Towards Modeling Thermoresponsive Polymer Networks: A Molecular Dynamics Simulation Study of N-Isopropyl Acrylamide Co-Oligomers

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Supporting Information

PART 1

Characteristics of the models.

System	Number of residues			Number and DP of backbone chains[a,b]	Number of water molecules	Polymer concentration[c] (%w/w)	Box size[c] (nm)	Density[c] ($g \cdot cm^{-3}$)
	PVA	MA	NIPAAm					
A-I	0	0	28	1 (28)	1890	10.7	3.95	0.9982
A-II	0	0	28	2 (14)	1890	10.7	3.95	0.9922
PMN-I	160	8	20	1 (28)	5189	9.15	5.64	0.9708
PMN-II	160	8	20	2 (14)	5217	9.20	5.62	0.9707

[a]The polymerization degree, DP, is reported in parenthesis.

[b]Data of MA-NIPAAm chains, in PMN-I and PMN-II systems.

[c]At the end of equilibration, T=323 K.

PART 2

Backbone conformational properties[a].

System	R_g [b](nm)	Ete[c] (nm)	$R_{G,TOT}$ [d] (nm)	R_g [b] (nm)	Ete[c] (nm)	$R_{G,TOT}$ [d] (nm)
	293 K			323 K		
A-I	1.29 ± 0.04	3.5 ± 0.1		0.67 ± 0.01	1.2 ± 0.2	
A-II	0.63 ± 0.02 0.59 ± 0.02	1.5 ± 0.1 1.18 ± 0.09		0.54 ± 0.02 0.52 ± 0.02	1.5 ± 0.2 1.0 ± 0.1	
PMN-I	1.11±0.02	2.9 ± 0.2	1.31 ± 0.01	0.91 ± 0.01	0.9±0.1	1.30 ± 0.02
PMN-II	0.79 ± 0.01 0.75 ± 0.01	2.0 ± 0.1 2.15 ± 0.07	1.07 ± 0.01 1.18 ± 0.02	0.78 ± 0.02 0.70 ± 0.03	2.2 ± 0.2 2.2 ± 0.2	1.12 ± 0.02 1.10 ± 0.02

[a]Time averaged on the last 5 ns trajectory.

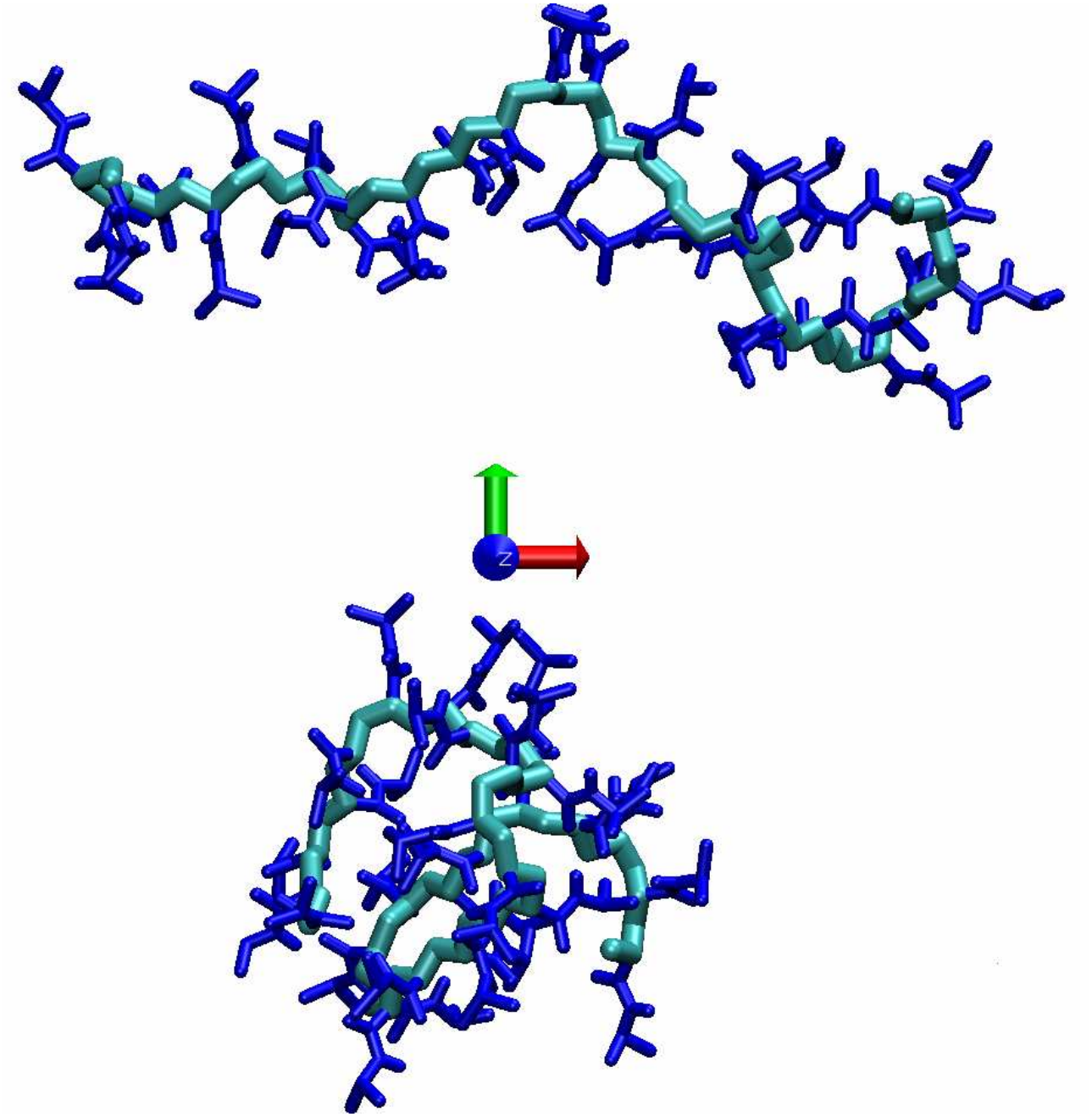
[b]Radius of gyration, including only backbone carbon atoms. For PMN systems, including only MA-NIPAAm backbone carbon atoms.

[c]End-to-end distance. For PMN systems, end-to-end distance of MA-NIPAAm chains.

[d]Radius of gyration, including PVA and MA-NIPAAm backbone carbon atoms.

PART 3

Projections in the xy plane of the final configuration of A-I at 293 K (top) and 323 K (bottom). The backbone chain is shown in azure. Water molecules are omitted.



PART 4

Autocorrelation function of the HB's between MA-NIPAAm residues and water, at 293 K (black lines) and 323 K (red lines). Semi-logarithmic plots.