Electronic Supplementary Information for

In silico cooling rate dependent crystallization and glass transition in n-alkanes

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Section S2 : R_{ee} distribution of C16 for fast cooling rates



Fig. S1: Root mean square deviation (RMSD) of C4, C16 and C50 during (I) temperature rescaling, (II) 5 ns NVT, and (III) 5 ns NPT equilibration trajectories.



Fig. S2: Representative snapshots of the liquid phase after the 100 ns NPT production run for (a) C12 at 310 K and (b) C16 at 370 K. Molecules colored according to their end-to-end distances.

Table S1: Box dimensions [in Å] and the heating temperature [in K] utilized for obtaining the 14 n-alkanes in the liquid phase.

<i>n</i> -Alkane	Box Dimensions $(x y z)$	Heating Temp.
C4	$(26\ 26\ 26)$	300
C6	$(30 \ 30 \ 24)$	300
C8	$(35 \ 35 \ 23)$	300
C10	$(40 \ 40 \ 21)$	300
C12	$(40 \ 40 \ 24)$	310
C14	$(47 \ 47 \ 20)$	330
C16	$(47 \ 47 \ 22)$	370
C18	$(47 \ 47 \ 25)$	350
C20	$(47 \ 47 \ 30)$	350
C22	$(47 \ 47 \ 31)$	400
C24	$(47 \ 47 \ 32)$	400
C30	(505036)	400
C40	$(50 \ 50 \ 52)$	400
C50	$(60 \ 60 \ 41)$	400

S1. Fitting polynomials to the density data

The simulated densities, ρ , for the four slower cooling rates ($\leq 1.2 \times 10^{12}$ K/min) of C12 and C16 are shown in Fig. S3. Evidently, ρ increases as the temperature decreases. At 6×10^{10} and 1.2×10^{11} K/min, the gradual rise of ρ in the liquid region changes to an abrupt surge during the liquid to crystal phase transition, which rises steadily on further cooling. Three regions (liquid, liquid to crystal transition, and crystal) are clearly seen in the figure. These are denoted as high temperature (HT), transition from liquid to crystal (TLC), and low temperature (LT). A similar trend is observed for $\gamma = 6 \times 10^{11}$ K/min, except that in the TLC region $\rho(T)$ does not rise as steeply. Hence, at these three γ 's, for HT, TLC and LT regions, we fitted ρ to a second order polynomial, a straight line, and a third order polynomial, respectively. At 1.2×10^{12} K/min, we were unable to detect the TLC region. So, we fitted ρ to two different second order polynomials in the HT and LT regions. The fitted equations are given in Table S2 and, graphically, in Fig. 2.

The simulated $\rho(T)$ values obtained at the three fastest γ 's ($\geq 3 \times 10^{12}$ K/min), which do not lead to a crystal phase, are shown in Fig. S4. The data show, as expected, that $\rho(T, n)$ increases monotonically with n. The presence of some noise in the data is also evident. Since our analysis requires very clean data, we fit it to analytical functions as described below. In addition, we have checked (Figs. S5 and S6) that, within limits, there is no dependence on the system size and box dimensions.



Fig. S3: The simulated density (ρ [kg/m³]) for the four slower cooling rates of (a) C12 and (b) C16 as calculated during the cooling trajectories.

γ [K/min]	Region	C12	C16
1.2×10^{12}	LT	$913.487 - 0.240798T - 0.0004825T^2$	$922.092 - 0.17973T - 0.0006415T^2$
	HT	$975.9 - 0.5592T - 0.000724T^2$	$1012.0 - 0.713253T - 0.0002235T^2$
6×10^{11}	LT	$924.165 - 0.290454T + 0.00026542T^2 - 0.000003T^3$	$939.289 - 0.327776T + 0.0011965T^2 - 0.0000058T^3$
	TLC	1113.74 - 1.30747T	1164.88 - 1.32585T
	HT	$1025.84 - 0.952251T + 0.0000155T^2$	$990.957 - 0.575389T - 0.00044034T^2$
1.2×10^{11}	LT	$958.736 - 0.336762T + 0.0010108T^2 - 0.0000049T^3$	$980.347 - 0.394589T + 0.0016577T^2 - 0.000006T^3$
	TLC	1531.9 - 2.864T	1669.25 - 3.03794T
	HT	$656.523 + 1.66114T - 0.00458158T^2$	$1122.74 - 1.37387T + 0.0007589T^2$
6×10^{10}	LT	$962.761 - 0.372754T + 0.00126T^2 - 0.00000576T^3$	$987.034 - 0.372402T + 0.0014012T^2 - 0.0000047T^3$
	TLC	3219.99 - 9.49938T	3226.81 - 8.43022T
	HT	$611.624 + 1.87464T - 0.00479748T^2$	$1117.43 - 1.33754T + 0.000699T^2$

