Supporting Information for

Energy-Renormalization for Achieving Temperature Transferable Coarse-Graining of Polymer Dynamics

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Supporting Figures

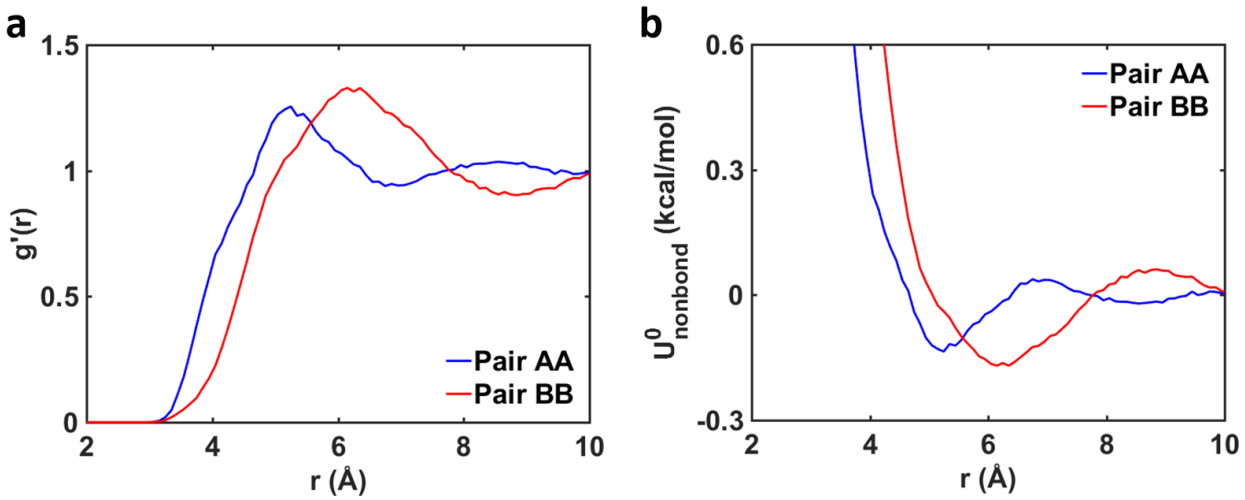

Figure S1. **(a)** All-atomistic radial distribution functions (RDF) $g'(r)$ between effective bead centers *AA* and *BB* used in the CG mapping scheme, and **(b)** their respective potentials $U^o_{nonbond}$ obtained via the Inverse Boltzmann method. The initial nonbonded LJ parameters are determined: $\sigma^0_{AA} = 4.60$ Å, $\sigma^0_{BB} = 5.06$ Å, $\varepsilon^0_{AA} = 0.136$ kcal/mol, and $\varepsilon^0_{BB} = 0.174$ kcal/mol.

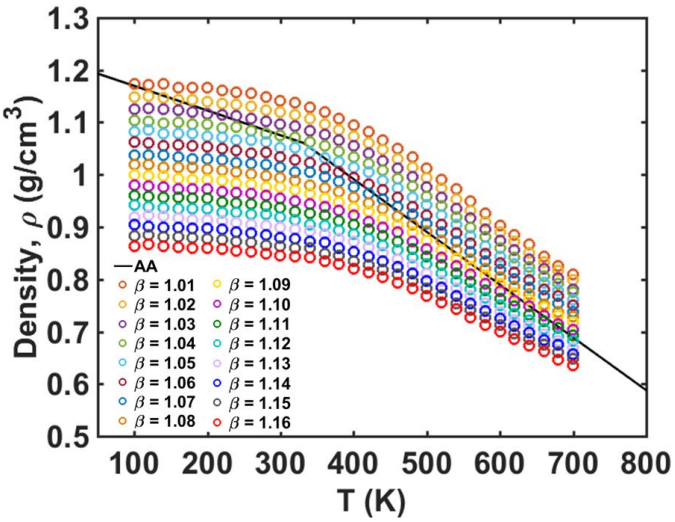

Figure S2. Density sweeps as function of temperature for AA (solid line) and CG (open symbols) models with varying β parameters from 1.01 to 1.16. Temperature-dependent β can be determined by matching the density results of AA model, leading to linear scaling relationship.

