2 Supplement

S.1 Supplementary Figures

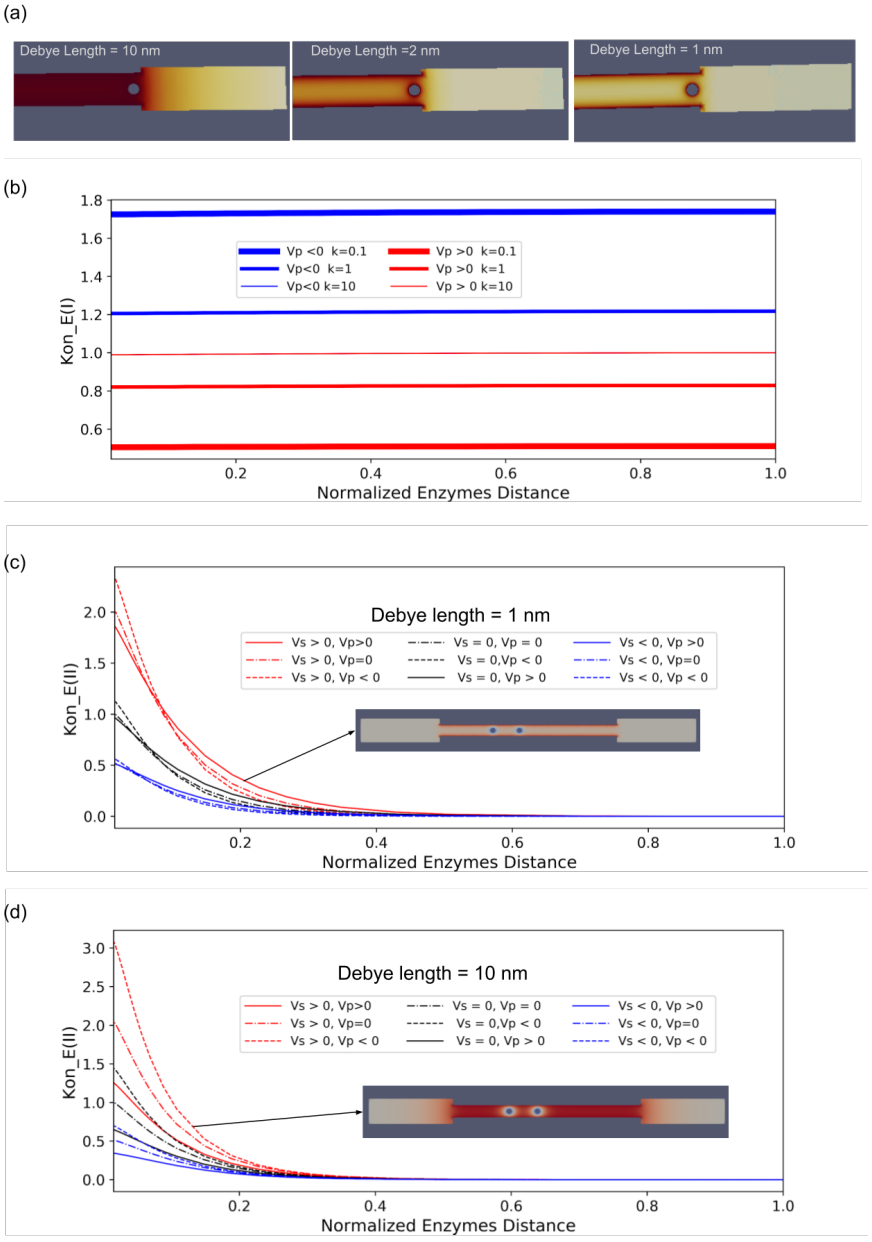

Figure S1: finite element method (FEM) predictions of small molecule reaction rates on a reactive nanoparticle confined to a nanoporous channel. a) Predictions of concentration gradient for different channel diameters b) Association rate at first reactive center as a function of ionic strength (κ^{-1}) and surface potential (V_p) c) and d) Association rate at secondary reactive center at 1 and 10 nm Debye lengths, respectively, for varied reactive center potentials (V_s). We anticipate similar trends to emerge in the zeolitic systems, as SiO_2/Me interactions are expected to influence diffusion rates.