Table S2: Polynomials used for fitting the temperature dependence of the density $[kg/m^3]$ of C12 and C16 at the four slower γ values.



Fig. S4: The simulated density (ρ [kg/m³]) of the 14 alkanes as obtained by averaging over three trajectories for each alkane and each γ = (a) 6 × 10¹³, (b) 6 × 10¹², and (c) 3 × 10¹² K/min.



Fig. S5: Comparison of $\rho(T)$ between 100 and 1000 molecules of C16, rapidly cooled at $\gamma = 6 \times 10^{13}$ K/min. It shows that increasing the number of molecules in our simulations ten-fold do not affect these data.



Fig. S6: Comparison of $\rho(T)$ between two different box dimensions [in Å] of C4, rapidly cooled at $\gamma = 6 \times 10^{13}$ K/min. It shows that the box dimensions have a negligible effect on the density versus temperature data.

The data for fast cooling rates is used to obtain T_g . Fig. S7 shows a fit of two intersecting straight lines in the range of T between 10 and 300 K. The intersection point of the two lines produces an initial guess for T_g , denoted T_g^* and listed in Table S3. Subsequently, we refit $\rho(T)$ in the two regions (LT and HT), above and below T_g^* , with appropriate polynomials. We find that a polynomial of order two can approximate the behaviour (of $\rho(T)$) satisfactorily in both LT and HT regions. These polynomials are listed in Table S4.



Fig. S7: Two straight lines fitted to the simulated density of C12 at $\gamma = (a) \ 6 \times 10^{13}$, (b) 6×10^{12} , (c) 3×10^{12} and (d) 1.2×10^{12} K/min. The intersection points, denoted T^* , are given in each panel, and summarized in Table S3.

Table S3: The guess values for T_g [K] (T_g^*) , as obtained from the intersection of the two straight lines in Fig. S7, at the three fastest cooling rates, γ , for the 14 *n*-alkanes.

<i>n</i> -Alkane	6×10^{13}	6×10^{12}	3×10^{12}
C4	100	93	93
C6	129	120	117
C8	152	152	146
C10	153	152	151
C12	184	182	179
C14	193	182	180
C16	205	202	196
C18	208	212	202
C20	211	208	190
C22	226	213	213
C24	228	229	219
C30	237	232	221
C40	240	223	225
C50	246	237	234

