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Article

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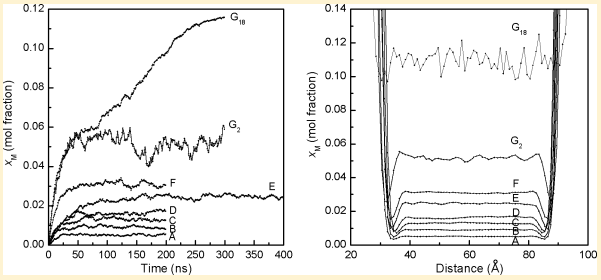
Supporting Information

ABSTRACT: [illegible]



[illegible] ~0.05 [illegible]

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Table 1. Details of Simulation Systems[a]

	N	N	T ( )	P (a)	$L_{x(y)}$ ( )	χ		a i a ( )
	3 0	1 00	25 .5	1.2	2 .	1.0	20	200
	640	1 00	25 .5	32 .5	2	1.0	20	200
	00	1 00	25 .5	2 .2	30.04	1.0	20	200
D	00	1 00	250.0	2 .4	2 . 2	1.0	20	200
	00	1 00	240.0	2 .	2 .	1.0	20	400
	00	1 00	25 .5	26.3	2 . 4	1.20	20	200
2	00	1 00	25 .5	24.5	2 . 2	1.30	2	300
1	00	1 00	25 .5	45.0	2 .3	1.30	1	300

[a] N a N a a a a , i . $L_{x(y)}$ i i a i i x-a y- i i . T, P, a χ a a , a a a i a − a a a i , i . a i i a a i . a ii , i a ifi i 2, i i a a i , a 1, i i a a i (ai i).

V i a a a a ff a ii a a a , a a ai a a i a a a i , i i i i i a a a i a a a i a i , a a a i i a i a a i .

■ E D

U i O ,[20] i i a fi a i a a fi a a i i ii a fi a i a a i a i (i i 30 × 30 × 2) a i i a i a i (30 × 30 × 5) i a a − a − a a i a , a i a a 3 a a i a i a i i 30 × 30 × 120 . N -H a a a i - a a a a , i a i 1.0 , a i NPT . a i - a a i a i-i i , a i i a i i a i x- a y- i i i i fi i z- i i . i i a ii i a i i . a i a i a a a fi i i i a i a i , a a i a fi a 1 00, a a a a i a a a x–y i i a i 30 × 30 a a i 3 0 a 00, i . 4 /2005 a[21] a i a i a i a O -U a[22] a . ifi − i i a i a i a a a , i a

$$\sigma_{MO} = (\sigma_M + \sigma_O)/2$$

$$\varepsilon_{MO} = \chi\sqrt{\varepsilon_M \varepsilon_O}$$

σ a ε a a a i a - a i a i i a aa a i a O a a a , i . a ii , χ i a a a i a i a a a , i a χ a 1 i i a a − i i . χ i i a i − a ii , i a a i ii . i D a .,[23] a χ a 1.0 i a a i ia a a i

a a i fi i i i a a i a 2 0–3 0 , a i i i a a 1 0 2 0 . a i a / a / a - a ii i a i 5% i a 40–400 a .[24] , fi a , a i a a a i i i i a 245 3 0 a a i i a a i i a / a i a a a a i a a . i a i a i χ a 1.20 a 1.30 a ii i i / a a a i . i , i a a a , − (a 1), a i a (T, P, a χ) a a ff a ii . a a , 20 i i i a i i a a a . , − a i ii i P, i a a i 1.2 2 .2 a T a i − , 25 .5 240 , a , , a iff i i χ, i a a i 1.0 1.30. ii a , a ( ) a i i a i a a a . i a ifi i 2, i i a a i i i a i , a 1, i i a a i (a i i). O a , − a i i ia i a i a ii . i a i , i a a a a i , a a a a a i i i i a . i ii fi , ii z- i i (i ., i i i a i a) i 120 a a a i i 1 a a a a i a a a a a i fi , ρ, a a ii fi , x (z) i a i , a i a . i a fi x (z) a ρ a i i 1. a i a , a i a a a , i a a i a ~15 i a i a i a i i , i i a , i i i , i a a i i a i a . a a i fi a a a a i i 2. a i a a (z 1 26 4) a i a a a (z 1 35 5 , ii , a i i 1 i a i) a i a i a , i a i a a (z 1 34 6) a

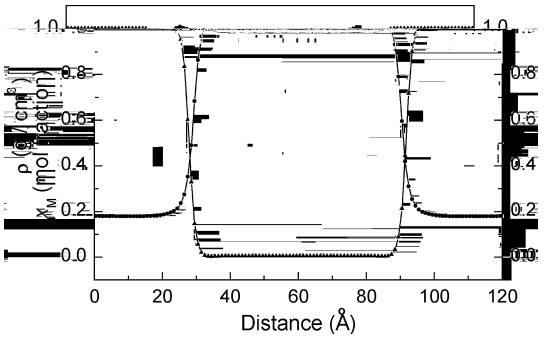

Figure 1. ia fi a i a , ai a a a a a a 100 a i. ia a ii (*x*) a i i (*ρ*).

