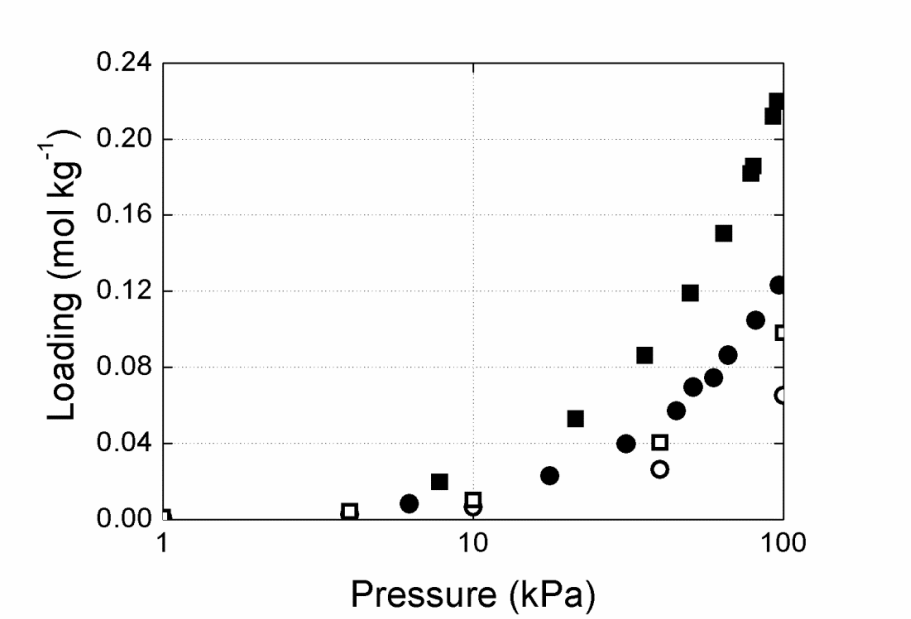

Figure S7: Experimental (full symbols) and computed (empty symbols) adsorption isotherms of argon in NaX Si/Al ratio=1.23 at 305 K (circles), and Na-MFI Si/Al ration=30 at 295 K. (squares) Available data from Dunne *et al.*[3] are included for comparison. Computed adsorption isotherms show the excess loading for a better comparison with experiments.

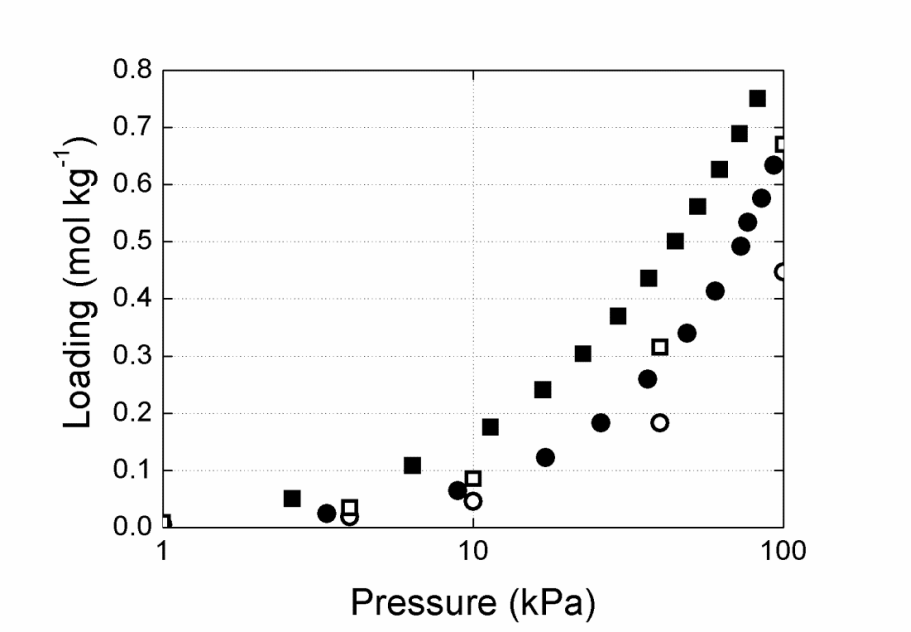

Figure S8: Experimental (full symbols) and computed (empty symbols) adsorption isotherms of methane in NaX Si/Al ratio=1.23 at 305 K (circles), and Na-MFI Si/Al ration=30 at 295 K. (squares) Available data from Dunne *et al.*[3] are included for comparison. Computed adsorption isotherms show the excess loading for a better comparison with experiments.

(1) Dunne, J. A.; Mariwals, R.; Rao, M.; Sircar, S.; Gorte, R. J.; Myers, A. L., Calorimetric Heats of Adsorption and Adsorption Isotherms .1. O-2, N-2, Ar, Co2, Ch4, C2h6 and Sf6 on Silicalite. *Langmuir.* **1996***, 12*, 5888-5895.
(2) Golden, T. C.; Sircar, S., Gas-Adsorption on Silicalite. *Journal of Colloid and Interface Science.* **1994***, 162*, 182-188.
(3) Dunne, J. A.; Rao, M.; Sircar, S.; Gorte, R. J.; Myers, A. L., Calorimetric Heats of Adsorption and Adsorption Isotherms .2. O-2, N-2, Ar, Co2, Ch4, C2h6, and Sf6 on Nax, H-Zsm-5, and Na-Zsm-5 Zeolites. *Langmuir.* **1996***, 12*, 5896-5904.