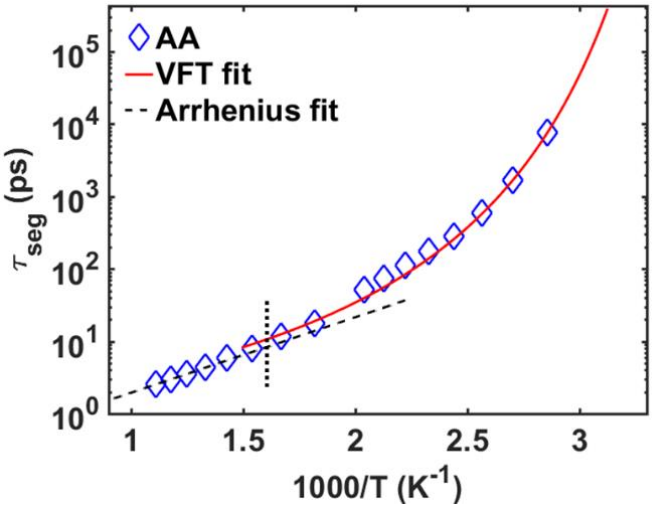

Figure S3. τ_{seg} as a function of temperature for the AA model. The solid curve shows the VFT fit of the data for AA model. The dashed slope shows the Arrhenius fit of τ_{seg} at high temperatures. The vertical dotted line marks T_A.

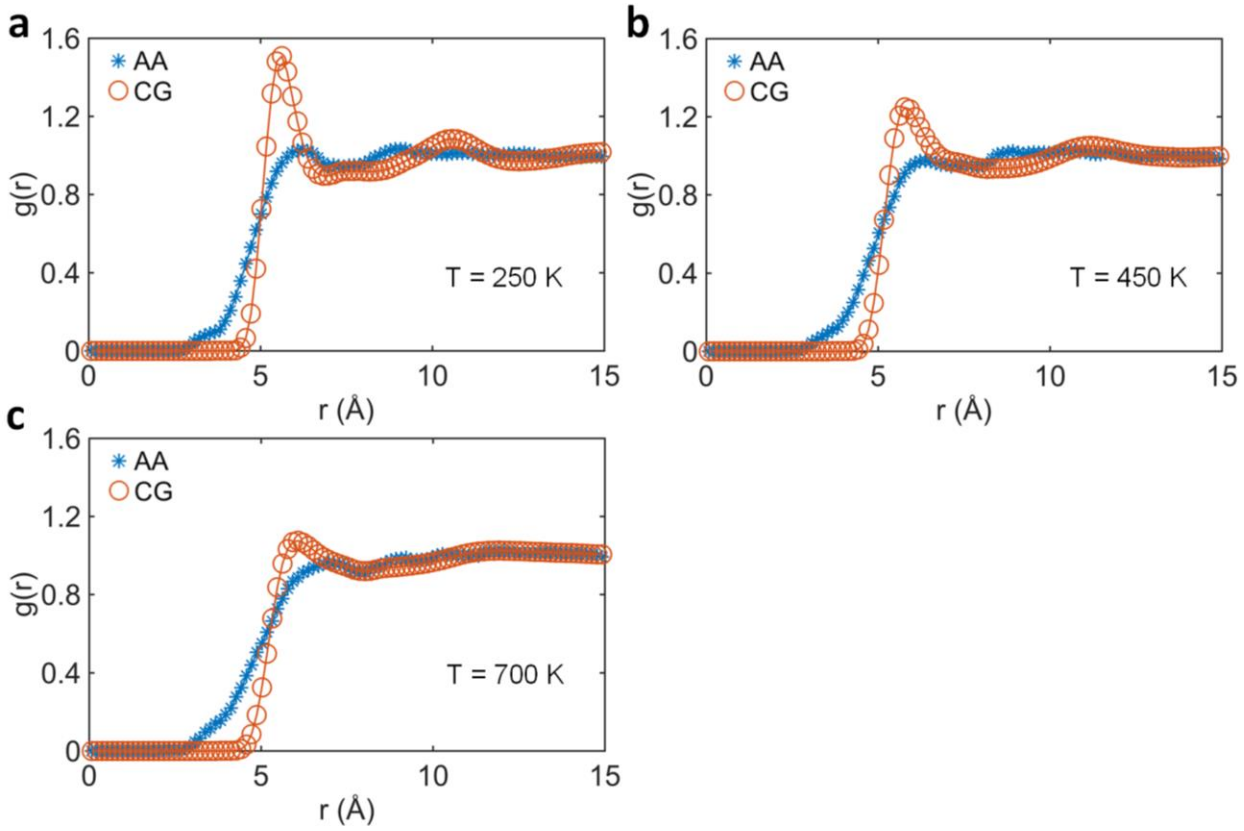

Figure S4. Comparison of the RDF $g(r)$ of all the CG bead sites within the AA and CG systems at different temperatures: **(a)** $T = 250$ K, **(b)** $T = 450$ K, and **(c)** $T = 700$ K.