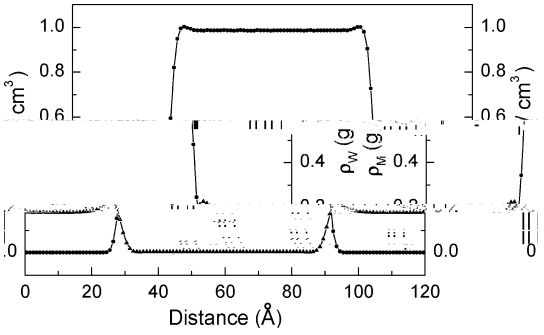

Figure 2. D i fi a (▲) a a (●) a a .

i. *x* (*z*) fi a a a , a i fi a a i i a 1a 2 i a i. a , i a , a 30 a fi (i., a 45– 5) i, a a i a i aa ff fi i.

a a a fi a a a a . i a , “a ” a a -a a a , a fi i i i , [13,25] a i a i a . a fi ia a 5.3 (fi ii i a – a a i i i i). a fi a i a i i a a .

E

i i *x* (*t*) (a a 45a 5) i i i 3. , i i a a a a a i i 100 . i i , a 200 i a i a a ii a . ii a , a a a 20 i a i , a a. i i a i i i a a a a a a i 1 20 a a i a i i a i , [13] i., a a -fi i i a i a a .

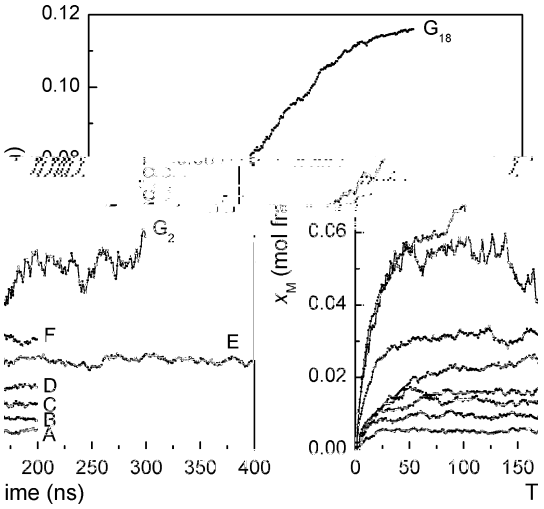

Figure 3. i i *x* (*t*) a . aa a a a i a fi (45– 5) i a i i a . a i a a a 1 .

a i a a i a fi i a . i i a a a – (i a 3a 4 , i a i). i a i a i , i a 2, a a i i fi a a i i 1 i a i (1) a a a - i . i, i a 100 a i a i a a a i a (a a) i i i .

i a 4 i i fi a , *x* (*z*) (a a a 100 i a i), a .

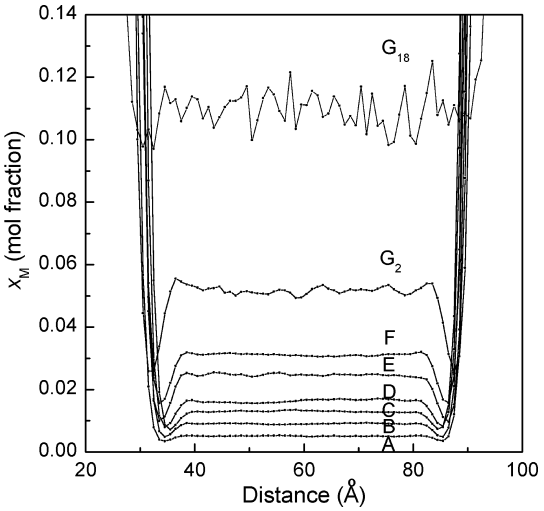

Figure 4. a fi *x* (*z*) a . aa a a a a 100 a i a i , a a i a a a l i a .

a i i a a i i i a a a fi (a. 40– 0), a i i a i a i (1). O a i i a 3a 4, a – 2 a a a a i i i a i a a a i . , i i a i i i , a

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Table 2. Structural Characterization of Methane Solutions under the Equilibrium (system A) and Metastable (systems B−G$_2$) Conditions[a]

	N	N	x	C ($^{-3}$)	C_a ($^{-3}$)	ρ (/ ^{3})	f
	4.5(2)	(1)	0.0051(2)	0.1 (1)	0.246(0)	0. 01(2)	0.214(0)
	.2(3)	(1)	0.00 1(4)	0.30(1)	0.22 (1)	1.0046(4)	0.201(0)
	12.2(3)	20(1)	0.0131(3)	0.45(1)	0.200(1)	1.02 4(3)	0.1 (0)
D	15.1(3)	05(1)	0.0164(3)	0.56(1)	0.255(1)	1.023 (4)	0.226(1)
	22.3( )	0(2)	0.024 ( )	0. 4(3)	0.365(3)	1.011 ( )	0.30 (2)
	2 .2(4)	2(1)	0.0310(5)	1.05(1)	0.240(1)	1.00 (5)	0.20 (1)
2	45. (15)	42(3)	0.0514(1)	1. 1(5)	0.2 (3)	0. 02(15)	0.24 (1)

