

SUPPLEMENTARY INFORMATION

Intracrystalline Transport Barriers Affecting the Self-Diffusion of CH₄ in Zeolites |Na₁₂|-A and |Na_{12-x}K_x|-A

Niklas Hedin¹, Przemyslaw Rzepka¹⁺, Alma Berenice Jasso-Salcedo^{1#}, Tamara L. Church¹, Diana Bernin^{2,3}*

¹ Department of Materials and Environmental Chemistry, Stockholm University, SE-106 91 Stockholm, Sweden

² Swedish NMR Centre, University of Gothenburg, SE-405 30 Göteborg, Sweden

³ Department of Chemistry and Chemical Engineering, Chalmers University of Technology, SE-412 96 Göteborg, Sweden

Email: niklas.hedin@mmk.su.se

+ Current address: Department of Chemistry and Applied Biosciences, ETH Zurich, 8093 Zurich, Switzerland

Current address: Cátedra CONACYT-COITTEC, Department of Biosciences and Agrotechnology, Centro de Investigación en Química Aplicada, Blvd. Enrique Reyna Hermosillo No.140 C.P. 25294 Saltillo, Coahuila, México

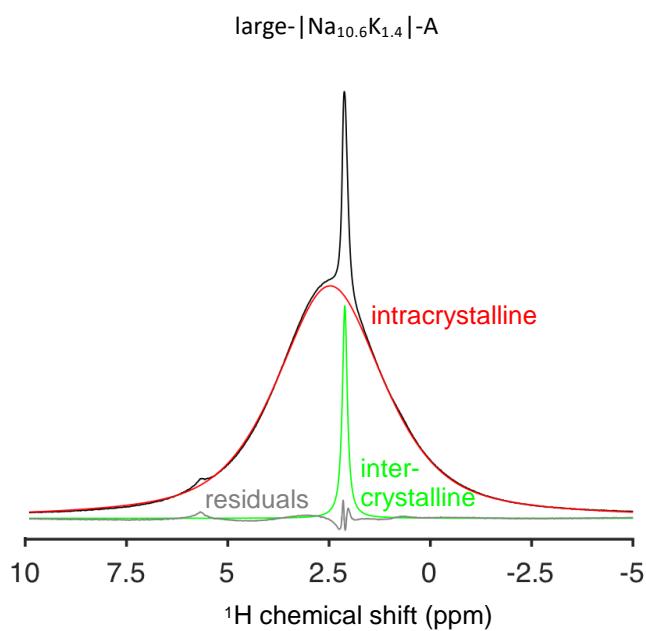


Figure S1. Example of a deconvoluted ¹H spectrum: large-|Na_{10.6}K_{1.4}|-A.

