



(a) MD simulations of Na-montmorillonite interlayers, some “doped” with one Cs⁺ or Sr²⁺ ion per interlayer (shown is a snapshot of the 2-layer hydrate of Na-montmorillonite with Na⁺ ions in blue, water O and H atoms in red and gray), yield **(b)** data on the diffusion coefficients of H₂O, Na⁺, Sr²⁺ and Cs⁺ in Na-montmorillonite interlayers (shown in the 2nd column for the 2-layer hydrate, normalized to the diffusion coefficient in bulk water, D_0) that are consistent with our previous *continuum scale* estimates of $D_{\text{interlayer}}/D_0$ in the interlayer portion of the pore space of smectite-rich porous media [3rd column (Bourg, 2004; Bourg et al., 2006, 2007)]. Our simulation data on $D_{\text{interlayer}}/D_0$ allowed us to reexamine our previous modeling of the continuum scale “apparent” diffusion coefficients (D_a) of H₂O, Na⁺, Sr²⁺ and Cs⁺ in bentonite clay barriers; shown here **(c)** are model predictions (thick line, with confidence intervals as thin lines) and experimental results on the ratio of the relative apparent diffusion coefficients (D_a/D_0) of Cs⁺ and H₂O in Na-bentonite (Bourg and Sposito, 2009).