

Quasi-Elastic Neutron Scattering (QENS) Studies of Zeolitic Diffusion

Hervé Jobic

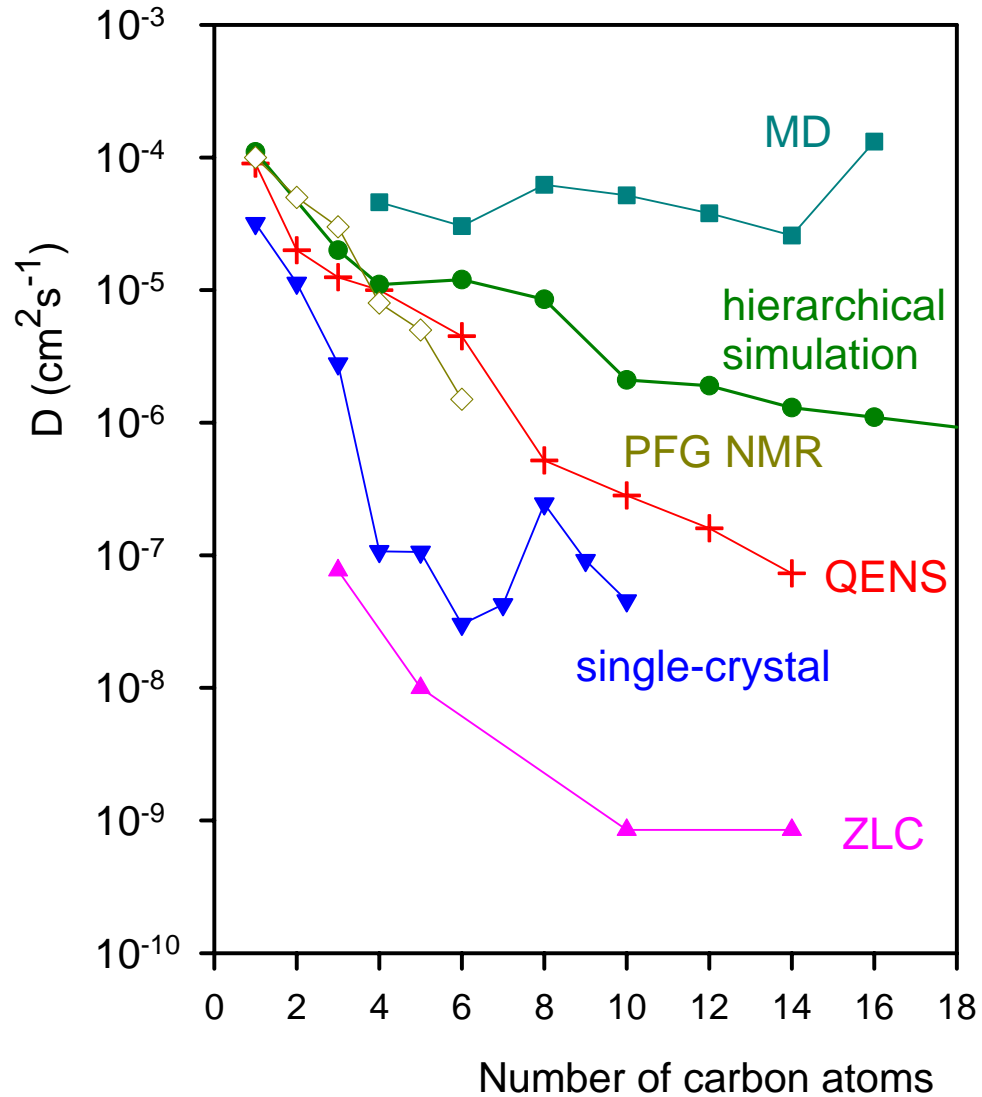
Institut de Recherches sur la Catalyse, CNRS, 2 avenue Albert Einstein,
69626 Villeurbanne



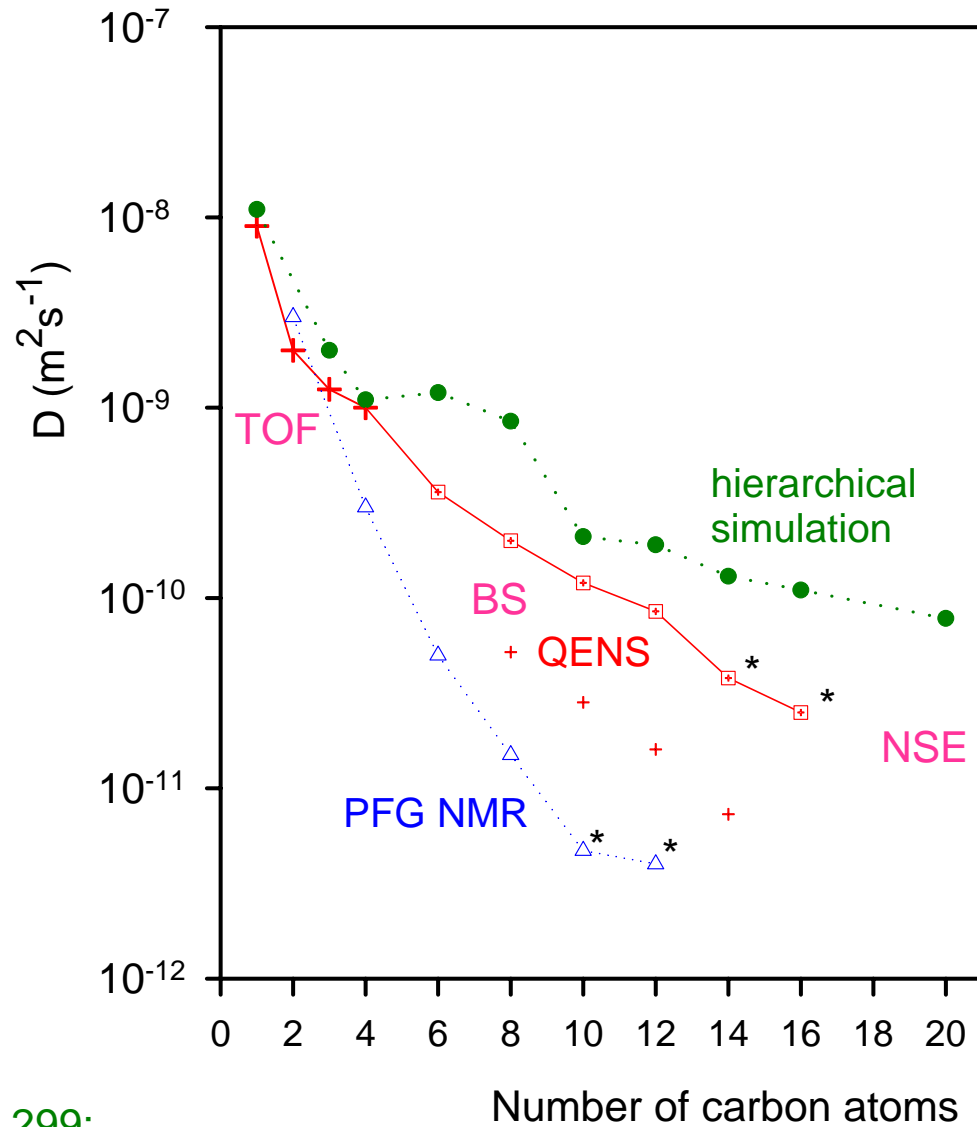
Leipzig, Oct 2006



Ds *n*-alkanes / MFI
(T = 300 K)