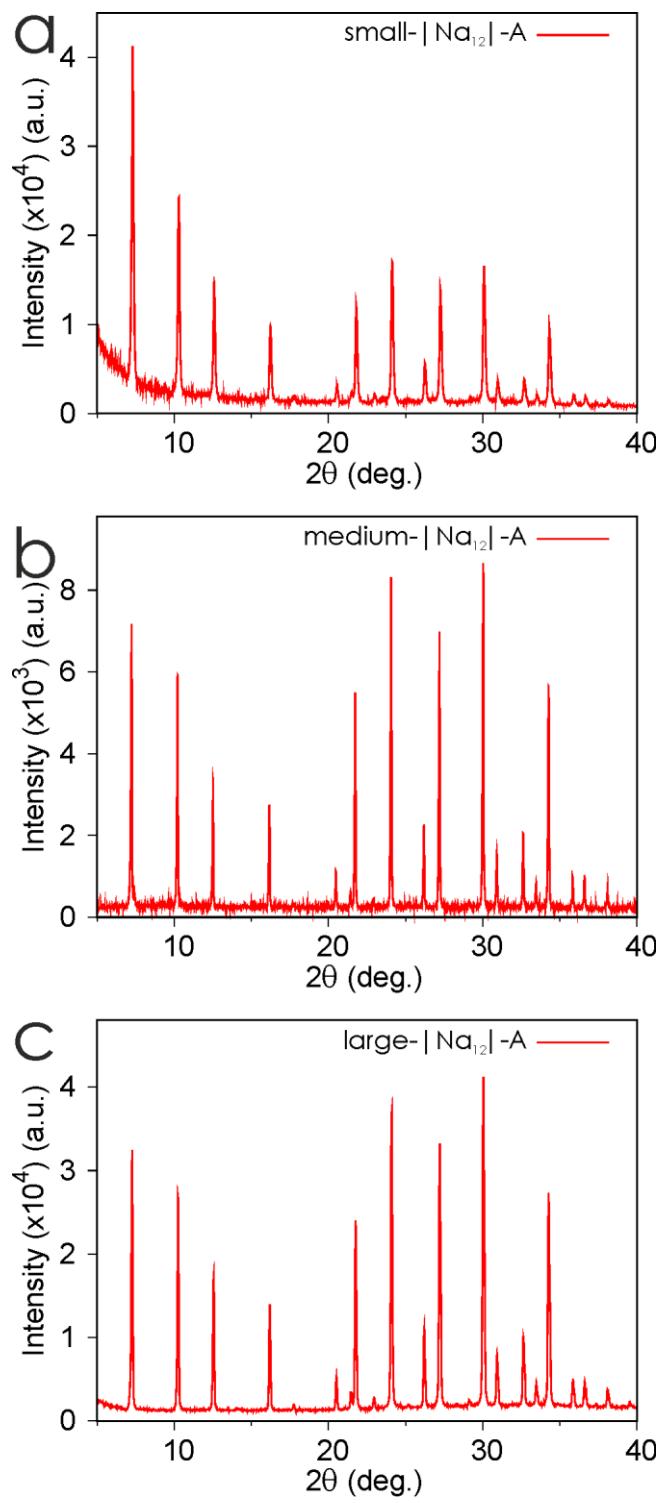


Figure S2. X-ray diffractograms of (a) small (b) medium and (c) large crystals of zeolite |Na₁₂|-A.

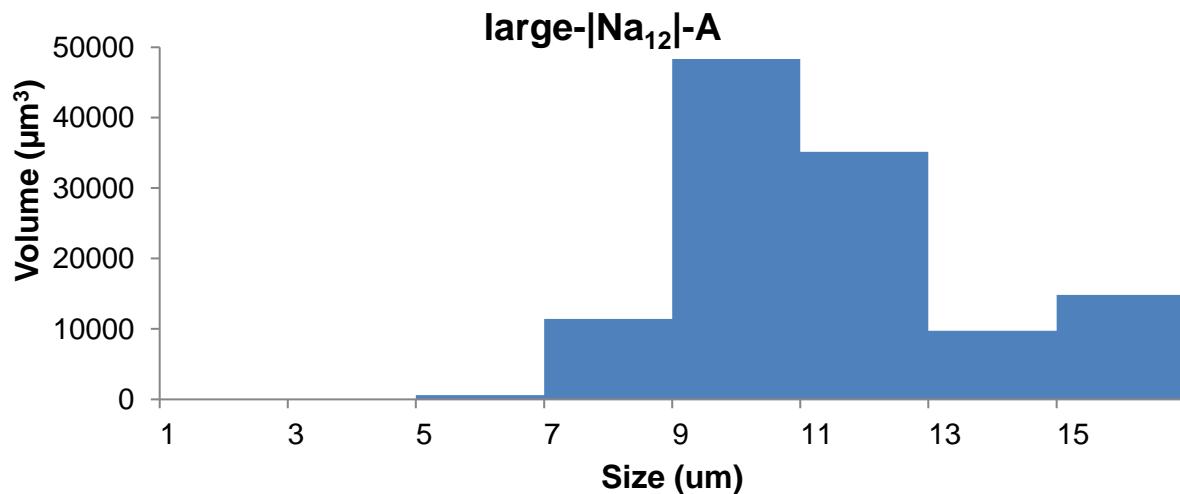
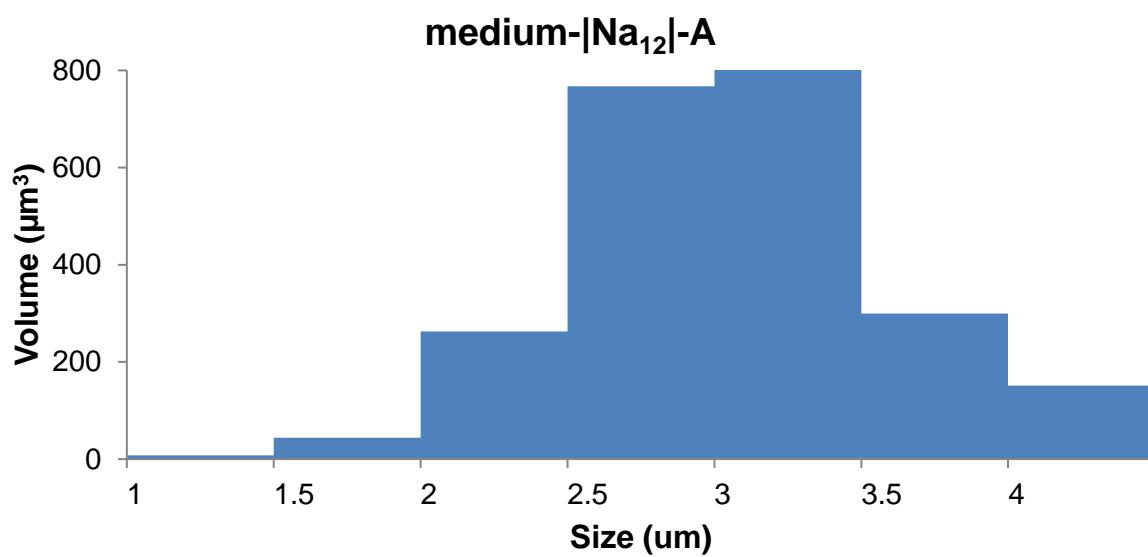
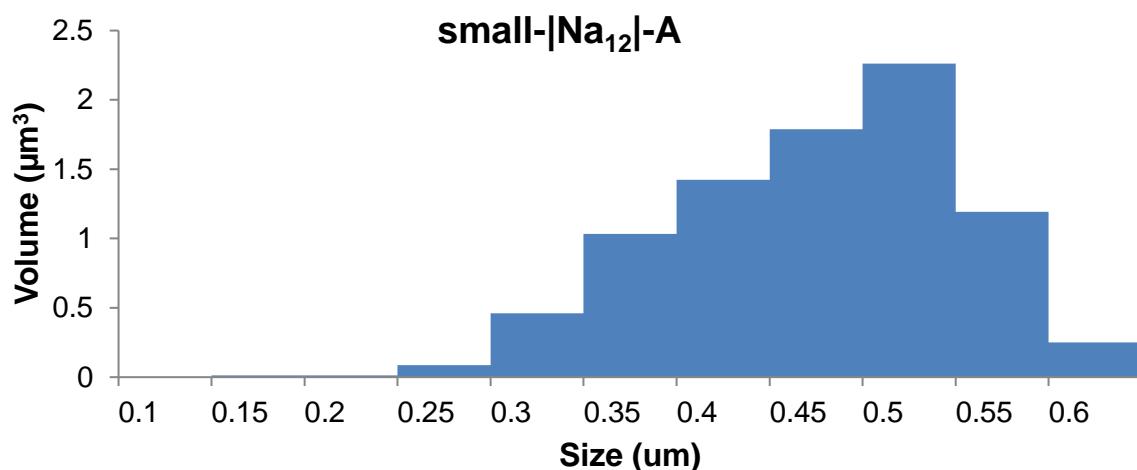