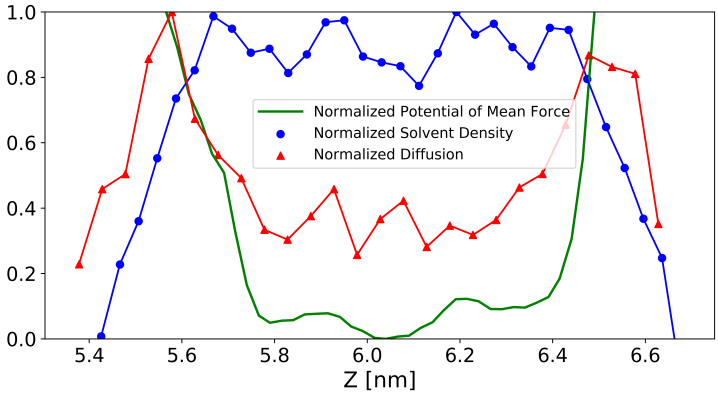

Figure S2: Predictions of methane diffusion (red), solvent density (blue) and potentials of mean force (green). Local diffusion coefficient close to the silica surfaces varies strongly from its value in the center of the channel. Small oscillations in potential of mean force graph farther from the edge in the center reflect oscillations in local water density, leading to small variation in local diffusivity. Zeolites present much narrower pores in comparison to the channel here, thus we anticipate the local water structure to be significantly more ordered in zeolitic frameworks.

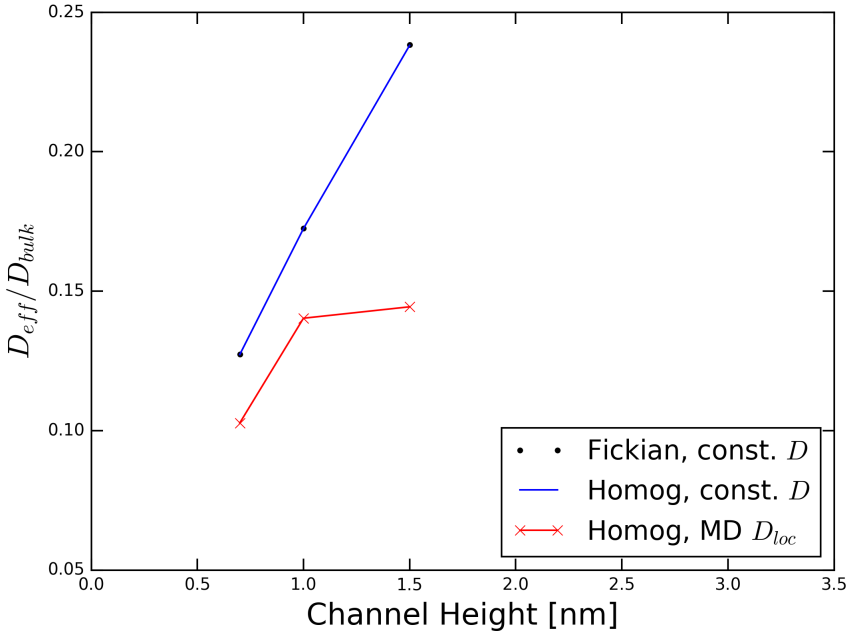

Figure S3: Normalized diffusion coefficient data for silicate channels of varying height. The 'Fickian' estimates are based on solving the standard Fickian diffusion equation for the domain in question for the steady-state concentration field, from which an effective diffusion constant is obtained as $D \approx -\left(\frac{\Delta c)}{\Delta x}\right) \langle J \rangle^{-1}$, where J is the flux along the boundary. The homogenization 'const' estimate follows from the method described in [2, 3], assuming a constant diffusivity. 'Homog, MD' utilizes diffusion coefficients determined directly from molecular dynamics simulations.

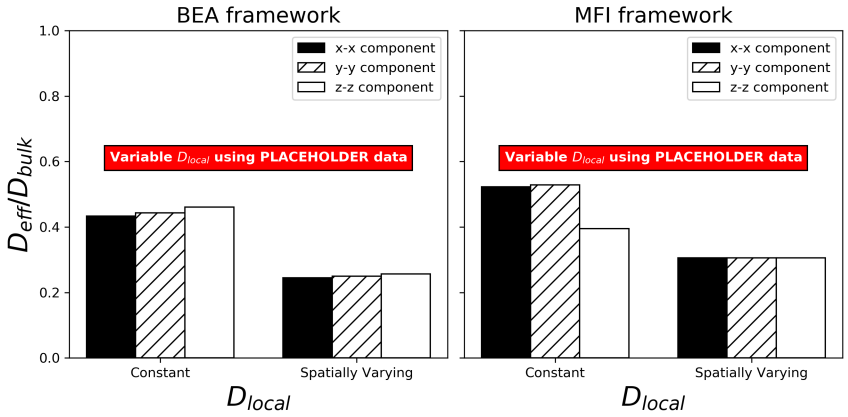

Figure S4: Normalized diffusion coefficients for BEA (left) and MFI (right) zeolite frameworks. Data are presented for constant and MD-determined diffusion coefficients. We are in the early stages of validating the MD-predicted diffusion data, therefore we are using representative data for the FEM modeling in these figures.