Supporting Tables

Table S1. Functional Form of Force Field and Potential Parameters for CG Model of PS.

Interaction	Potential form	Parameters
A-A Bond Length	$U_{bondAA}(l) = k\left(l - l_0\right)^2$	k = 80.69 kcal/mol·Å^2 l_0 = 2.568 Å
A-B Bond Length	$U_{bondAB}(l) = k\left(l - l_0\right)^2$	k = 224.6 kcal/mol·Å^2 l_0 = 2.871 Å
A-A-A Angle	$U_{angleAAA}(\theta) = -\mathrm{k}_b T \ln\left[a_1 \exp-\left(\frac{\theta-\theta_1}{b_1}\right)^2 + a_2 \exp-\left(\frac{\theta-\theta_2}{b_2}\right)^2 + a_3 \exp-\left(\frac{\theta-\theta_3}{b_3}\right)^2\right]$	a_1 = 2.277e-1 a_2 = 5.588e-1 a_3 = -5.497e-1 b_1 = 10.76° b_2 = 19.27° b_3 = 18.78° θ_1 = 177.1° θ_2 = 148.8° θ_3 = 148.5°
A-A-B Angle	$U_{angleAAB}(\theta) = -\mathrm{k}_b T \ln\left[a_1 \exp-\left(\frac{\theta-\theta_1}{b_1}\right)^2 + a_2 \exp-\left(\frac{\theta-\theta_2}{b_2}\right)^2 + a_3 \exp-\left(\frac{\theta-\theta_3}{b_3}\right)^2\right]$	a_1 = 1.451e-1 a_2 = 1.767e-2 a_3 = 3.199e-2 b_1 = 6.762° b_2 = 9.745° b_3 = 11.01° θ_1 = 141.5° θ_2 = 93.22° θ_3 = 134.7°
A-A-A-A Dihedral Angle	$U_{dihedralAAAA}(\phi) = A\cos(\phi)$	A (atactic) = 0.5 (kcal/mol)
B-A-A-B Dihedral Angle	$U_{dihedralBAAB}(\phi) = \sum_{k=1}^{5} A_k \cos^{k-1}(\phi)$	*meso* A_1 = 4.236 (kcal/mol) A_2 = -1.274 (kcal/mol) A_3 = 0.5337 (kcal/mol) A_4 = -0.8179 (kcal/mol) A_5 = -0.4622 (kcal/mol) *racemo* A_1 = 3.762 (kcal/mol) A_2 = 0.3631 (kcal/mol) A_3 = 2.128 (kcal/mol) A_4 = -0.9691 (kcal/mol) A_5 = -1.880 (kcal/mol)
Non-bonded	$U_{nonbond} = 4\varepsilon(T)\left[\left(\frac{\sigma(T)}{r}\right)^{12} - \left(\frac{\sigma(T)}{r}\right)^{6}\right] + S_{LJ}(r)$	$\varepsilon_{AA} = \alpha(T)\times 0.136$ (kcal/mol) $\sigma_{AA} = \beta(T)\times 4.60$ (Å) $\varepsilon_{BB} = \alpha(T)\times 0.174$ (kcal/mol) $\sigma_{BB} = \beta(T)\times 5.06$ (Å)

Table S2. Functional Form of Temperature Dependent Energy-Renormalization Factors for the CG Nonbonded Potential.

Scaling factor	**Functional form**	**Parameters**
$\alpha(T)$	$\alpha(T)=\frac{\alpha_A-\alpha_g}{1+\exp\left[-k(T-T_T)\right]}+\alpha_g$	α_A = 2.33, α_g = 3.60 T_T = 475.2 K k = 0.0185 K^{-1}
$\beta(T)$	$aT+b$	a = 1.718×10^{-4}K^{-1}, b =0.9905

Table S3. Comparison of the ratios of characteristic temperatures of simulation results described in the main text and prediction of the generalized entropy theory (GET) for flexible-stiff class of polymer.

Predictions	T_A/T_g	T_g/T_0	T_A/T_0	T_l/T_0
AA	2.14	1.11	2.38	2.22
CG	2.15	1.11	2.39	2.23
GET	1.70	1.09	1.86	-