Figure S3. Volume for each class of particle size, measured from the SEM images in Figure 1.

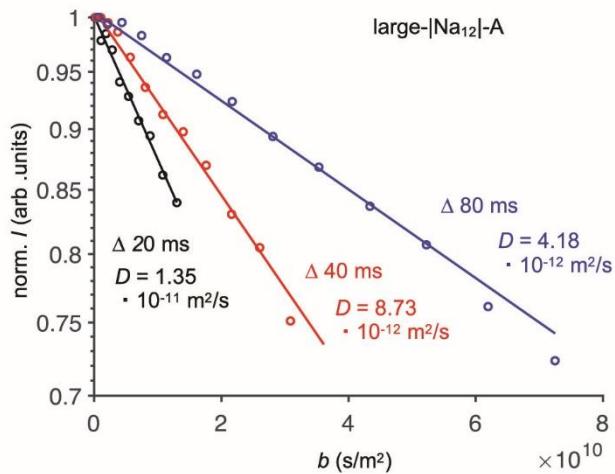


Figure S4. PGSTE attenuation curves (circles) and fitting (line) for the diffusion of CH₄ in large-|Na₁₂|-A.

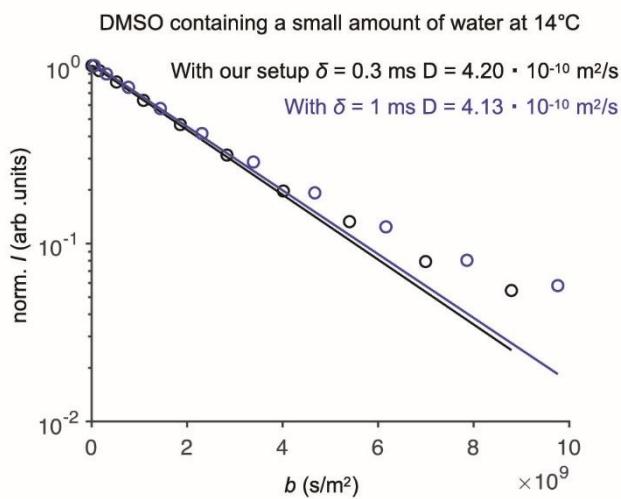


Figure S5. PGSTE attenuation curves (circles) and fitting (line) for the diffusion of DMSO with a small amount of water at a temperature of 14 °C. Recorded with short/identical settings (black) and somewhat longer (blue) gradient pulses.

