Diffusion and Friction Dynamics of Probe Molecules in Liquid *n*-Alkane Systems: A Molecular Dynamics Simulation Study

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Supplementary Materials

The log-log plots of the self-diffusion coefficient (D_{self}) of liquid *n*-alkanes, and those of the diffusion coefficients of MY1 (D_{MY1}) and MY2 (D_{MY2}) in liquid *n*-alkane systems *vs* the molecular weight (M) of liquid *n*-alkanes at four different temperatures shown in Figs.1 and 2 are obtained from S.Table 1 and the log-log plots of the friction coefficient (ζ_{self}) of liquid *n*-alkanes, and those of the friction coefficients of MY1 (ζ_{MY1}) and MY2 (ζ_{MY2}) in liquid *n*-alkane systems *vs* the molecular weight (M) of liquid *n*-alkanes at four different temperatures shown in Figs.3 and 4 are obtained from S.Table 2.

S.Table 1. Logarithm of diffusion coefficients D(10^{-6} cm^2/s) of *n*-alkanes, MY1, and MY2 in *n*-alkanes at T = 318, 418, 518, and 618 K.

n-alkane	D_{self}				D_{MY1}				D_{MY2}			
	318K	418K	518K	618K	318K	418K	518K	618K	318K	418K	518K	618K
$C_{12}H_{26}$	1.198	1.642	1.943	2.191	1.656	2.069	2.313	2.489	0.728	1.482	2.035	2.275
$C_{20}H_{42}$	0.689	1.264	1.598	1.864	1.360	1.890	2.197	2.411	0.357	1.243	1.850	2.149
$C_{28}H_{58}$	0.351	1.027	1.386	1.641	1.152	1.760	2.128	2.361	0.137	1.057	1.753	2.070
$C_{36}H_{74}$	0.084	0.810	1.224	1.491	1.036	1.664	2.054	2.335	-0.001	0.920	1.674	2.013
$C_{44}H_{90}$	-0.112	0.668	1.066	1.361	0.920	1.585	2.013	2.305	-0.065	0.869	1.598	1.982
$C_{80}H_{162}$	-0.645	0.194	0.615	0.933	0.603	1.378	1.880	2.240	-0.229	0.708	1.422	1.863

$C_{120}H_{242}$	-0.934	-0.086	0.324	0.653	0.423	1.241	1.806	2.199	-0.331	0.609	1.302	1.790
$C_{160}H_{322}$	-1.048	-0.270	0.119	0.438	0.284	1.136	1.749	2.165	-0.414	0.555	1.216	1.733
$C_{200}H_{402}$	-1.142	-0.362	0.009	0.321	0.185	1.068	1.710	2.137	-0.469	0.502	1.160	1.685
$C_{240}H_{482}$	-1.189	-0.431	-0.075	0.220	0.115	1.011	1.680	2.114	-0.514	0.467	1.118	1.652
$C_{280}H_{562}$	-1.232	-0.489	-0.147	0.130	0.056	0.962	1.656	2.095	-0.552	0.438	1.082	1.620
$C_{320}H_{642}$	-1.280	-0.540	-0.208	0.055	0.005	0.920	1.635	2.080	-0.585	0.413	1.051	1.591
$C_{360}H_{722}$	-1.314	-0.582	-0.260	-0.024	-0.037	0.885	1.618	2.065	-0.613	0.392	1.026	1.573
$C_{400}H_{802}$	-1.348	-0.624	-0.311	-0.059	-0.080	0.850	1.600	2.050	-0.640	-0.370	1.002	1.550

S.Table 2. Logarithm of friction coefficients ζ (g/ps·mol) of *n*-alkanes, MY1, and MY2 in *n*-alkanes at T = 318, 418, 518, and 618 K.

n-alkane	ζ_{self}				ζ_{MY1}				ζ_{MY2}			
	318K	418K	51 K	618K	318K	418K	518K	618K	318K	418K	518K	618K
$C_{12}H_{26}$	2.850	2.768	2.680	2.570	2.367	2.301	2.225	2.134	2.609	2.516	2.436	2.368
$C_{20}H_{42}$	3.072	2.996	2.918	2.838	2.418	2.354	2.288	2.207	2.657	2.567	2.491	2.429
$C_{28}H_{58}$	3.218	3.144	3.071	2.997	2.445	2.383	2.322	2.250	2.687	2.598	2.521	2.463
$C_{36}H_{74}$	3.331	3.256	3.182	3.110	2.462	2.401	2.340	2.274	2.704	2.611	2.541	2.486
$C_{44}H_{90}$	3.422	3.346	3.272	3.204	2.478	2.415	2.354	2.290	2.711	2.619	2.554	2.500
$C_{80}H_{162}$	3.694	3.616	3.541	3.472	2.513	2.453	2.391	2.326	2.723	2.630	2.581	2.530
$C_{120}H_{242}$	3.856	3.798	3.724	3.654	2.531	2.470	2.409	2.348	2.726	2.639	2.598	2.547
$C_{160}H_{322}$	3.974	3.915	3.857	3.791	2.545	2.483	2.421	2.359	2.731	2.645	2.610	2.555
$C_{200}H_{402}$	4.064	4.014	3.995	3.890	2.553	2.492	2.431	2.369	2.735	2.647	2.619	2.566
$C_{240}H_{482}$	4.130	4.090	4.031	3.962	2.562	2.500	2.439	2.377	2.737	2.651	2.627	2.574
$C_{280}H_{562}$	4.202	4.162	4.100	4.404	2.569	2.507	2.446	2.383	2.739	2.654	2.633	2.580
$C_{320}H_{642}$	4.249	4.209	4.160	4.098	2.575	2.513	2.450	2.388	2.741	2.657	2.639	2.586
$C_{360}H_{722}$	4.301	4.259	4.205	4.148	2.580	2.518	2.454	2.393	2.743	2.660	2.644	2.591
$C_{400}H_{802}$	4.352	4.309	4.250	4.196	2.584	2.522	2.460	2.397	2.744	2.662	2.648	2.596