System-Size Corrections for Self-Diffusion Coefficients Calculated from Molecular Dynamics Simulations. The Case of CO_2, *n*-Alkanes and Poly(ethylene glycol) Dimethyl Ethers

Supplementary Material

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Table S1. Molecular dynamics simulation results for carbon dioxide and *n*-alkanes.

	T (K)	P (bar)	N	L (nm)	ρ (kg m^{-3})	D (10^{-9} m^2 s^{-1})	η (10^{-5} Pa s)
carbon dioxide	323.15	200	250	2.853	783 (3)	18.9 (0.5)	7.5 (0.1)
			500	3.600		19.5 (0.6)	
			1000	4.536		20.2 (0.1)	
			2000	5.720		20.5 (0.3)	
methane	150.15	500	500	3.174	417 (2)	6.5 (0.2)	11.6 (0.1)
			1000	3.999		6.6 (0.2)	
			2000	5.039		6.8 (0.1)	
			4000	6.349		6.9 (0.1)	
propane	400.15	45	500	7.553	84 (4)	195 (4)	1.3 (0.1)
			1000	9.533		197 (3)	
			2000	12.008		199 (3)	
			4000	15.134		200 (2)	
n-hexane	400.15	30	500	5.057	553 (4)	13.7 (0.2)	10 (0.1)
			1000	6.371		13.9 (0.2)	
			2000	8.027		14.1 (0.2)	
			4000	10.113		14.4 (0.2)	
n-hexadecane	400.15	1	250	5.097	710 (3)	2.5 (0.1)	35 (1)
			500	6.423		2.62 (0.07)	
			1000	8.092		2.72 (0.08)	
			2000	10.196		2.77 (0.06)	

Table S2. Molecular dynamics simulation results for poly(ethylene glycol) dimethyl ethers.

	T (K)	P (bar)	N	L (nm)	ρ (kg m^{-3})	D (10^{-9} m^2 s^{-1})	η (10^{-5} Pa s)
G1	400	30.3975	125	2.933	745 (2)	8.5 (0.2)	16.6
			250	3.689		9.0 (0.5)	
			500	4.649		9.0 (0.3)	
			1000	5.854		9.3 (0.3)	
			2000	7.377		9.49 (0.06)	
			4000	9.295		9.6 (0.1)	
G2	400	1.01325	125	3.209	842 (1)	3.95 (0.06)	34.8
			250	4.046		3.82 (0.2)	
			500	5.097		3.98 (0.06)	
			1000	6.424		4.0 (0.1)	
			2000	8.090		4.11 (0.03)	
			4000	10.193		4.23 (0.09)	
G3	400	1.01325	125	3.459	895(1)	1.9 (0.1)	68.0
			250	4.354		1.9 (0.1)	
			500	5.491		2.01 (0.07)	
			1000	6.917		2.03 (0.04)	
			2000	8.717		2.04 (0.03)	
			4000	10.980		2.09 (0.03)	
G4	400	1.01325	125	3.678	927 (1)	0.98 (0.05)	113.1
			250	4.634		1.07 (0.03)	
			500	5.838		1.12 (0.04)	
			1000	7.358		1.14 (0.02)	
			2000	9.269		1.15 (0.02)	
			4000	11.679		1.19 (0.03)	

Table S3. Experimental density, self-diffusion coefficient and viscosity of the studied systems.

	T (K)	P (bar)	ρ (kgm^{-3})	D (10^{-9} m^2/s)	η (10^{-5} Pa s)
carbon dioxide	323.15	200	784.29[1]	23.579[2] 22.760[3]	6.8674[1]
methane	150.15	500	417.53[1]	8.456[4]	9.8431[1]
propane	400.15	45	92.158[1]	-	1.3831[1]
n-hexane	400.15	30	557.50[1]	13.015[5,6]	13.052[1]
n-hexadecane	400.15	1	698.30[7]	1.874[8]	52.67[9] 55.92[9–11]
G1	400	30.3975	741.6[12, a, b]	-	18[12, a, c]
G2	400	1.01325	834.8[13, b]	-	29[13, c]
G3	400	1.01325	882.4[13, b]	-	50[13, c]
G4	400	1.01325	913.1[13, b]	-	75[13, c]

[a] Based on experimental data at 1 atm. [b] Extrapolated from linear fit to experimental data at low temperatures. [c] Extrapolated from experimental data at low temperatures using the Vogel-Tamman-Fulcher (VTF) equation[14].

