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Addition/Correction

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Correction to "How Electrostatics Influences Hydrodynamic Boundary Conditions: Poiseuille and Electro-Osmostic Flows in Clay Nanopores"

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An error was found in the simulations using the CLAYFF force field. The calculations were performed with ε_O = 0.0371 kcal mol^{-1} as Lennard-Jones parameter for surface oxygen atoms, instead of ε_O = 0.1554 kcal mol^{-1}. We have thus performed new simulations with the appropriate values. The new results are indistinguishable from the previous one in the case of pyrophyllite: The velocity profiles and the conclusions remain the same.

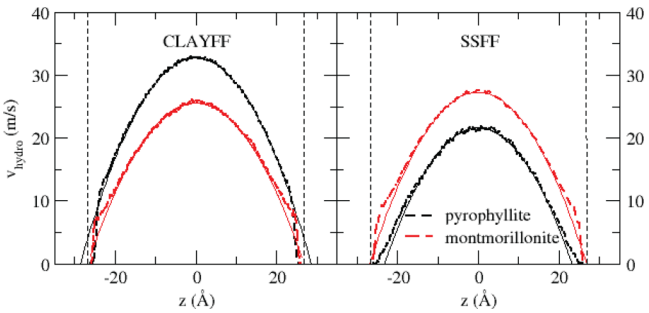

Figure 2. Hydrodynamic velocities (F_{hydro} = 0.75 cal/mol/Å) as a function of z, for pyrophyllite (black) and montmorillonite (red) simulated with CLAYFF (left) and SSFF (right). The simulation results (dashed lines) are reported together with fits by parabolas (solid lines). The vertical dashed lines indicate the location of the clay surface oxygen atoms.

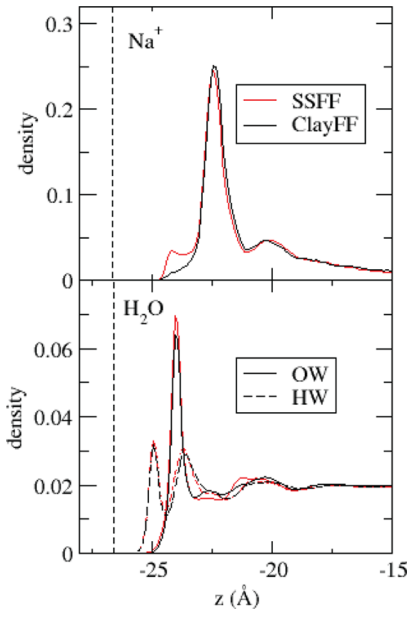

Figure 5. Density profiles in montmorillonite for the CLAYFF (black) and SSFF (red) force fields: Na^+ (top), water oxygen atoms (bottom, solid lines), and water hydrogen atoms (bottom, dashed lines). The vertical dashed lines indicate the location of the clay surface oxygen atoms.

However, important differences are observed with montmorillonite. The new hydrodynamics and density profiles corresponding to Figures 2 and 5 of ref 1 are given below. The results indicate that the predictions of the CLAYFF and Skipper−Smith (SSFF) force field are in very good agreement in that case. In particular, in montmorillonite, slip boundary conditions should be used also with CLAYFF, contrary to our previous conclusion, and Table 2 should be modified according to: b = 1.4 ± 0.3 Å with η = 0.70 ± 0.02 cP and $L_{hyd}/2$ = 25.4 ± 0.02 Å. The paragraph entitled "Comparing Force Fields: Role of Local Interactions" can thus only be viewed as a discussion of the influence of the local structure on the hydrodynamic boundary conditions (with an incorrect force field) and not as a proper comparison between the CLAYFF and SSFF force fields.

REFERENCES

(1) Boţan, A.; Marry, V.; Rotenberg, B.; Turq, P.; Noetinger, B. *J. Phys. Chem. C* **2013**, *117*, 978−985.

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