Alkane	γ	LT polynomial	HT polynomial
$\overline{\mathrm{C4}}$	a	$838.946 - 0.342659T - 0.0019604T^2$	$859.78 - 0.591931T - 0.0015425T^2$
	b	$845.224 - 0.233776T - 0.0028635T^2$	$887.875 - 0.900991T - 0.0007103T^2$
	с	$846.924 - 0.283607T - 0.0021943T^2$	$889.63 - 0.891206T - 0.000781T^2$
$\overline{\mathrm{C6}}$	a	$862.737 - 0.283433T - 0.0012444T^2$	$892.916 - 0.535245T - 0.0009954T^2$
	b	$870.301 - 0.274908T - 0.0010688T^2$	$908.76 - 0.625862T - 0.0008901T^2$
	с	$872.183 - 0.298993T - 0.0008229T^2$	$920.962 - 0.718704T - 0.0007142T^2$
C8	a	$873.849 - 0.242314T - 0.0009137T^2$	$868.207 - 0.0711586T - 0.0018098T^2$
	b	$883.713 - 0.245242T - 0.0008397T^2$	$920.3 - 0.459999T - 0.00105T^2$
	с	$887.276 - 0.23529T - 0.0009432T^2$	$944.0 - 0.666T - 0.0006T^2$
$\overline{\mathrm{C10}}$	a	$887.399 - 0.245286T - 0.0010596T^2$	$849.001 + 0.190003T - 0.0022909T^2$
	b	$896.353 - 0.273116T - 0.0006795T^2$	$946.565 - 0.584028T - 0.0007226T^2$
	с	$897.686 - 0.246077T - 0.0008698T^2$	$931.998 - 0.4262T - 0.0011201T^2$
$\overline{\text{C12}}$	a	$888.941 - 0.245822T - 0.0006045T^2$	$911.691 - 0.314576T - 0.000896T^2$
-	b	$897.526 - 0.208267T - 0.0006966T^2$	$914.305 - 0.21007T - 0.001209T^2$
	с	$902.253 - 0.214936T - 0.0006855T^2$	$906.692 - 0.0854423T - 0.0015655T^2$
C14	a	$900.038 - 0.222829T - 0.0007542T^2$	$909.038 - 0.182999T - 0.0011925T^2$
	b	$909.155 - 0.205129T - 0.0007395T^2$	$949.976 - 0.400206T - 0.0008758T^2$
	\mathbf{c}	$914.359 - 0.201053T - 0.0007466T^2$	$964.529 - 0.484683T - 0.0007496T^2$
C16	a	$897.092 - 0.23334T - 0.0004244T^2$	$892.593 - 0.0758474T - 0.0010939T^2$
	b	$908.363 - 0.178671T - 0.0006071T^2$	$939.411 - 0.278839T - 0.0008793T^2$
	\mathbf{c}	$914.866 - 0.213012T - 0.0004795T^2$	$970.162 - 0.4734T - 0.000554T^2$
C18	a	$898.832 - 0.19269T - 0.0005725T^2$	$941.098 - 0.444017T - 0.0003427T^2$
	b	$910.674 - 0.201991T - 0.0004854T^2$	$933.003 - 0.2092T - 0.000944T^2$
	с	$919.651 - 0.203735T - 0.0004464T^2$	$945.002 - 0.2073T - 0.001072T^2$
C20	a	$902.216 - 0.236602T - 0.0003037T^2$	$913.578 - 0.181133T - 0.0008074T^2$
	b	$916.12 - 0.174619T - 0.0005879T^2$	$924.418 - 0.112277T - 0.0010858T^2$
	\mathbf{c}	$921.158 - 0.210741T - 0.0003235T^2$	$930.128 - 0.0947573T - 0.0011880T^2$
C22	a	$900.916 - 0.188962T - 0.0005333T^2$	$904.105 - 0.129629T - 0.0008554T^2$
	b	$912.973 - 0.203802T - 0.0003669T^2$	$951.024 - 0.29636T - 0.0007287T^2$
	\mathbf{c}	$920.502 - 0.170217T - 0.0005747T^2$	$973.454 - 0.422577T - 0.0005477T^2$
C24	a	$900.491 - 0.180628T - 0.0005189T^2$	$905.71 - 0.134513T - 0.000821T^2$
	b	$914.589 - 0.164562T - 0.0005588T^2$	$912.153 - 0.0179512T - 0.0011562T^2$
	\mathbf{c}	$920.855 - 0.162579T - 0.0005394T^2$	$941.002 - 0.16009T - 0.0009727T^2$
C30	a	$902.16 - 0.163578T - 0.0005393T^2$	$916.044 - 0.2112T - 0.000591T^2$
	b	$919.493 - 0.178622T - 0.0004191T^2$	$945.856 - 0.210938T - 0.0007838T^2$
	\mathbf{c}	$922.729 - 0.158729T - 0.0004956T^2$	$948.169 - 0.200344T - 0.0008237T^2$
C40	a	$906.058 - 0.175071T - 0.0003932T^2$	$928.418 - 0.23678T - 0.0005226T^2$
	b	$923.126 - 0.164432T - 0.0004335T^2$	$925.569 - 0.0567517T - 0.0009452T^2$
	\mathbf{c}	$926.632 - 0.152479T - 0.0004547T^2$	$947.133 - 0.15867T - 0.000834T^2$
C50	a	$908.812 - 0.16986T - 0.0003842T^2$	$900.004 - 0.03421T - 0.000795T^2$
	b	$924.417 - 0.149638T - 0.000433T^2$	$921.548 - 0.01135T - 0.0009723T^2$
	\mathbf{c}	$927.184 - 0.162153T - 0.000353T^2$	$950.96 - 0.157952T - 0.0008053T^2$

Table S4: Polynomials (in T) fitted to the density ρ [kg/m³] of the 14 alkanes for γ = (a) 6×10^{13} , (b) 6×10^{12} , and (c) 3×10^{12} K/min.