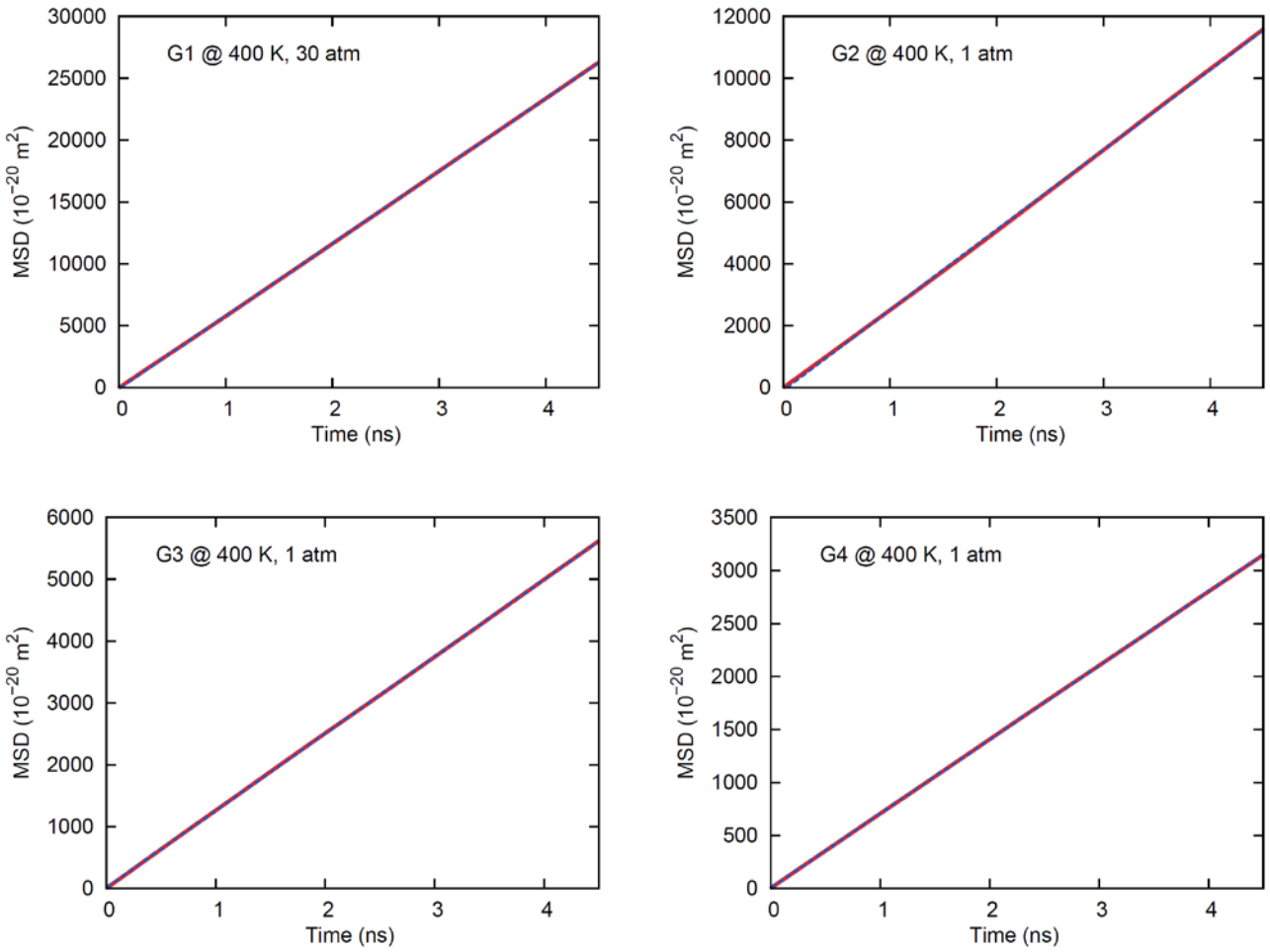

Figure S1. Calculated mean square displacements (solid red lines) as a function of time for the glymes based on simulations of the largest box sizes and the fitting results to the Einstein relation (dashed blue lines).

