Structure and Dynamics of Aqueous and Aqueous-Hydrocarbon Fluids between Charged Surfaces

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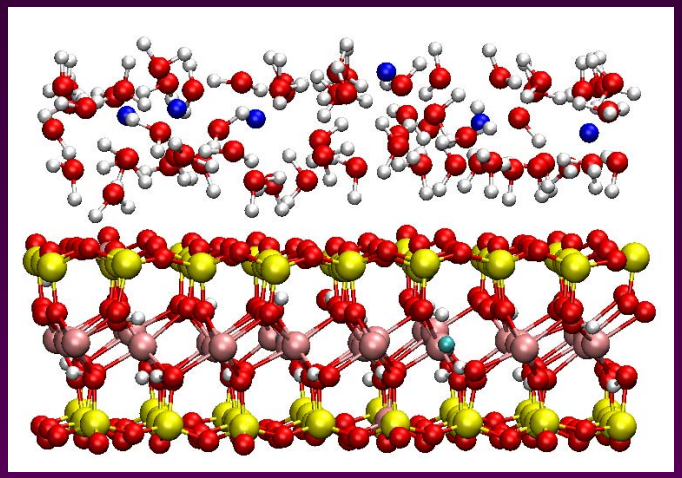
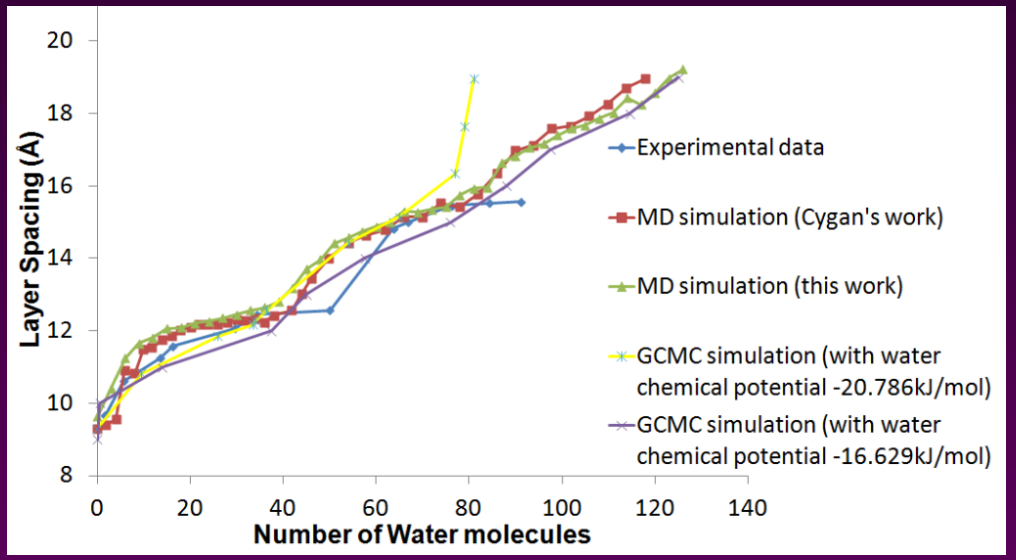


A snapshot of the two-layer aqueous hydration film near Na-montmorillonite clay surface



Swelling curves predicted by molecular simulations agree with experimental results for a Na-montmorillonite clay

Chemical potential for methane (kJ/mol)	-24.94	-16.63	-8.31	+8.31	+24.94
Number of methane molecules	0	5	30	36	49
Number of water molecules	123	110	68	65	46
Methane number fraction	0	0.0455	0.4412	0.5538	1.0652

When water chemical potential is fixed, the variation of the chemical potential of methane determines the methane content in the clay aqueous-hydrocarbon mixture