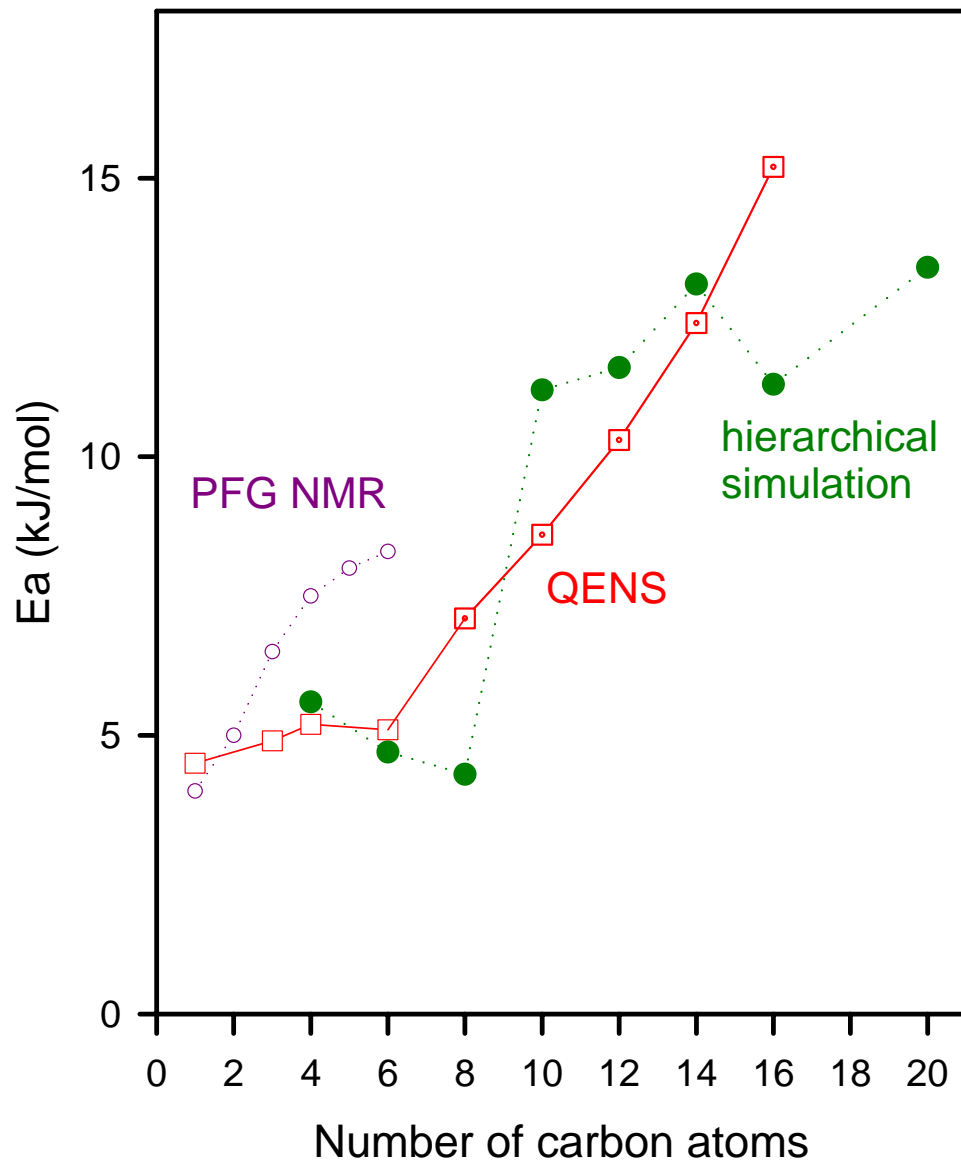


Ds *n*-alkanes / silicalite
(T = 300 K)

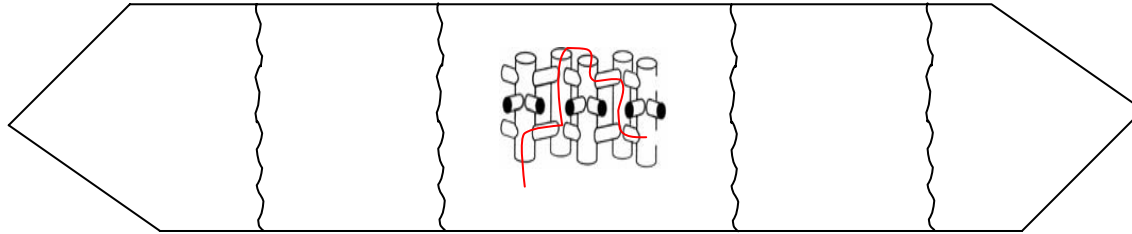


Microp. Mesop. Mater. 90 (2006) 299;
J. Phys. Chem. B 110 (2006) 1964

Ea *n*-alkanes / silicalite

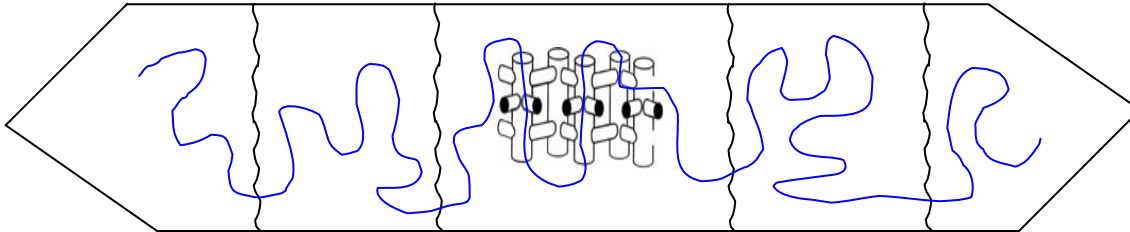


QENS

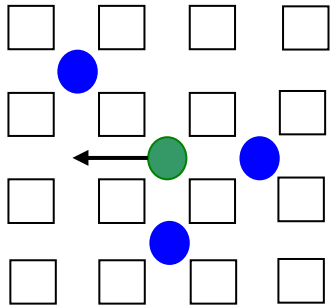


$\approx \text{nm}$

PFG NMR

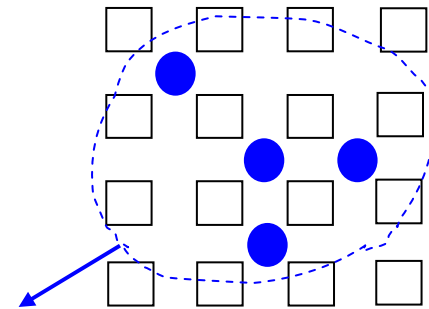


$\approx \mu\text{m}$



$$\frac{\partial G_S(\mathbf{r}, t)}{\partial t} = D_s \nabla^2 G_S(\mathbf{r}, t)$$

hydrogenated molecules

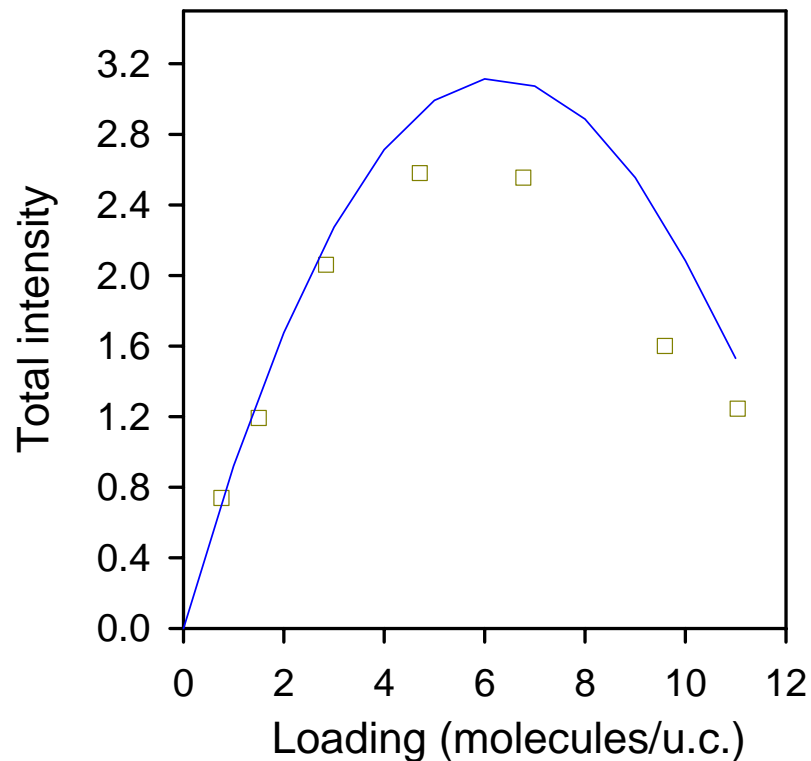
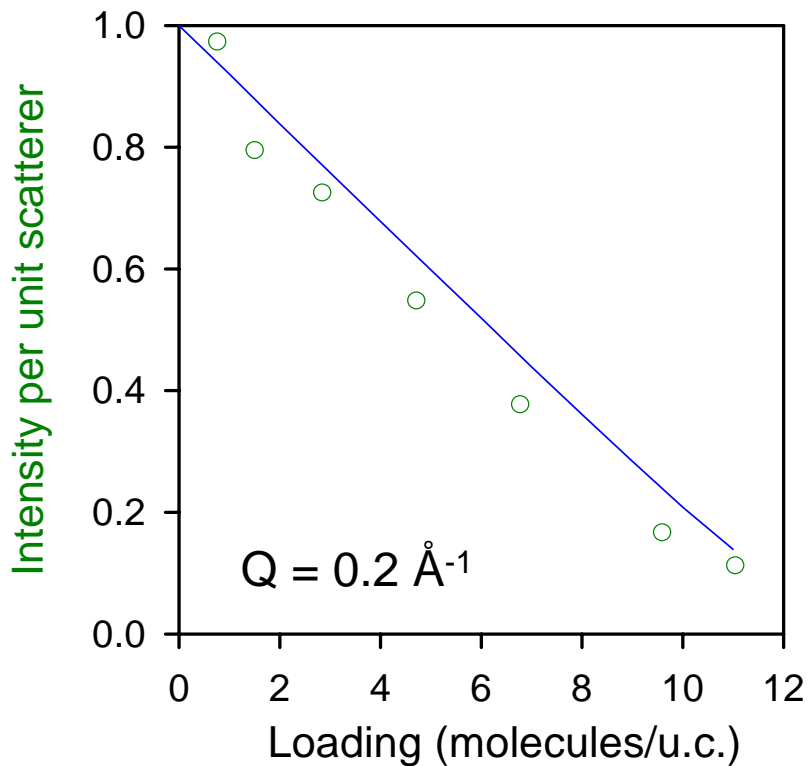