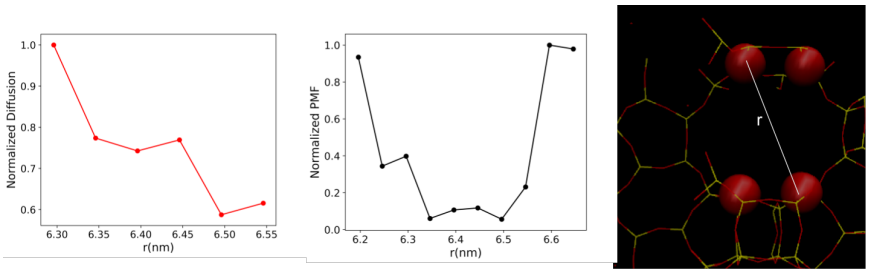

Figure S5: Potentials of mean force (left) and local diffusion rates (right) along a cross section of a BEA channel. The PMF maxima coincide with the location of oxygens forming the channel wall (right).

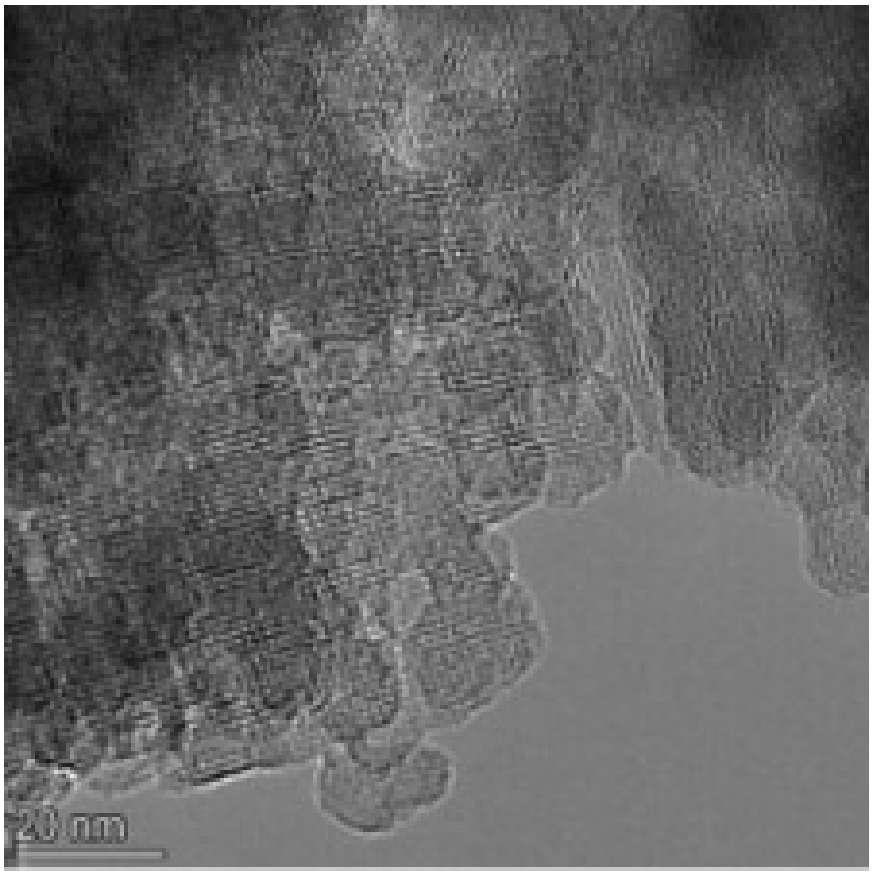

Figure S6: tunneling electron microscopy (TEM) data of an zeolite powder. The pores are just below the diffraction limit, which yields a spurious criss-cross pattern in the image. Subsequent data collection will be performed at higher resolution to resolve the pores.