

Supplementary Material

A comparison of atomic-level and coarse-grained models for liquid hydrocarbons from
molecular dynamics configurational entropy estimates

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Supplementary Tables – captions

Table s 1 Single-fragment configurational entropies (AL model) of the alkane chains from MD simulations of liquid hydrocarbons. Entropies are calculated using 800 configurations collected over simulation periods of different lengths. The number of atoms used for the fitting procedure, the relative contribution of overall rotation to absolute entropy, and the simulation temperature are also reported. All entropies are given in $\text{J} \cdot \text{K}^{-1} \cdot \text{mol}^{-1}$. Fragments (fc) nomenclature refers to Figure 1. See Table 2 and Methods section for definitions of entropy codes.

Table s 1 Single-fragment configurational entropies (AL model) for chain fragments of liquid hydrocarbons.^a

system	fc	$S_{ch}^i(fc)$	$S_{ch}^{ip}(fc)$	$S_{ch}^{ir}(fc)$	$S_{ch}^{irp}(fc)$	nr. atoms fit	$s_{ch}^r(fc)$	time period [ns]	T [K]
		[J · K ⁻¹ · mol ⁻¹]					[%]		
Dodecane	A	229	57	310	77	12	26	2.5	303
	B	217	54	286	71	12	24	2.5	303
	C	229	57	310	77	12	26	2.5	303
Tetradecane ^b	A	240	60	314	78	14	23	2.5	303
	B	175	58	229	76	14	23	2.5	303
	C	175	58	229	76	14	23	2.5	303
	D	240	60	314	78	14	23	2.5	303
Hexadecane	A	264	66	330	82	16	20	25	323
	B	247	62	309	77	16	20	25	323
	C	246	61	309	77	16	20	25	323
	D	262	65	329	82	16	20	25	323
Octadecane ^c	A	273	68	334	83	18	18	25	323
	B	254	63	316	79	18	20	25	323
	C	131	65	163	81	18	20	25	323
	D	253	63	316	79	18	20	25	323
	E	272	68	334	83	18	18	25	323
<i>cis</i> -9-octadecene ^c	A	272	68	332	83	18	18	25	303
	B	248	62	311	78	18	20	25	303
	C	119	59	165	82	18	28	25	303
	D	248	62	311	78	18	20	25	303
	E	272	68	333	83	18	18	25	303

a. Results are averaged over 128 alkane chains simulated. Standard deviations around the average (over all molecules) are not reported (smaller than 0.5 J K⁻¹ mol⁻¹ in all cases).

b. Note: fragments B and C only include 3 united atoms.

c. Note: fragment C only includes 2 united atoms.

Supplementary Figures

Figure s 1 Single-molecule internal and internal plus rotational configurational entropies for AL hexadecane (C16) at 323 K, from concatenated 200 ns trajectories of $m = 1 \dots 16$ individual chains (500 configurations per trajectory). Internal $S_{ch}^i(ch)$ (continuous line) and internal plus rotational $S_{ch}^{ir}(ch)$ (dashed line) entropies were calculated for 16 randomly chosen chains (out of 128 in the simulated system). Vertical dotted lines separate the 16 individual trajectories. Error bars are smaller than $0.5 \text{ J} \cdot \text{K} \cdot \text{mol}^{-1}$ (not displayed). See Table 2 and Methods section for definitions of entropy codes.

Figure s 2 Correlation between the inverse of the relative contribution $s_{ch}^r(ch)$ (Eq. (3)) of rotational entropy to the total entropy for hydrocarbon chains and the average radius of gyration R_{gyr} , based on simulations with the AL model at temperatures specified in Table 3.

Figure s 1

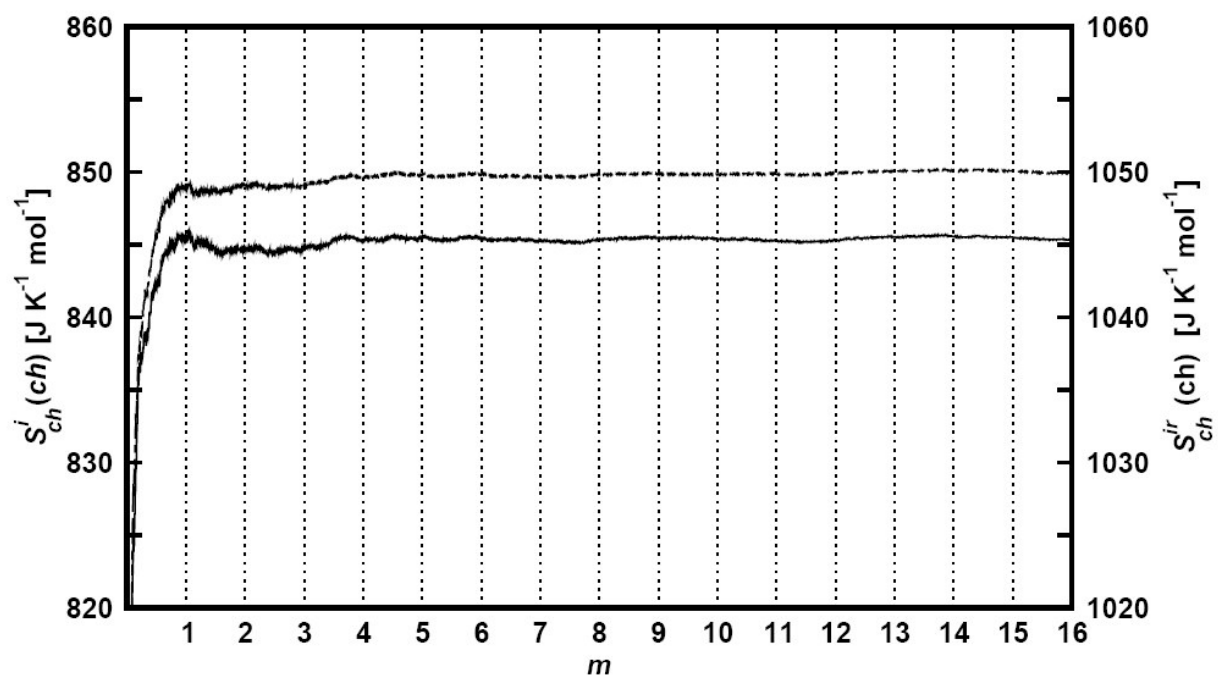


Figure s 2