$$\frac{\partial \rho(\mathbf{r}, t)}{\partial t} = D_t \nabla^2 \rho(\mathbf{r}, t)$$

deuterated molecules
+ O₂, N₂, CO₂, SF₆...

$$D_t = D_0 \frac{d \ln p}{d \ln c} = D_0 \Gamma$$

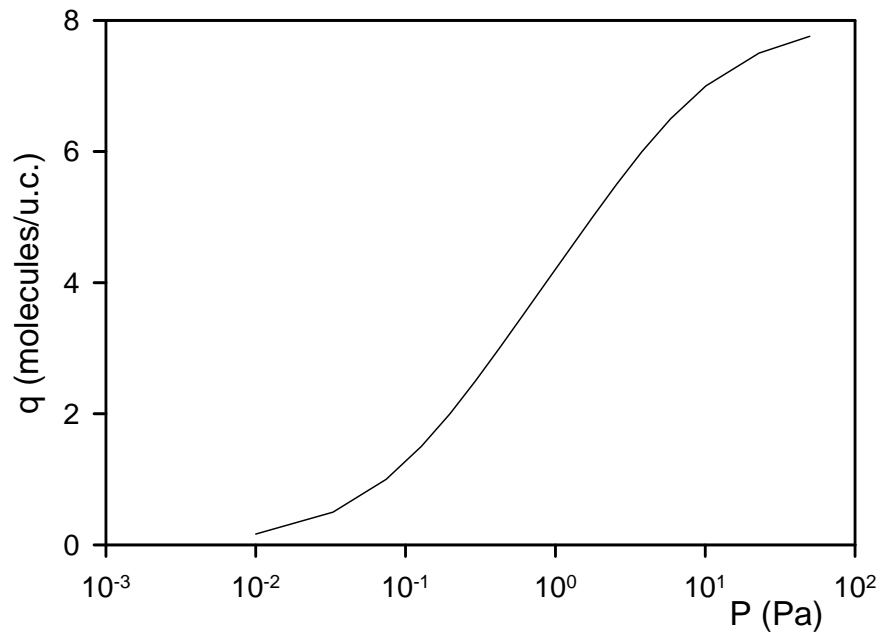
C₂D₆ in silicalite @ 300K



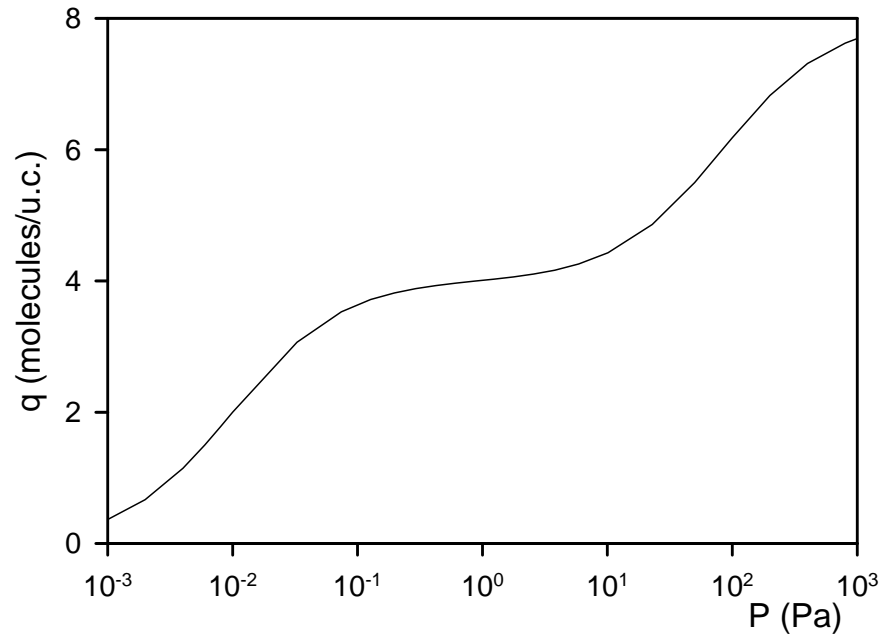
$$S(Q)_{Q \rightarrow 0} = \frac{\langle N^2 \rangle - \langle N \rangle^2}{\langle N \rangle} = \rho k_B T \kappa_T$$

$$\kappa_T = \frac{1}{\rho k_B T} \left(\frac{d \ln q}{d \ln p} \right)$$

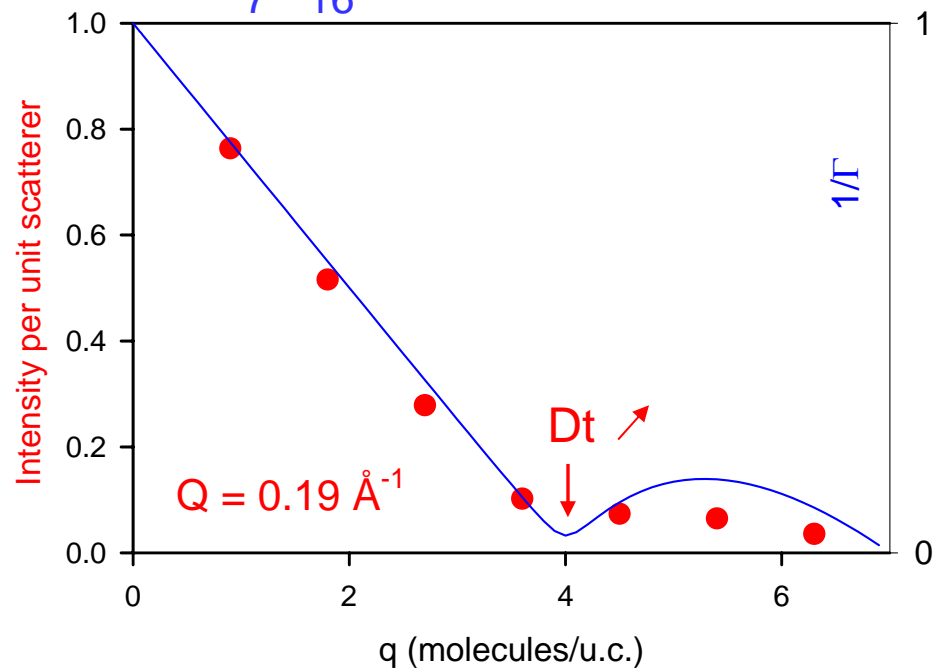
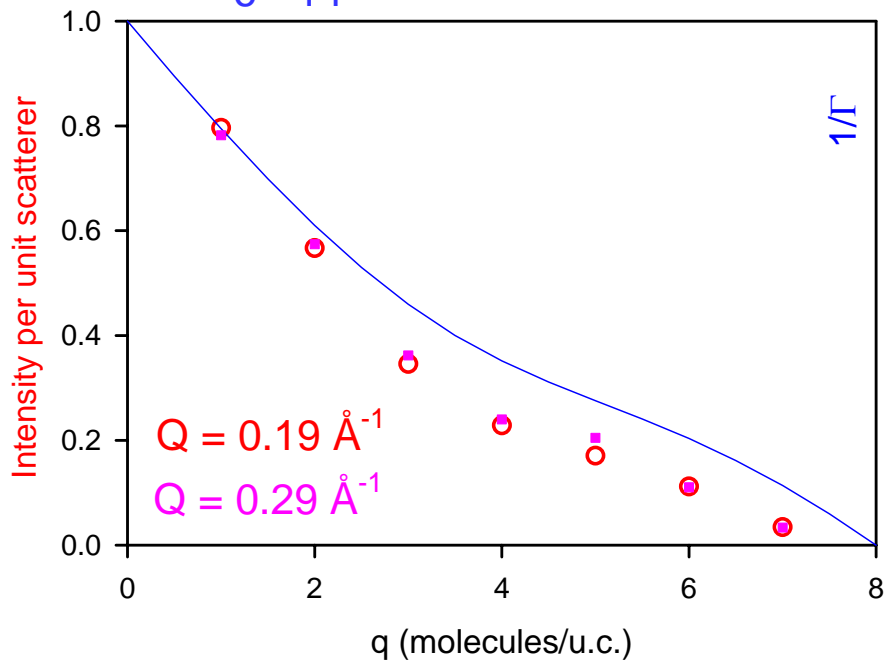
$$S(Q)_{Q \rightarrow 0} = \frac{d \ln q}{d \ln p} = \frac{1}{\Gamma}$$