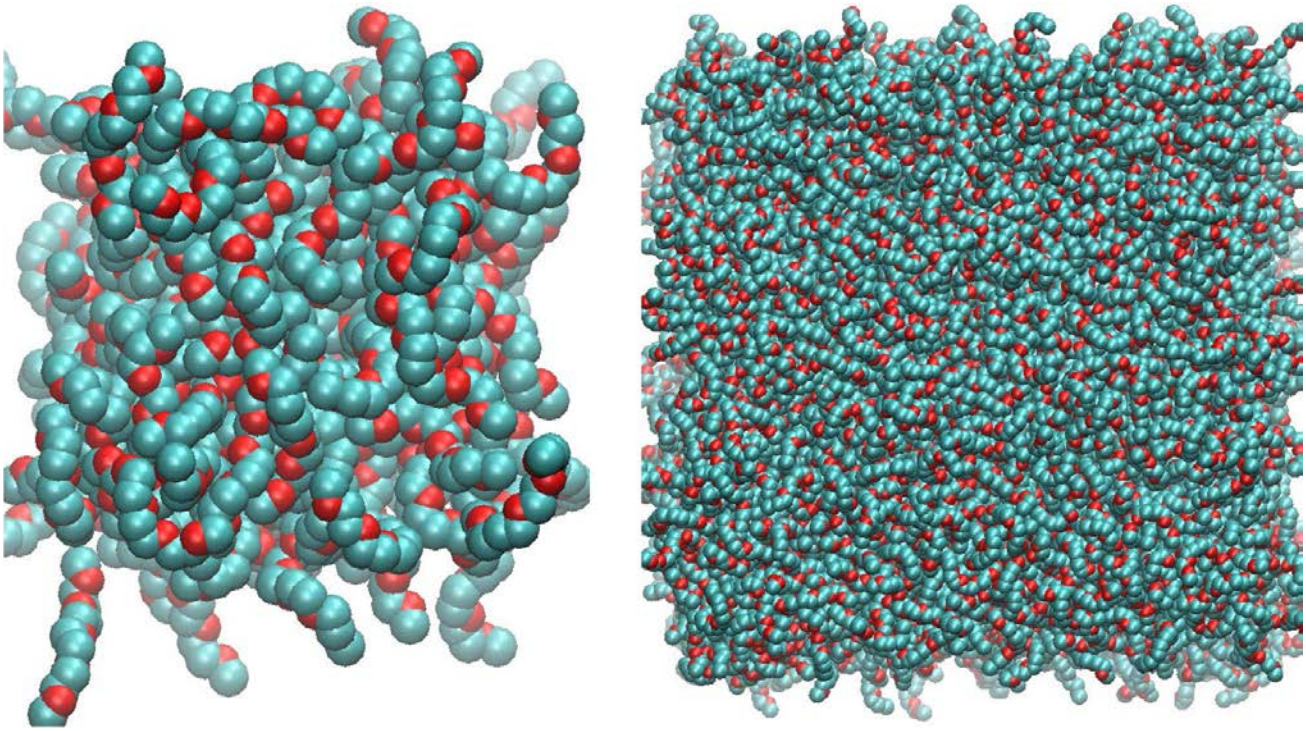

Figure S2. Snapshots of simulation boxes containing 125 (left) and 4000 (right) G4 molecules. Carbons are shown in cyan and oxygens in red.

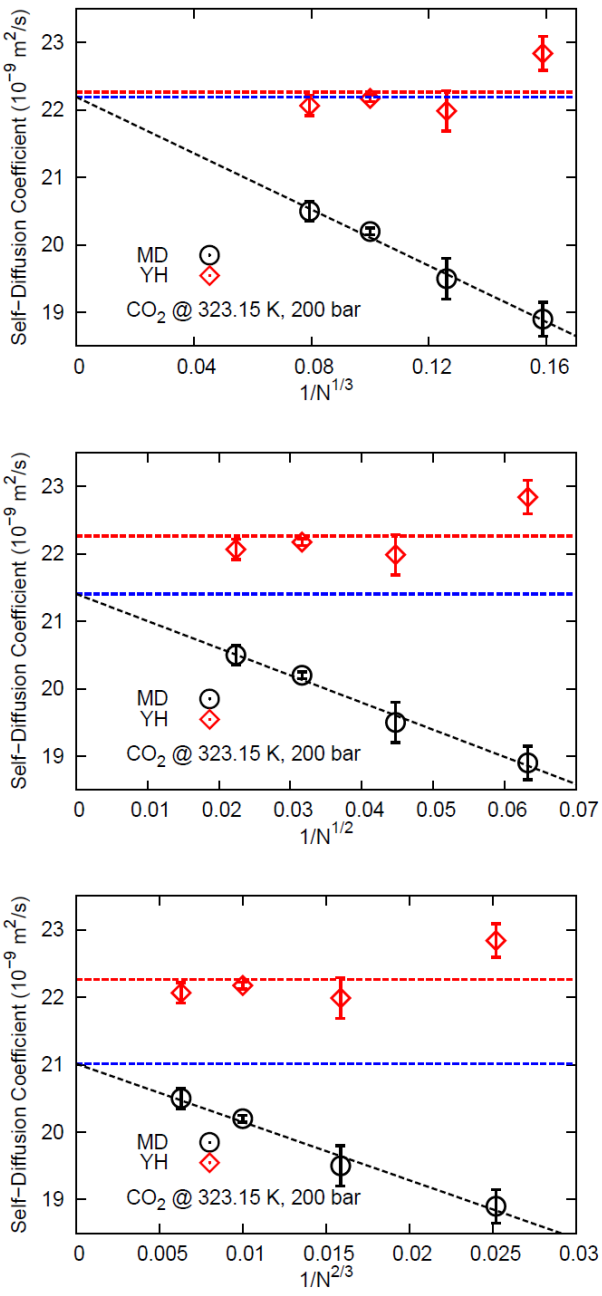

Figure S3. The fitting results (black dashed lines) of the calculated self-diffusion coefficients of CO_2 (black circles) as a function of $1/N^{1/3}$, $1/N^{1/2}$ or $1/N^{2/3}$, respectively. The extrapolated $D_{\infty,MD}$ (blue dashed lines) using the three different exponents are almost equal to each other. The corrected self-diffusion coefficients using the YH method are shown as red diamonds and the red dashed lines are the average.

