Supplementary file

Molecular insights into two-phase flow in clay nanopores during gas hydrate recovery: Wettability-induced multiple pathways of water lock formation

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Table S1. The number of molecules in each simulation system at different water saturation in pore

S_w	Molecule type	Molecule number		
		NPss	NPgg	NPsg
0	CH_4	439	442	449
0.1	CH_4	359	375	428
	H_2O	484	484	484
0.2	CH_4	347	354	364
	H_2O	875	875	875
0.3	CH_4	281	292	316
	H_2O	1230	1230	1230
0.4	CH_4	250	239	284
	H_2O	1488	1488	1488
0.5	CH_4	181	209	198
	H_2O	1887	1887	1887
1.0	H_2O	3280	3280	3280

Table S2. Parameters for the flexible SPC water model (Amira et al., 2004), OPLS-UA methane (Martin and Siepmann, 1998), and the CLAYFF force field (Cygan et al., 2004). σ and ε are the Lennard-Jones parameters, in units of nm and kJ/mol, respectively; q is the partial charge of an atom in units of elementary charge (e); m is the atomic mass in units of g/mol

atom	ε (kJ/mol)	σ (Å)	q (e)	m (g/mol)
H_2O				
O	0.65	3.16552	-0.82	16.0
H	0	0	0.41	1.008
CH_4	1.23	0.373	0	16.0
Kaolinite				
Al	1.3298×10^{-6}	4.2713	1.575	26.98
Si	1.8402×10^{-6}	3.3020	2.1	28.055
O^b	0.1554	3.1655	-1.050	15.994
O^h	0.1554	3.1655	-0.950	15.994
H	0	0	0.425	1.008

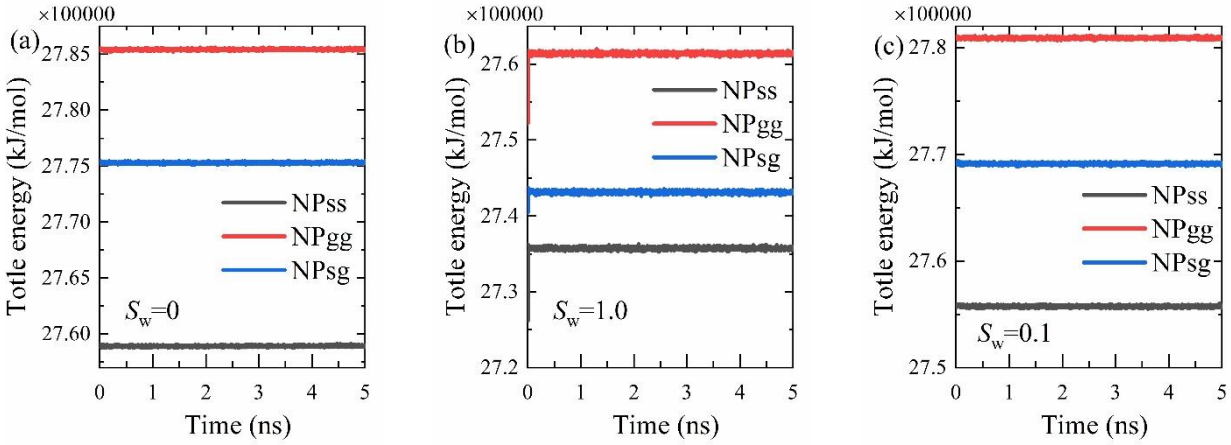

Fig. S1. The system energy profiles as a function of simulation time for different water saturation levels

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