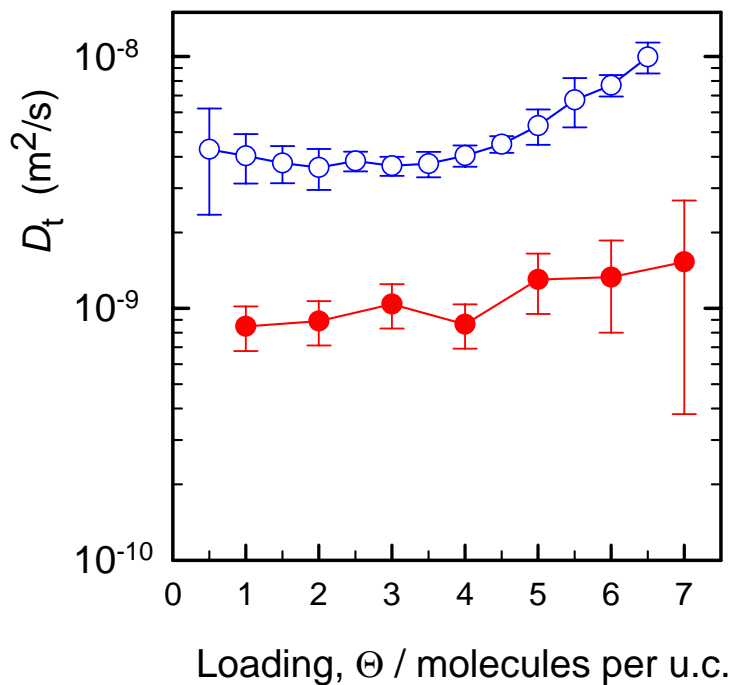
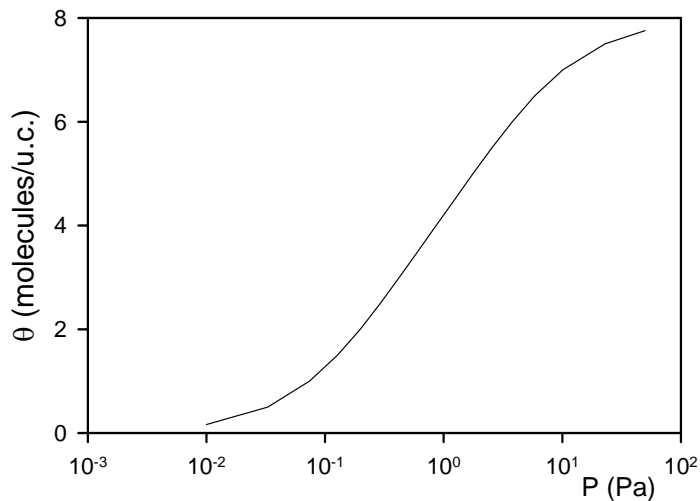
$n\text{-C}_6\text{D}_{14}$ / silicalite @ 300K



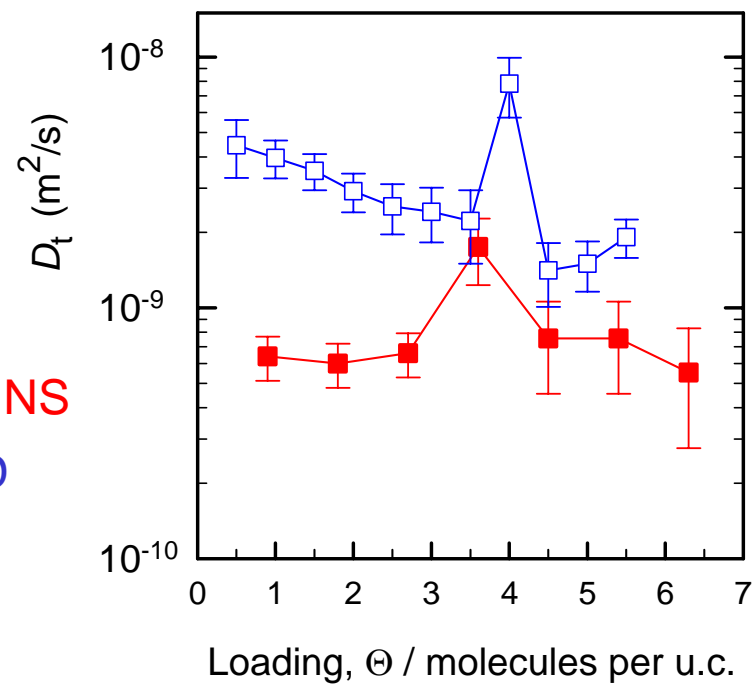
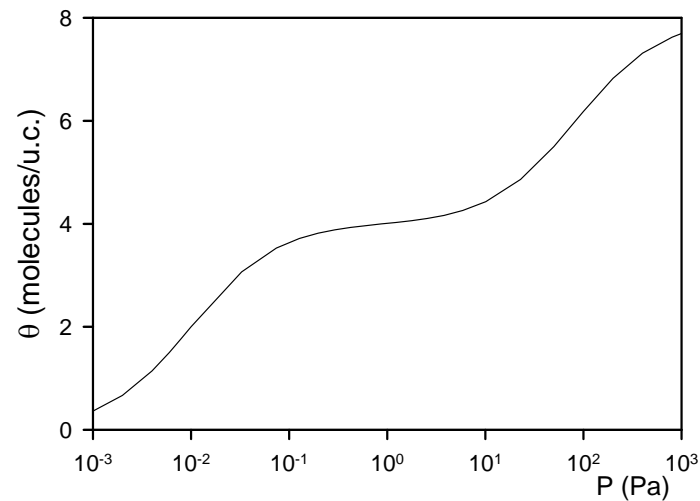
$n\text{-C}_7\text{D}_{16}$ / silicalite @ 300K