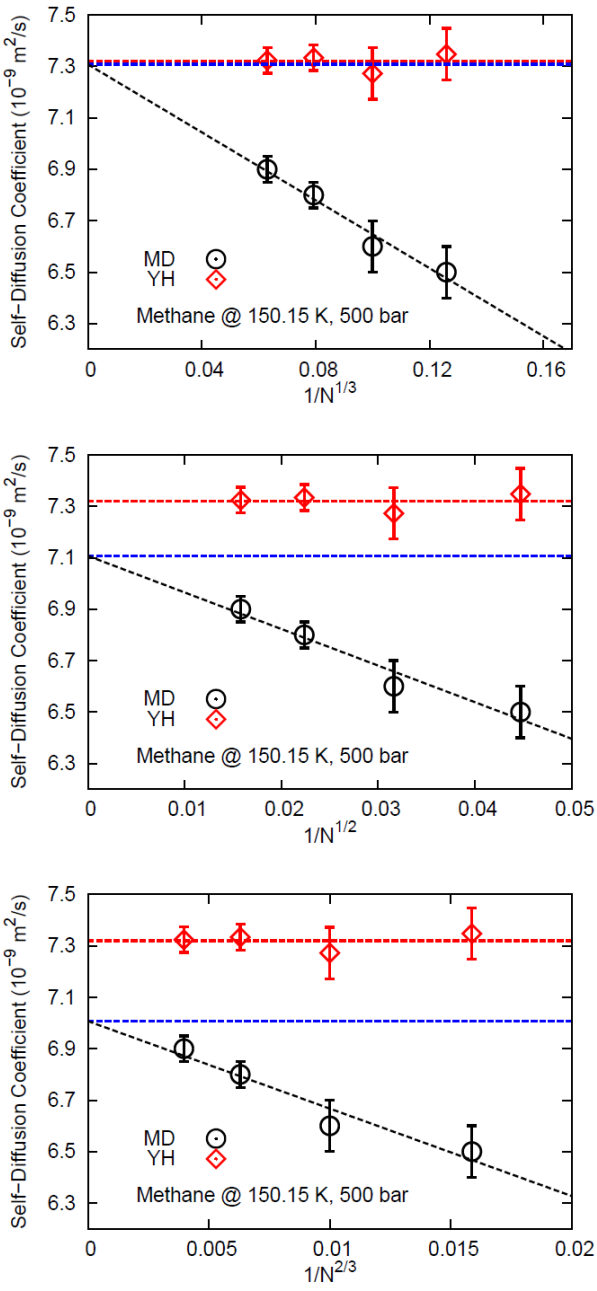

Figure S4. The fitting results (black dashed lines) of the calculated self-diffusion coefficients of methane (black circles) as a function of $1/N^{1/3}$, $1/N^{1/2}$ or $1/N^{2/3}$, respectively. The extrapolated $D_{\infty,MD}$ (blue dashed lines) using the three different exponents are almost equal to each other. The corrected self-diffusion coefficients using the YH method are shown as red diamonds and the red dashed lines are the average.