[a] a a a a i a a (i., 45 ≤ z ≤ 5). a 100 . N a N a a a a i i fi a x 1 N /(N + N)a i a i C 1 N /V, V i a i a a. a a i C_a 1 N_a /V, N_a i a . ρ i a a i a i , a f_a i a i i a a a a a a a a a a i fi i .[13] i a a a a a , a a 20 i — a i 2.

a i i a i a a a . — 2, i i i a a a a a a " " a x a i i a 2. i i a , i ifi a a i a a a a a ii i i i fi i a a i a i i (i 5) a i

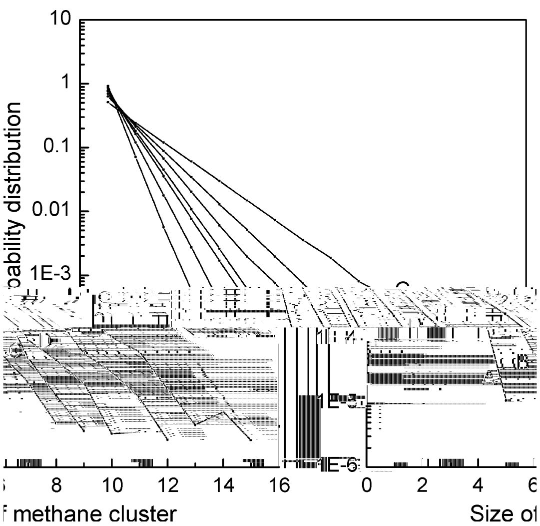

Figure 5. a ii i i i fi i a a i a i i .

a a i a a i i a i a fi (i., 45 ≤ z ≤ 5) a a a — a a - a a a a i a . N i i i i a i a ii 2 (a 2), a a i i a a a a a . i a i a a i (i) a (i 1 i i 5), 2% i 52% i 2, a i i (i) a i i a 5- a i i i 0.004 x i 0.0266 2. i i , a i a i i a i i a ii . i i i i i i , a i i a i i a , a -a a i a , i ia i .

a 6a a 3 13).

a a i i 5 i i a i i i i i , i ia i a i i i i i, i a a , a . ii i , a ii i i i i i (−G_n/kT), G_n i i i a n a , i 5 a i ia a i , G_n/kT, i a i a i n. i i i i i a ia a i ,[26] i i G_n a a ii a (a i a $n^{2/3}$)a a a i (a i a n^1), a i ia a a a i i a a i . i i i a a i a a i i , a a a i i 5 a i i a 3 a i

Table 3. Free Energies for Methane Cluster Formation[a]

	$\Delta G_1/kT$		$\Delta G_1/kT$
	2.55		1.11
	1. 1		0. 1
	1.56	2	0. 0
D	1.42		

[a] ΔG_1 i a a a i i a i ai a i i i 5.

a a i i ifi a a a (kT) 2. iff i ia a i a i i a i a i i i a , a i a a i i a a i i i a a a i .

■ D C

fi , a 25 .5 a 1.2 a. i i a i i 4 /2005 a i 250 a i a i a a a a a i a ,[24] a ia a a i i i fi . , i a a a i , i i a a i a ii i a i . a a x

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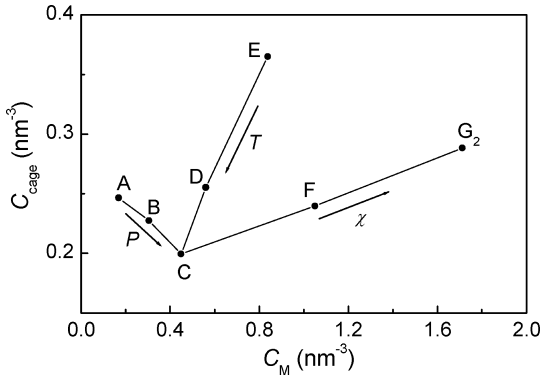

Figure 6.

[illegible] ($\sim$ [illegible]) [illegible] 0.05, [illegible] 1. [illegible] .4 [illegible] 0.0 [illegible] ($\sim$ .6 [illegible]) [illegible] 0.0 [illegible] ($\sim$ .0 [illegible]) [illegible] C [illegible] 2, [illegible] 1 .1 [illegible] $\sim$0.05 [illegible] (i.e., C 1-1. [illegible]) [illegible] [32] [illegible] [33] [illegible] [10,11] [illegible] [12,1] [illegible] χ, [illegible]

■ C G [illegible]

[illegible]

[illegible] 1 −31% [illegible] ([illegible] 2). [illegible] $\sim$0.05 [illegible] 1. [illegible]

■ A [illegible] CA EDC [illegible] E

● [illegible] pp [illegible] g [illegible]

[illegible]

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