n-hexane / silicalite @ 300K

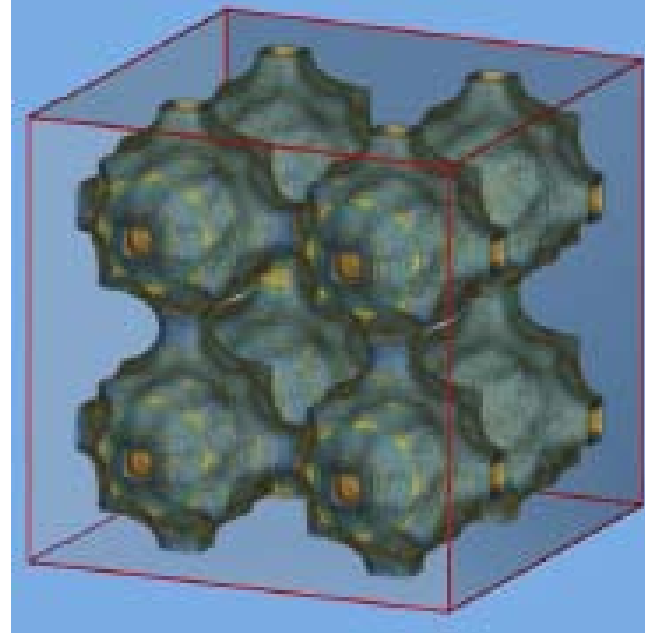
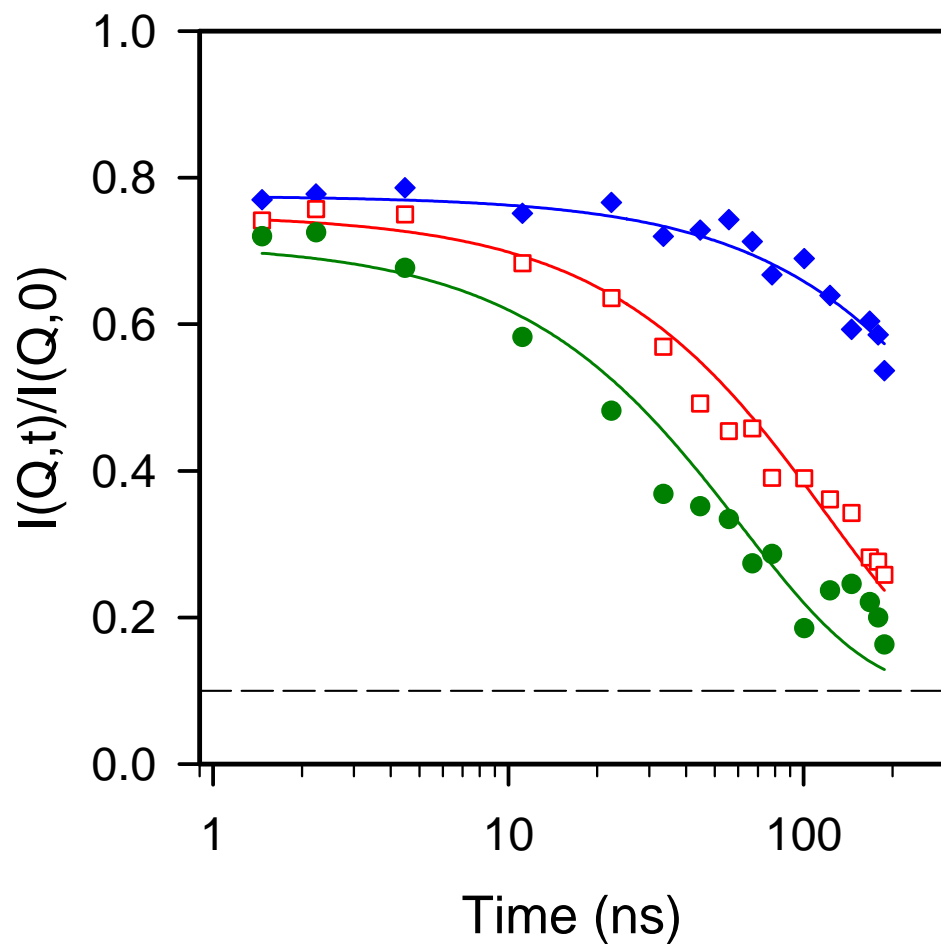


n-heptane / silicalite @ 300K



n-alkanes in NaCaA (5A)

($T = 475$ K, $Q = 0.2 \text{ \AA}^{-1}$)