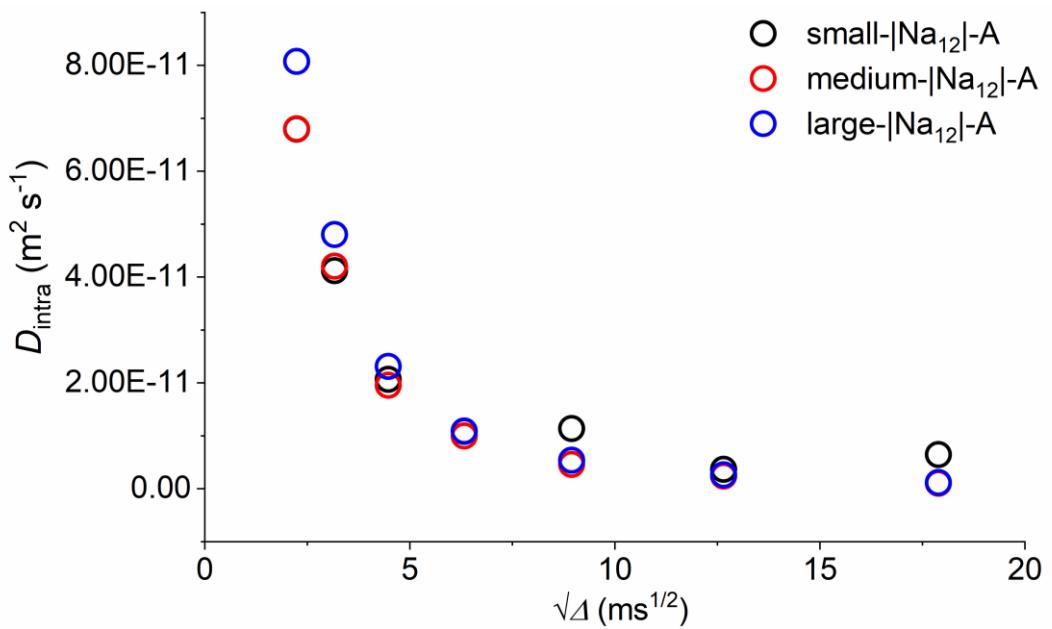


Figure S6. Diffusion coefficients (D_{intra}) for adsorbed CH₄ (1 atm, 298 K) on small-, medium-, and large-|Na₁₂|-A as a function of square root of the diffusion time ($\sqrt{\Delta}$).

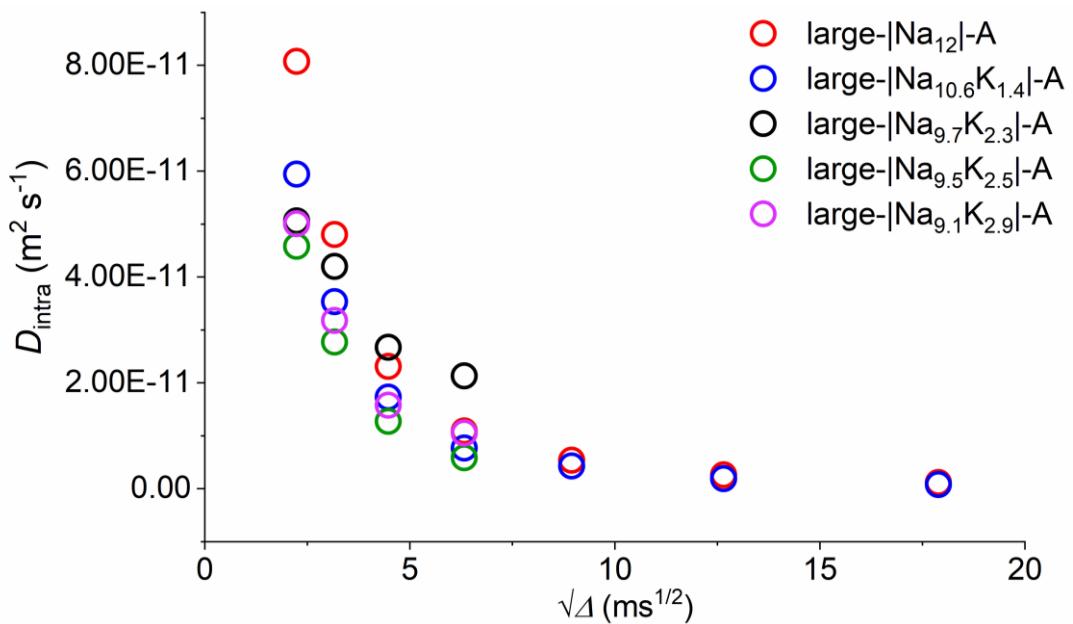


Figure S7. Diffusion coefficients (D_{intra}) for adsorbed CH₄ (1 atm, 298 K) on large-|Na_{12-x}K_x|-A as a function of square root of the diffusion time ($\sqrt{\Delta}$).