Supporting Information

Microsecond Molecular Dynamics Simulation of Methane Hydrate Formation in Humic-Acid-Amended Sodium Montmorillonite

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Table S1. Nonbond Parameters for the CLAYFF force field

Species	Symbol	Nonbond parameters		
		q/e	σ (Å)	ε (kJ/mol)
hydroxyl hydrogen	ho	+0.4250	0	0
hydroxyl oxygen with substitution	ohs	-1.0808	0.3166	0.6502
hydroxyl oxygen	oh	-0.9500	0.3166	0.6502
bridging oxygen with octahedral substitution	obos	-1.1808	0.3166	0.6502
bridging oxygen	ob	-1.0500	0.3166	0.6502
octahedral magnesium	mgo	+1.3598	0.5264	3.778×10^{-6}
octahedral aluminum	ao	+1.5750	0.4271	5.564×10^{-6}
tetrahedral silicon	st	+2.1000	0.3302	7.701×10^{-6}
aqueous sodium ion	Na	+1.0000	0.2350	0.5443

Table S2. Bond Parameters for the CLAYFF force field

Bonds			
Species i	Species j	b_0/nm	k_b/kJ·mol^{-1}·nm^{-2}
ho	ohs	0.1	463532.808
ho	oh	0.1	463532.808

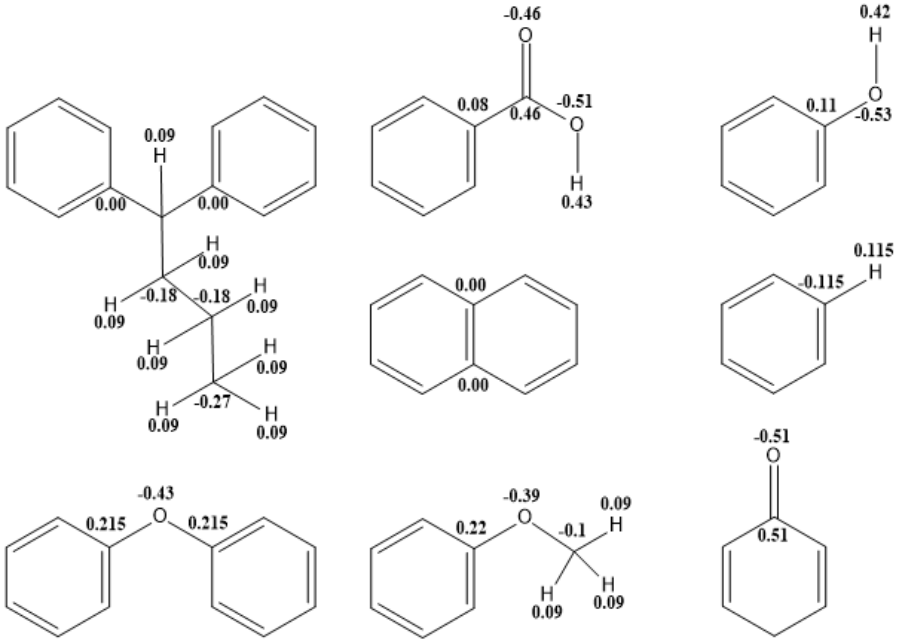

Figure S1. Partial charges for atoms in typical functional groups in LHA molecule.