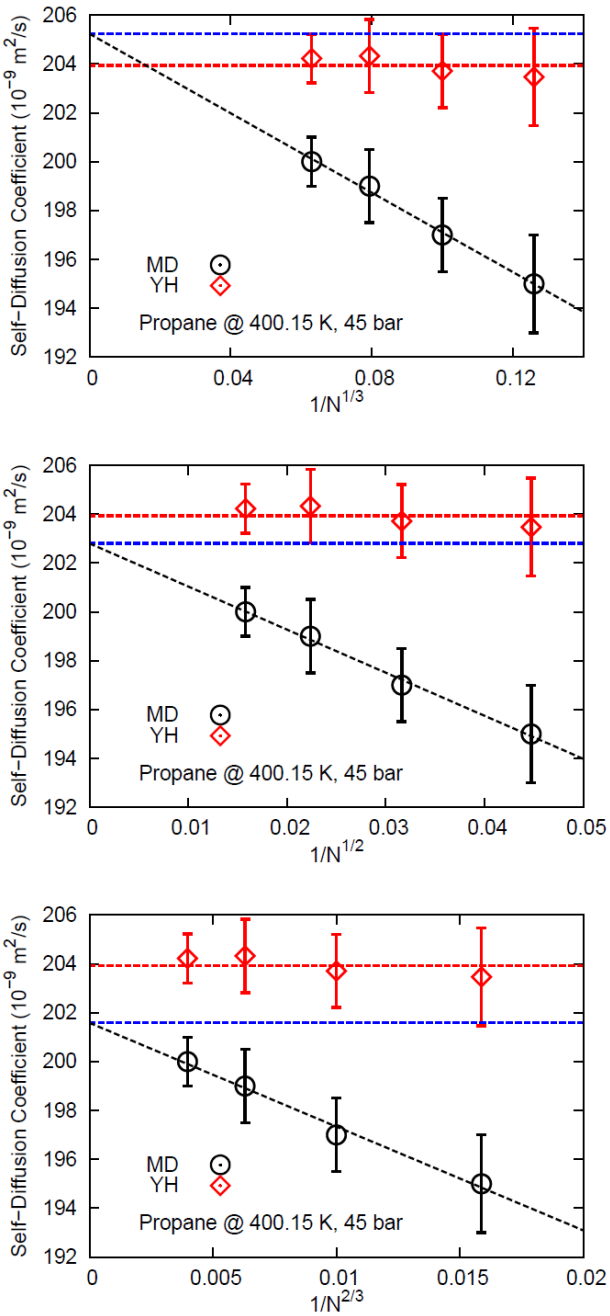

Figure S5. The fitting results (black dashed lines) of the calculated self-diffusion coefficients of propane (black circles) as a function of $1/N^{1/3}$, $1/N^{1/2}$ or $1/N^{2/3}$, respectively. The extrapolated $D_{\infty,MD}$ (blue dashed lines) using the three different exponents are almost equal to each other. The corrected self-diffusion coefficients using the YH method are shown as red diamonds and the red dashed lines are the average.

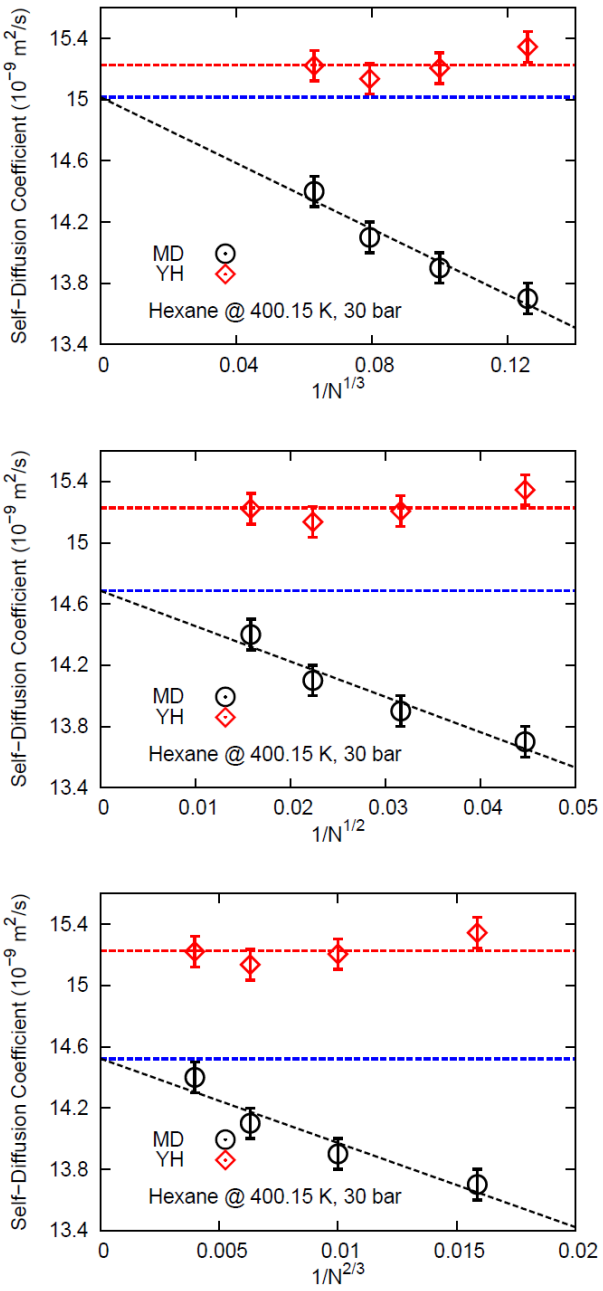

Figure S6. The fitting results (black dashed lines) of the calculated self-diffusion coefficients of n-hexane (black circles) as a function of $1/N^{1/3}$, $1/N^{1/2}$ or $1/N^{2/3}$, respectively. The extrapolated $D_{\infty,MD}$ (blue dashed lines) using the three different exponents are almost equal to each other. The corrected self-diffusion coefficients using the YH method are shown as red diamonds and the red dashed lines are the average.