Table S5: Fraction of crystalline molecules (χ , in %), obtained from our intra- and intermolecular measures by averaging over all frames in the temperature range $10 \le T \le 150$ K for the seven cooling rates of C12 and C16.

$\overline{\gamma}$	Intramolecular	C12 [%]	C16 [%]	Intermolecular	C12 [%]	C16 [%]
6.0×10^{13}		3.63	0.00		10.17	4.67
6.0×10^{12}		11.39	4.31		12.54	10.48
3.0×10^{12}		16.61	9.53		16.25	10.16
1.2×10^{12}		32.25	10.06		32.85	17.64
6.0×10^{11}		37.58	40.22		36.13	49.41
1.2×10^{11}		80.58	83.89		76.28	81.53
6.0×10^{10}		88.0	93.68		90.94	92.05



Fig. S8: Discontinuity in the first derivative of ρ with respect to T, $(\frac{\partial \rho}{\partial T})_P$, indicating a 2ndorder glass transition (Ehrenfest nomenclature) for rapidly cooled C16. In this example, T_g hardly varies with γ . Compare with Fig. 3 in the main text.



Fig. S9: Geometry of three consecutive carbon atoms in a fully stretched *n*-alkane.



Fig. S10: Hairpin geometry of C16 obtained by implementing the TTTTGGTGGTTTT conformation in gview 6. Note the alternating CC distances (red distances, in Å) between the two tails of the hairpin. The averaged distance is 4.2 Å.

S2. R_{ee} distribution of C16 for fast cooling rates

In comparison with the end-to-end distance distributions of liquid and glassy C12 (at the two largest γ 's) in Fig. 6 of the main text, the corresponding R_{ee} distributions of C16 for are shown in Fig. S11. The distribution for the liquid exhibits a single broad peak at 15.6 Å (vs. 12.1 Å for C12), and is otherwise featureless (as for C12). However, the dominant peak for the glass, obtained at the fastest rate (γ_{max} , black line) appears at 16.3 Å rather than at 15.6 Å (whereas for C12 the two peaks coincide). In fact, the whole γ_{max} distribution for C16 has stronger intensities for the near-linear

conformers (at large R_{ee}) than the liquid, and weaker intensities for the bent rotamers (at small R_{ee}). Hence, unlike C12, the γ_{max} rate is not fast enough for trapping the dominant C16 conformers that existed in the SCL for $T > T_g$. While for C12 a peak for the lowest energy, linear conformer (at 13.9 Å) appears already at γ_{max} , the corresponding peak for C16 (at 19 Å) appears only when $\gamma < \gamma_{max}$. Possibly, for a larger *n* there are more low-energy near-linear conformers to compete and interfere with the search for the linear global minimum. In panel b, we show a few (of the many) rotamers corresponding to the peaks of the γ_{max} distribution. A representative conformer with $R_{ee} = 19$ Å is also shown, taken from the slower γ distribution in pane a.



Fig. S11: End-to-end distance distributions and representative conformers for C16. (a) R_{ee} distributions for liquid C16 (cyan line), and for glassy C16 obtained by cooling at the rates of 6×10^{13} K/min (black line, γ_{max}) and 6×10^{12} K/min (red line). The R_{ee} values (in Å) for major γ_{max} peaks are marked. In contrast to C12 (Fig. 6), there is no trace for the stretched C16 conformer at 19 Å for the fastest γ . However, a conspicuous peak appears once γ is made an order of magnitude smaller. (b) Representative rotamers corresponding to peaks in the γ_{max} distribution of panel a.



Fig. S12: R_{ee} distributions for C12 (top) and C16 (bottom) over the whole R_{ee} range, see Figure S11 for detail. Note that a small peak at 4 Å does not appear here, and that the stretched conformer peak is dominant at the slower cooling rate.