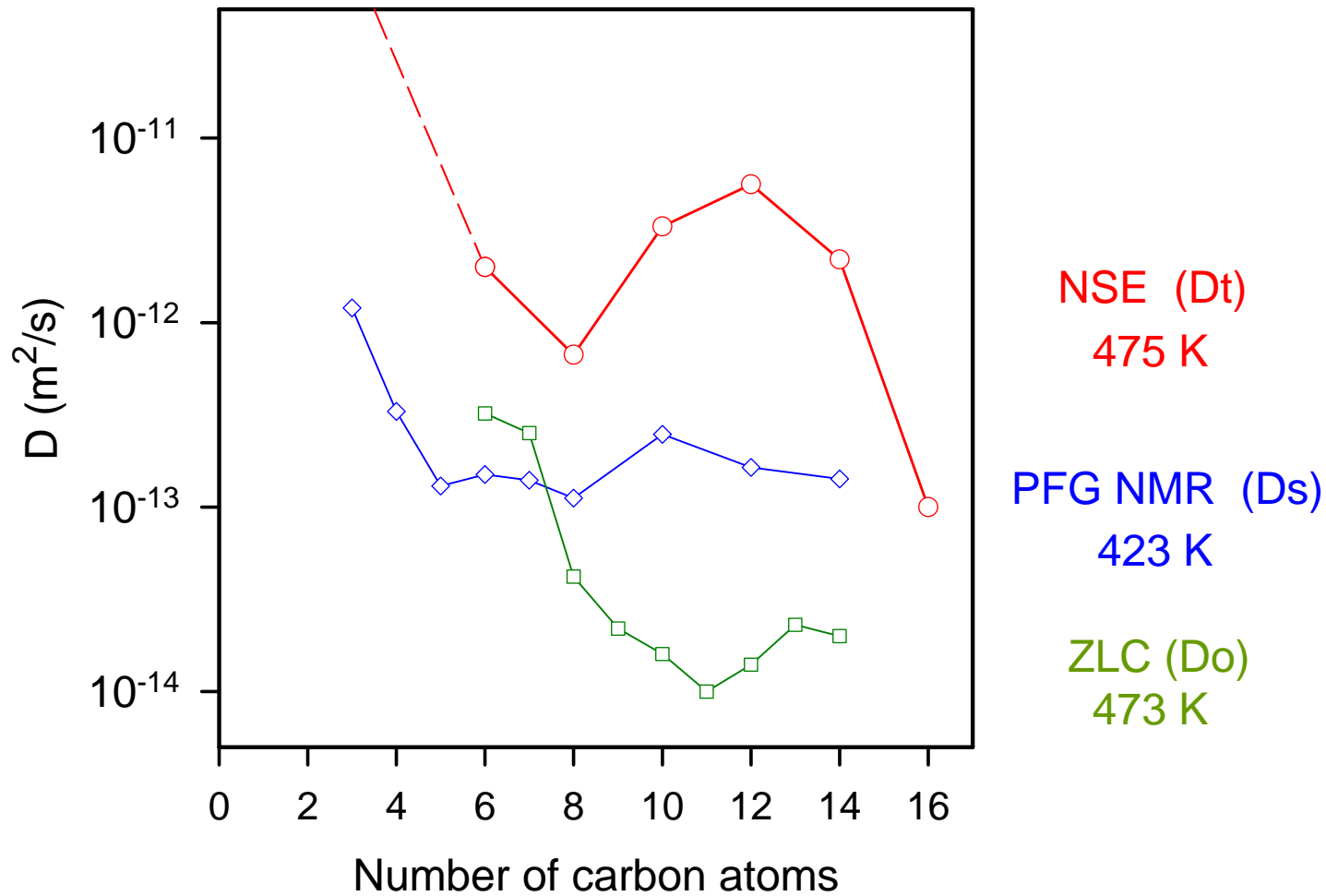
octane

decane

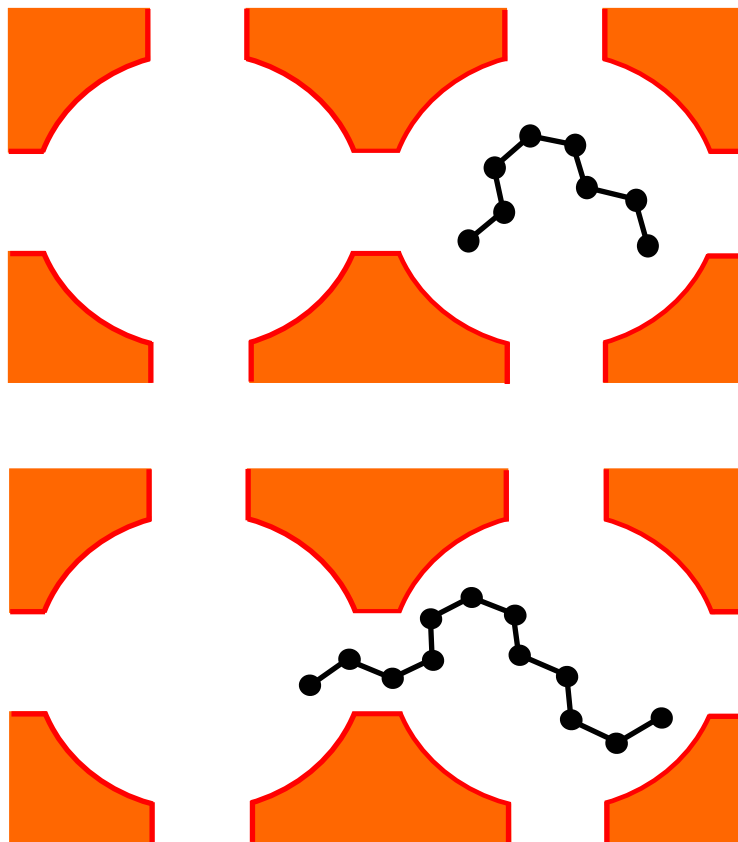
dodecane

12 C / cage

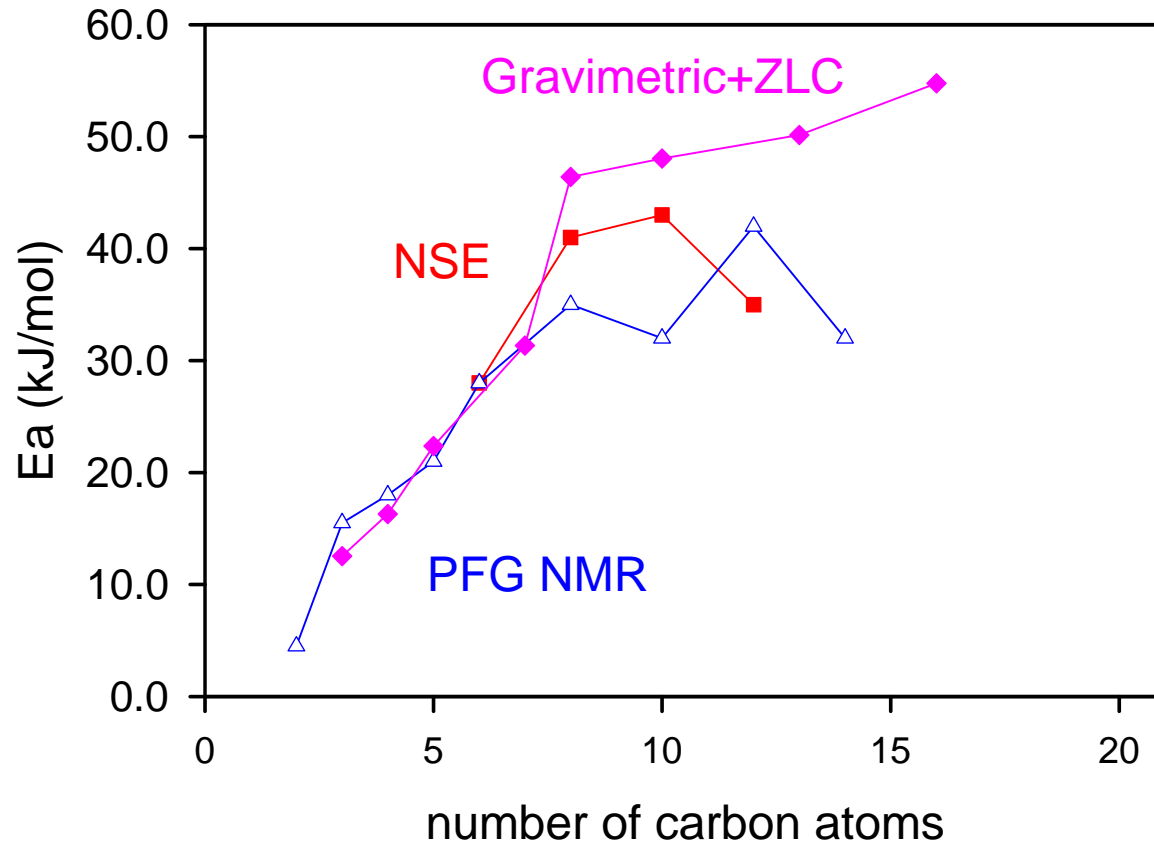
n-alkanes in 5A



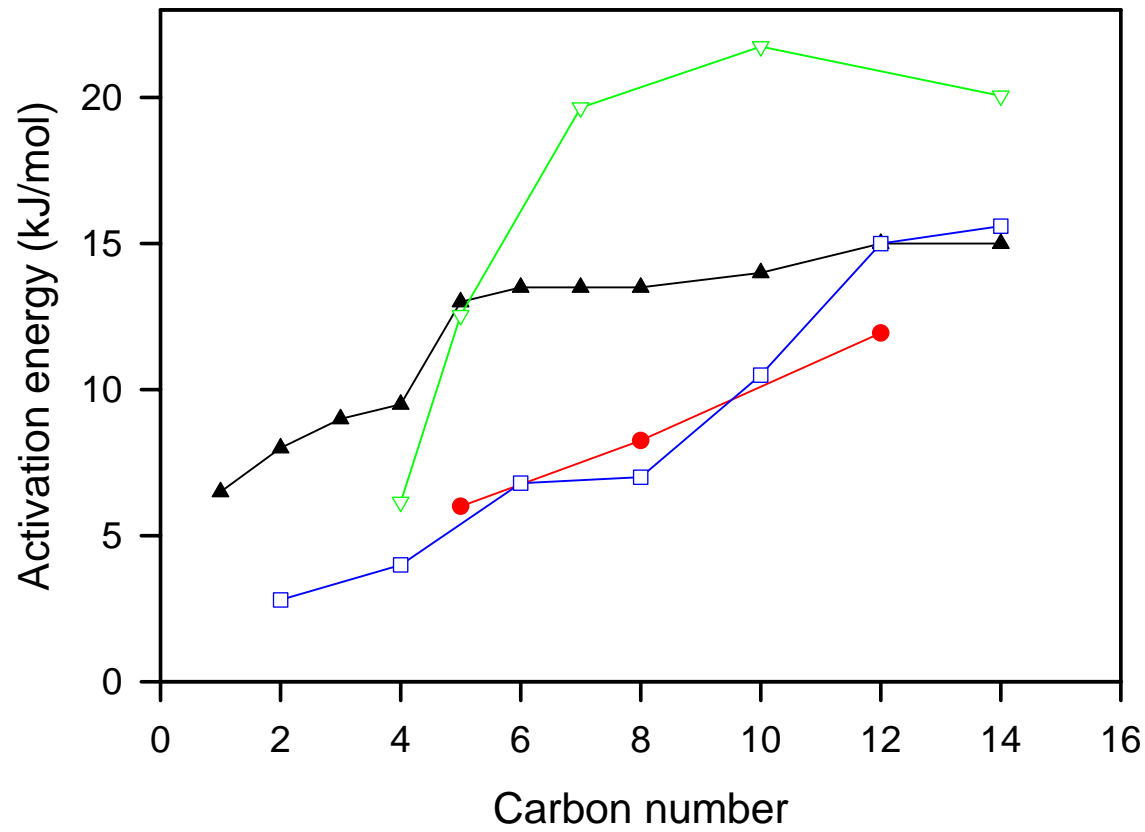
'Window effect'