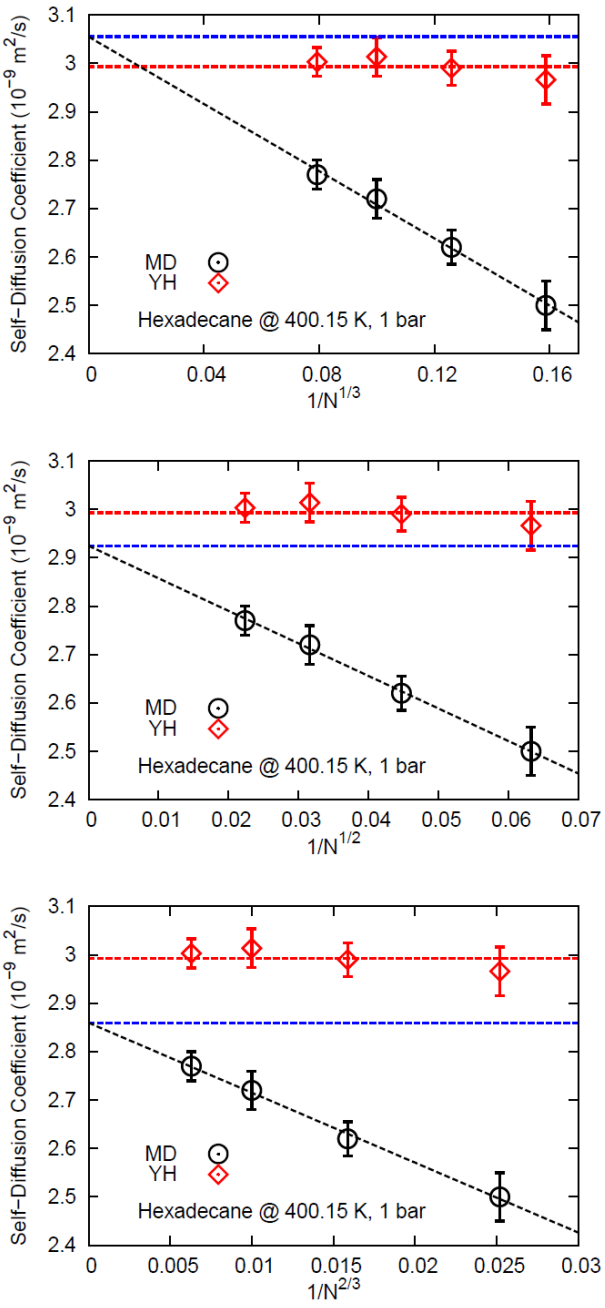

Figure S7. The fitting results (black dashed lines) of the calculated self-diffusion coefficients of n-hexadecane (black circles) as a function of $1/N^{1/3}$, $1/N^{1/2}$ or $1/N^{2/3}$, respectively. The extrapolated $D_{\infty,MD}$ (blue dashed lines) using the three different exponents are almost equal to each other. The corrected self-diffusion coefficients using the YH method are shown as red diamonds and the red dashed lines are the average.

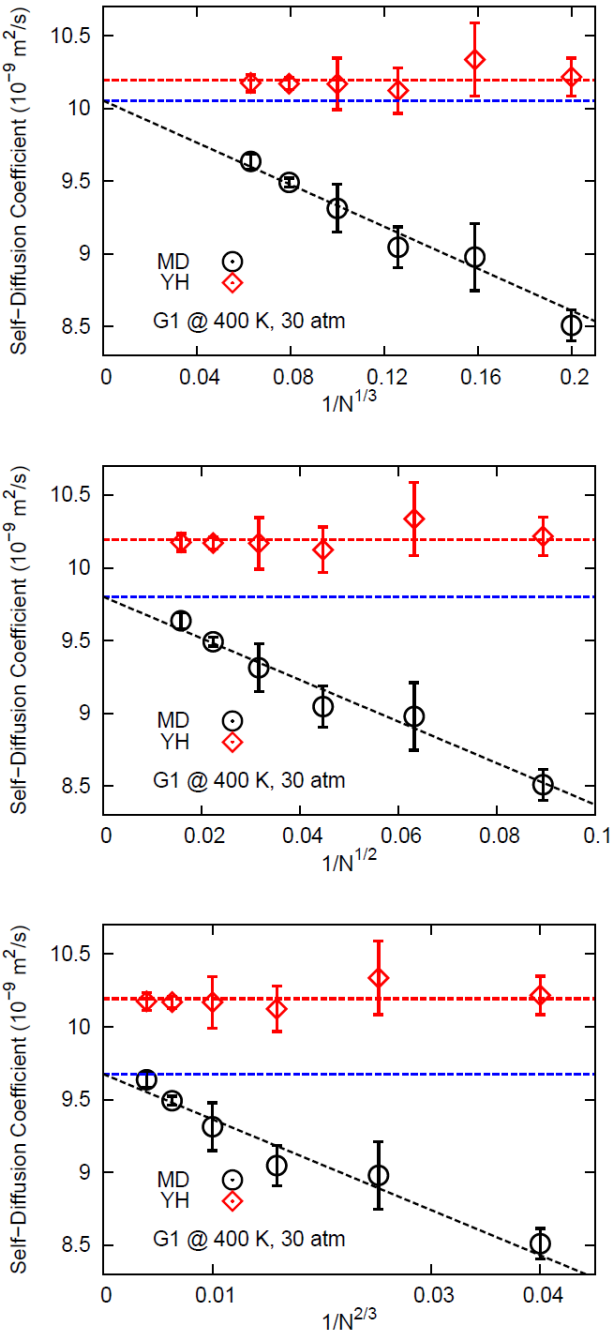

Figure S8. The fitting results (black dashed lines) of the calculated self-diffusion coefficients of G1 (black circles) as a function of $1/N^{1/3}$, $1/N^{1/2}$ or $1/N^{2/3}$, respectively. The extrapolated $D_{\infty,MD}$ (blue dashed lines) using the three different exponents are almost equal to each other. The corrected self-diffusion coefficients using the YH method are shown as red diamonds and the red dashed lines are the average.