Fig. S13: R_{ee} distributions for C18 (top) and C20 (bottom), see Figure S11 for detail. Note that a small peak at 4 Å appears here for the first time, and that the stretched conformer peak is less prominent than for C12 and C16.



Fig. S14: A representative hairpin conformer of C20 extracted from the alkane glass coordinates at 10 K, after cooling subject to the fastest γ .



Fig. S15: Representative snapshots of C16, as obtained at the end of cooling at 7 rates (fastest to slowest rates are shown in the order from a to g) at 10 K. Five different colors have been chosen based on R_{ee} values. Compare with Fig. 9 in the main text for C12.



Fig. S16: Enthalpy, H at three fastest cooling rates, ($\gamma \ge 3 \times 10^{12}$ K/min) for C4, C6, C8 and C10.



Fig. S17: Enthalpy, H at three fastest cooling rates, ($\gamma \ge 3 \times 10^{12}$ K/min) for C14, C18, C20 and C22.



Fig. S18: Enthalpy, H at three fastest cooling rates, ($\gamma \ge 3 \times 10^{12}$ K/min) for C24, C30, C40 and C50.

Table S6: Two intersecting straight lines (in T) fitted to the enthalpy H in the high- and low-temperature regions (HT and LT, respectively), of the 14 alkanes for $\gamma = (a) \ 6 \times 10^{13}$, (b) 6×10^{12} , and (c) 3×10^{12} K/min.

Alkane	γ	LT	HT
$\overline{\mathrm{C4}}$	a	-16 + 0.28T	-19 + 0.31T
	\mathbf{b}	-17 + 0.28T	-19.7 + 0.31T
	с	-17 + 0.275T	-19.7 + 0.31T
$\overline{\mathrm{C6}}$	a	-20 + 0.4T	-27.5 + 0.45T
	b	-21 + 0.39T	-28.5 + 0.45T
	\mathbf{c}	-21.3 + 0.39T	-29.5 + 0.455T
$\overline{\mathrm{C8}}$	a	-25.6 + 0.51T	-36.5 + 0.58T
	b	-28.3 + 0.506T	-41.5 + 0.595T
	с	-29 + 0.51T	-41.5 + 0.595T
C10	a	-26 + 0.63T	-36 + 0.695T
	b	-29 + 0.626T	-44 + 0.725T
	с	-30 + 0.63T	-43.8 + 0.72T
C12	a	-37 + 0.745T	-56 + 0.85T
	b	-41 + 0.744T	-61.7 + 0.86T
	с	-43.5 + 0.747T	-66 + 0.88T
C14	a	-38 + 0.87T	-61 + 0.99T
	b	-43 + 0.87T	-69 + 1.01T
	с	-44.5 + 0.865T	-70 + 1.005T
C16	a	-51.5 + 0.985T	-78 + 1.115T
	b	-58 + 0.985T	-91 + 1.15T
	с	-61 + 0.985T	-94 + 1.15T
C18	\mathbf{a}	-58 + 1.11T	-85 + 1.24T
	b	-64.9 + 1.11T	-102 + 1.28T
	с	-68 + 1.11T	-103 + 1.28T
C20	a	-62.5 + 1.22T	-90 + 1.35T
	b	-72 + 1.223T	-108 + 1.4T
	с	-75 + 1.22T	-114 + 1.415T
C22	a	-68 + 1.35T	-102 + 1.5T
	b	-75 + 1.33T	-123 + 1.55T
	с	-81 + 1.34T	-129 + 1.57T
C24	a	-72.5 + 1.465T	-111 + 1.63T
	b	-82 + 1.46T	-135 + 1.69T
	с	-89 + 1.47T	-142 + 1.71T
C30	a	-90 + 1.83T	-139 + 2.04T
	b	-102 + 1.82T	-161 + 2.08T
<u></u>	с	-105 + 1.817	-170 + 2.17
C40	a	-119 + 2.41T	-188 + 2.77
	b	-137 + 2.42T	-217 + 2.76T
	с	-140 + 2.47	-222 + 2.761T
C50	a	-145 + 3.07	-230 + 3.35T
	b	-164 + 2.997	-273 + 3.45T
	с	-170 + 3.0T	-273 + 3.44T