Ea *n*-alkanes in 5A

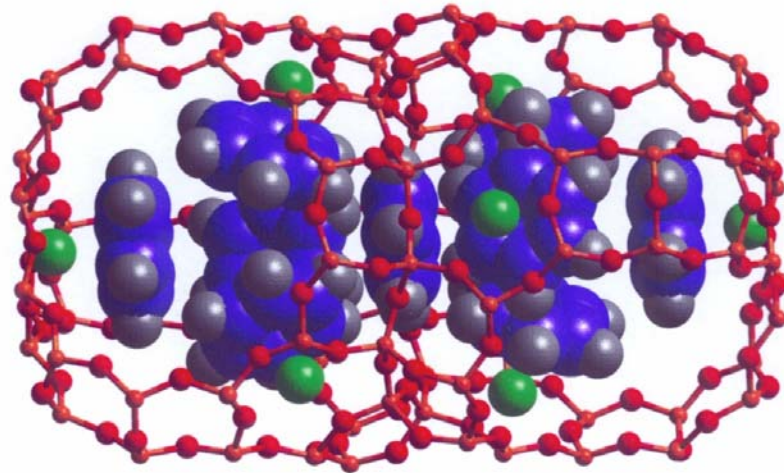
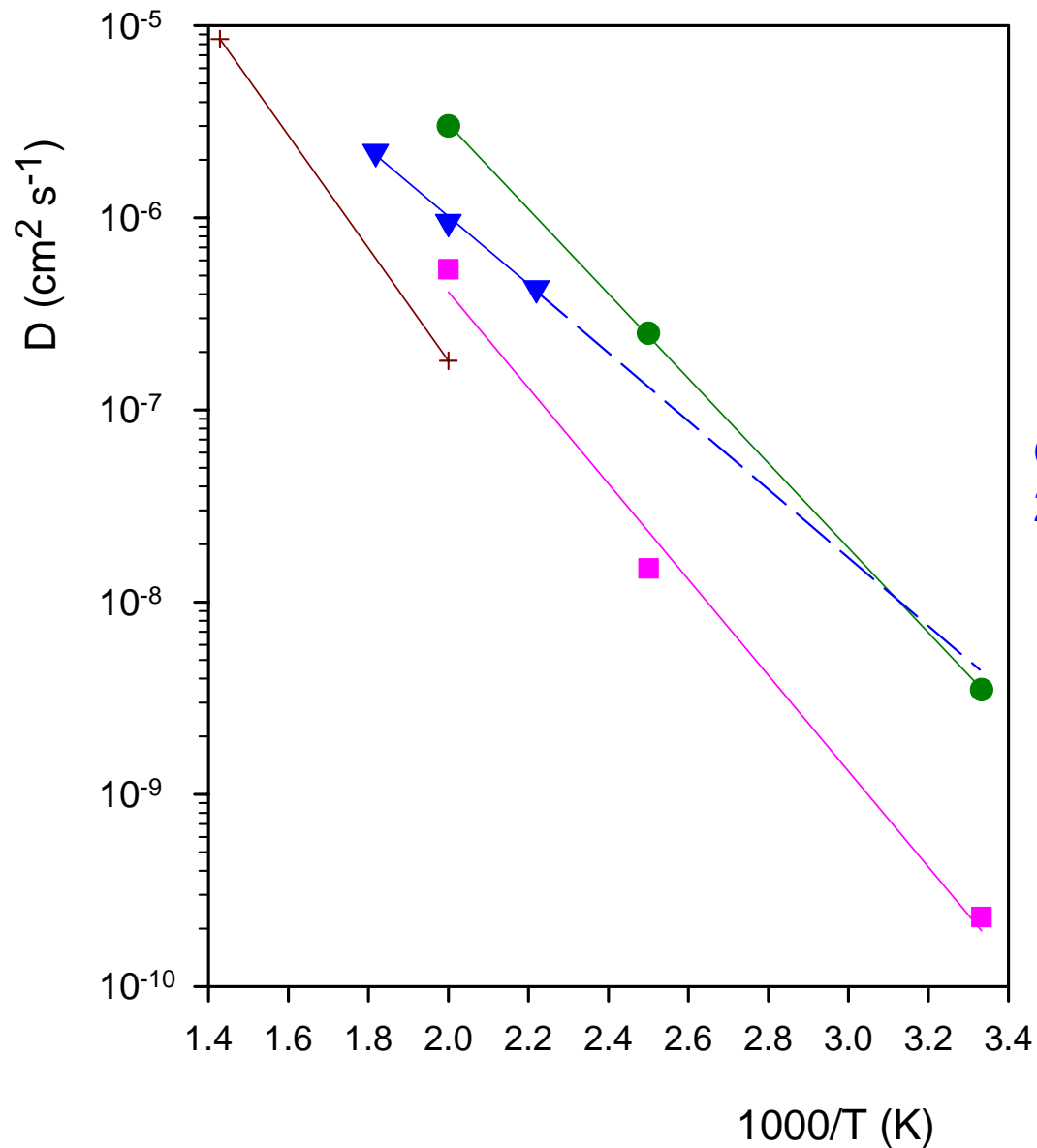