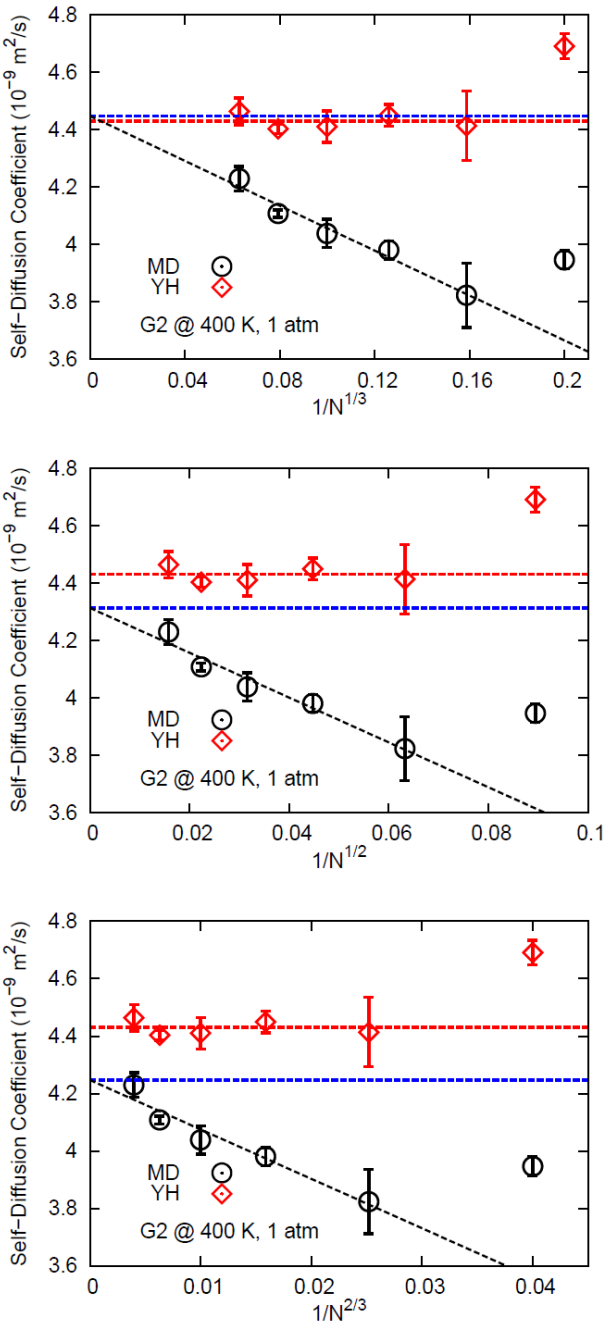

Figure S9. The fitting results (black dashed lines) of the calculated self-diffusion coefficients of G2 (black circles) as a function of $1/N^{1/3}$, $1/N^{1/2}$ or $1/N^{2/3}$, respectively. The extrapolated $D_{\infty,MD}$ (blue dashed lines) using the three different exponents are almost equal to each other. The corrected self-diffusion coefficients using the YH method are shown as red diamonds and the red dashed lines are the average.

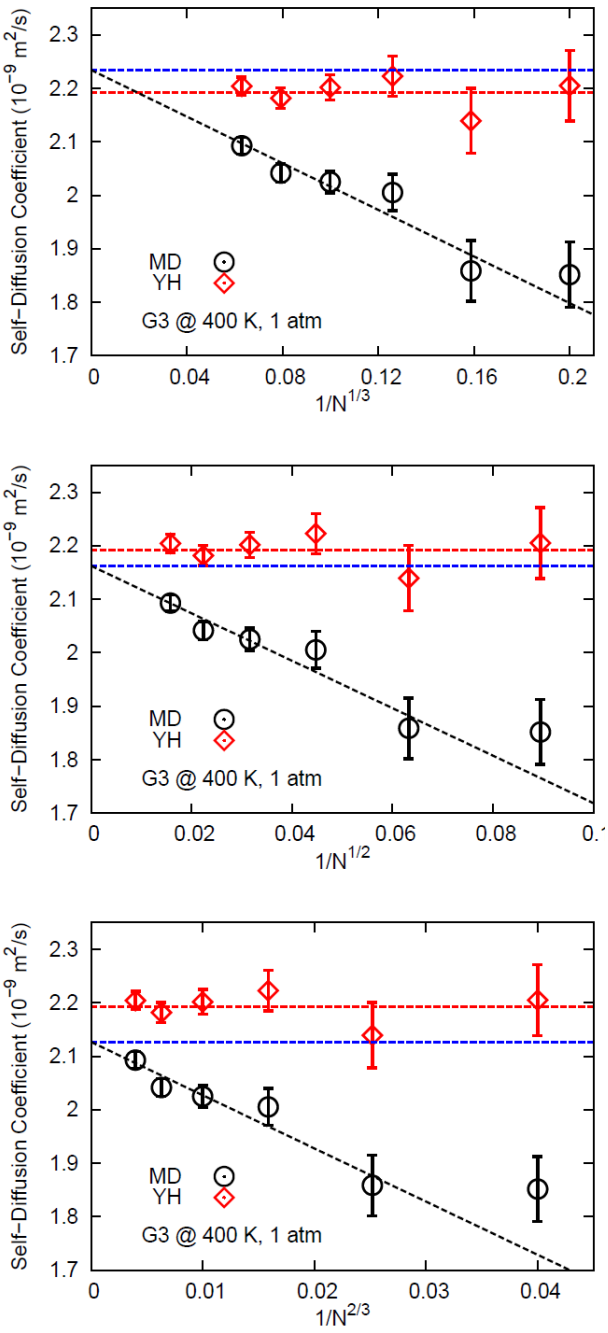

Figure S10. The fitting results (black dashed lines) of the calculated self-diffusion coefficients of G3 (black circles) as a function of $1/N^{1/3}$, $1/N^{1/2}$ or $1/N^{2/3}$, respectively. The extrapolated $D_{\infty,MD}$ (blue dashed lines) using the three different exponents are almost equal to each other. The corrected self-diffusion coefficients using the YH method are shown as red diamonds and the red dashed lines are the average.

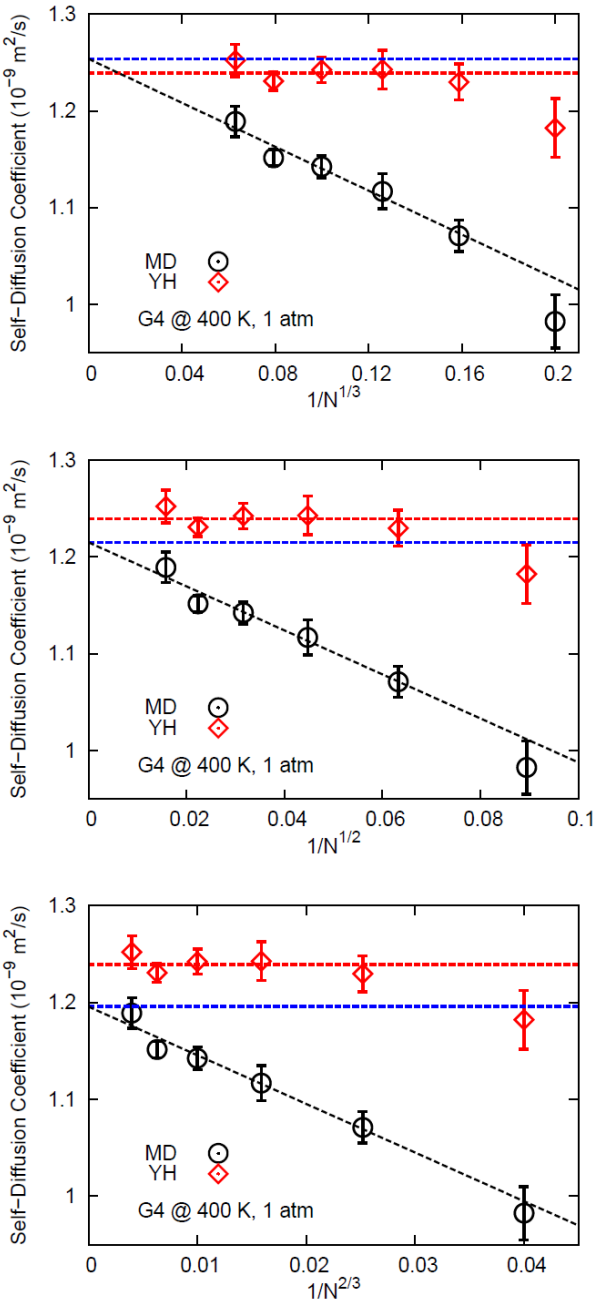

Figure S11. The fitting results (black dashed lines) of the calculated self-diffusion coefficients of G4 (black circles) as a function of $1/N^{1/3}$, $1/N^{1/2}$ or $1/N^{2/3}$, respectively. The extrapolated $D_{\infty,MD}$ (blue dashed lines) using the three different exponents are almost equal to each other. The corrected self-diffusion coefficients using the YH method are shown as red diamonds and the red dashed lines are the average.

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