Ea alkanes/NaX



- (▽) ZLC
- (▲) PFG NMR
- (□) Simulations
- (●) QENS

Ds Benzene/NaY



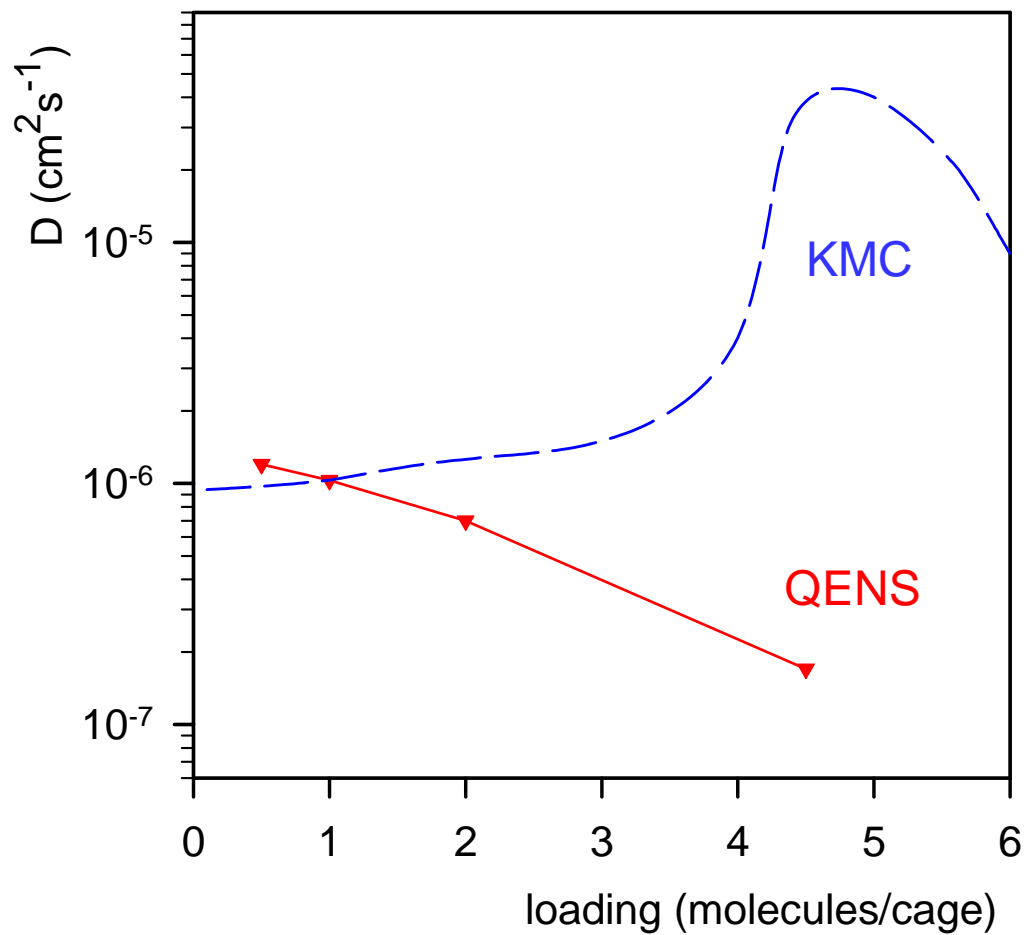
MD

QENS
2 mol./cage

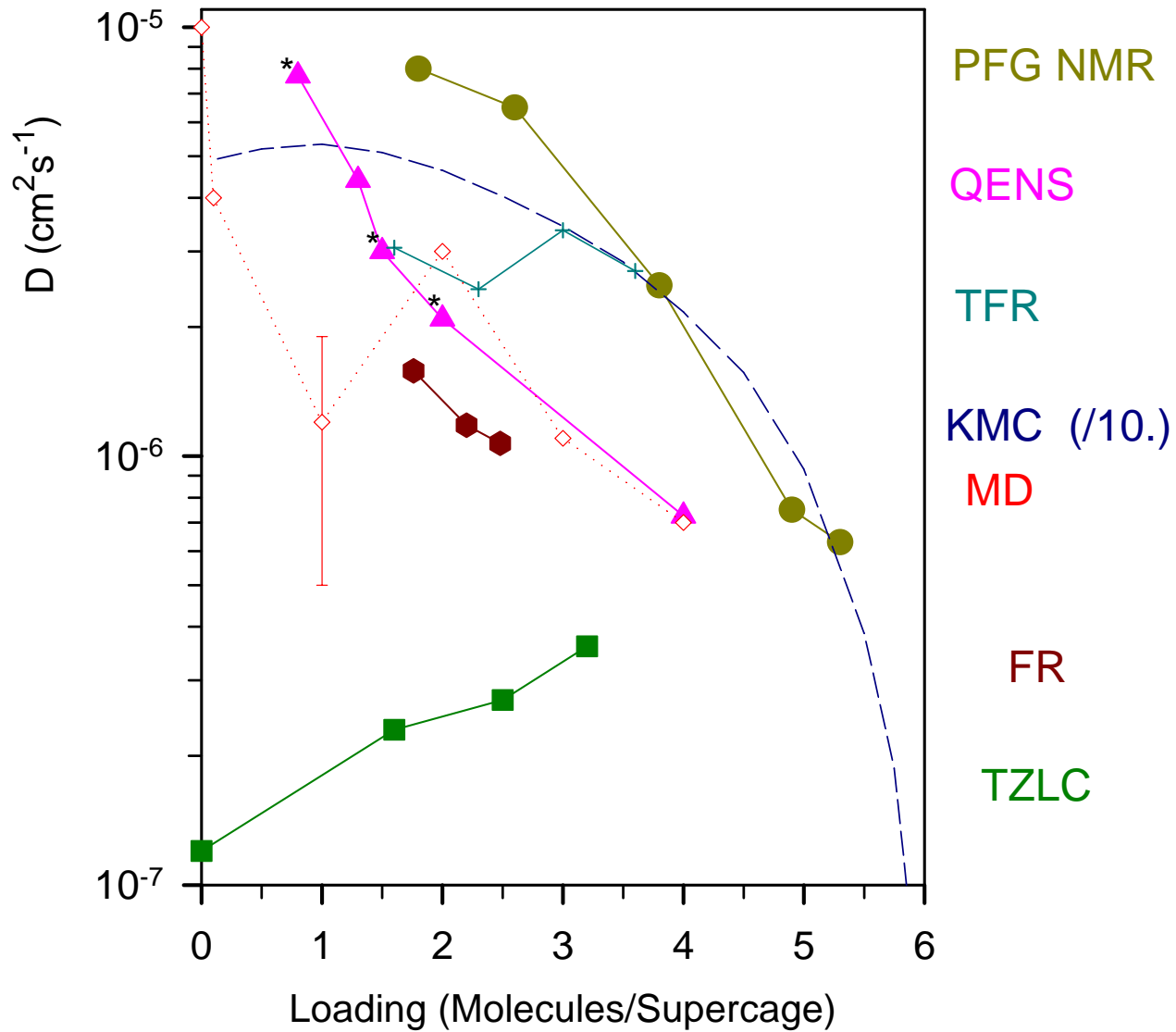
KMC

CRCD

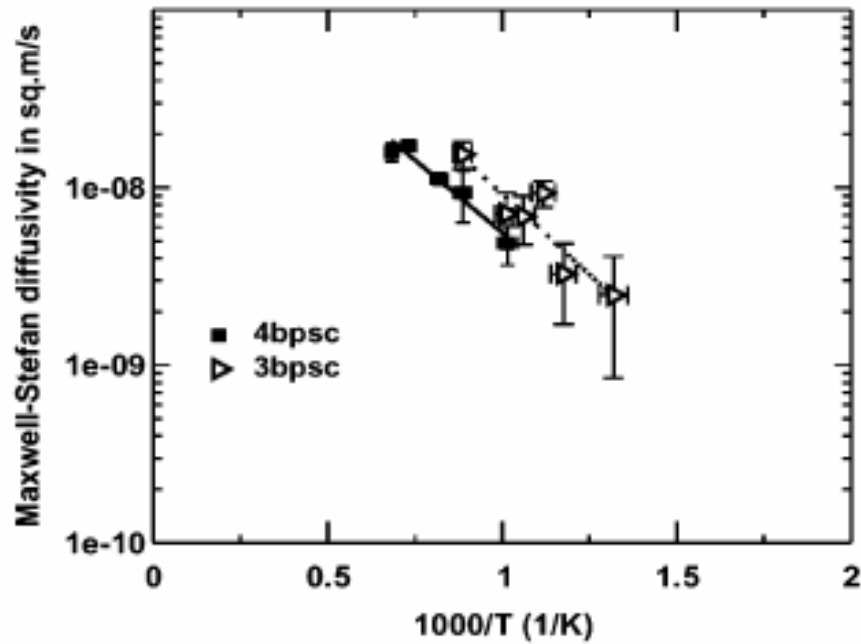
Ds Benzene/NaY @ 480 K



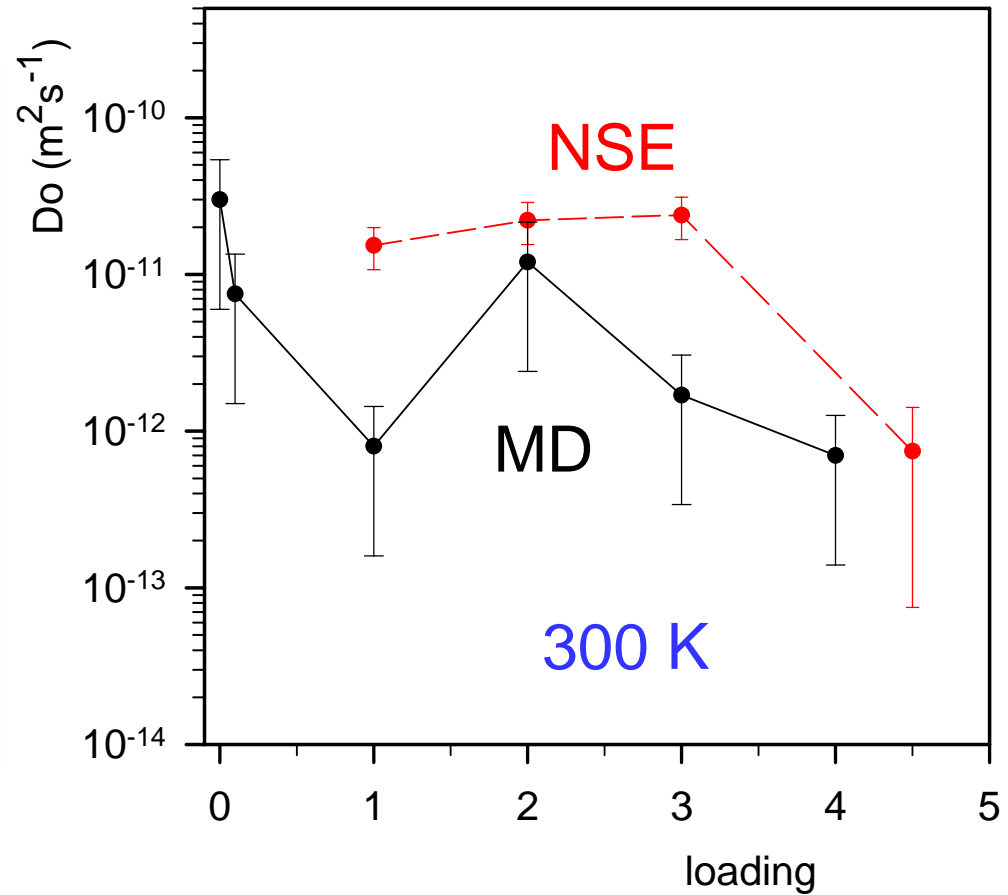
Ds Benzene / NaX (T = 468 K)



Do Benzene/NaX



JPC B 108 (2004) 17171



Micropor. Mesopor. Mater. 90 (2006) 307

Systems to be studied

NaCaA: *n*-alkanes, methanol

Silicalite: linear & branched alkanes, methanol

NaX/NaY: alkanes

aromatics; benzene in NaX: PFGNMR-QENS/TZLC

methanol in NaX; agreement: PFG NMR, ZLC, TFR (V. Bourdin)

AIPO-5

Ferrierite

Mixtures