Supplementary material Equilibrium swelling of biocompatible thermo-responsive copolymer gels

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Figures



Figure S-1: Parameter ϕ_{n0} versus molar fraction of comonomers ψ . Circles: treatment of observations (Lee and Huang, 2000) on P(NIPAm-HEMA) gels. Solid line: results of simulation.



Figure S-2: Parameter χ versus temperature T. Circles: experimental data on POx gels. A – PEtOx, Christova et al. (2003), B – PEtOx, Seguet et al. (2020), C – PIPOx, Jerca et al. (2018). Solid lines: results of simulation.



Figure S-3: Parameters χ_{max} (A), g_1 (B) and \bar{g}_2 (C) versus molar fraction ψ of comonomers. Symbols: treatment of observations on P(EtOx-HEMA), P(EtOx-HPA) and P(EtOx-MMA) copolymer gels (\circ – HEMA, \bullet – HPA, \ast – MMA). Solid lines: results of simulation.



Figure S-4: Parameter χ versus temperature T. Circles: experimental data on PMEO₂MA gels. Solid lines: results of simulation. A – macroscopic gel (Iizawa et al., 2012), B – core-shell microgel with Au core and gel shell (Lapresta-Fernandez et al., 2014), C – microgel particle (Cai et al., 2007), D – nanocomposite gel (Xia et al., 2015).



Figure S-5: Parameter χ versus temperature *T*. Circles: experimental data (Xia et al., 2015) on P(MEO₂MA–OEGMA₄₇₅) nanocomposite gels with various molar fractions ψ of OEGMA monomers. Solid lines: results of simulation.



Figure S-6: Parameters χ_1 and ϕ_{n0} versus molar fraction ψ of OEGMA monomers. Circles: treatment of observations on P(MEO₂MA-OEGMA_M) copolymer gels. Solid lines: results of simulation.



Figure S-7: Parameter χ versus temperature *T*. Symbols: experimental data (Paris and Quijada-Garrido, 2009) on P(MEO₂MA-OEGMA₄₇₅) (A) and P(MEO₂MA-OEGMA₂₀₈₀) (B) copolymer gels with various molar fractions ψ of OEGMA monomers. Solid lines: results of simulation.



Figure S-8: A – Parameter χ versus temperature *T*. Circles: experimental data (Gawlitza et al., 2014) on P(MEO₂MA-OEGMA₅₀₀) microgels with various molar fractions ψ of OEGMA monomers. Solid lines: results of simulation. B – Parameter χ_1 versus molar fraction ψ of OEGMA monomers. Circles: treatment of observations. Solid line: results of simulation.



Figure S-9: A, B – Degree of swelling Q versus temperature T. Circles: experimental data (Liu et al., 2013) on (MEA-OEGA) microgels with molar fractions $\psi = 0.1$ (A) and 0.3 (B) of OEGA₄₈₀ monomers. Solid lines: results of simulation. C, D – Parameter χ versus temperature T. Circles: treatment of experimental data. Solid lines: results of simulation.

Tables

Table S-1: Material parameters for N-substituted acrylamide gels.

Gel	χ_0	χ_1	$\chi_{ m max}$	g_1	Q_0	\bar{g}_2	β	$T_{\rm c}$ °C
PNNPAm	-3.147	0.123	-0.10	0.075	13.3	2.00	0.60	24.8
PNIPAm	-2.098	0.079	0.60	0.075	13.3	0.45	0.45	34.1
PNCPAm	-0.752	0.031	0.70	0.075	13.3	0.45	0.15	46.1
PDEAm	0.167	0.018	0.82	0.050	4.0	3.00	0.50	35.9

Table S-2: Material parameters for P(NIPAm-HEMA) gels with various molar fractions ψ of HEMA monomers.

ψ	χ_0	χ_1	$\chi_{ m max}$	g_1	Q_0	\bar{g}_2	β	$T_{\rm c}$ °C
0.0	-2.098	0.0791	0.49	0.123	9.5	0.8	0.4	32.7
0.1	-1.732	0.0712	0.49	0.123	5.5	0.8	0.4	31.2
0.3	-0.999	0.0554	0.49	0.123	2.7	0.8	0.4	26.9

Table S-3: Material parameters for poly(N-vinylcaprolactam) macro- and microgels.

Figure	χ_0	χ_1	$\chi_{ m max}$	g_1	\bar{g}_2	β	β_1	$T_{\rm c}$ °C
4A	-0.463	0.0396	0.72	0.05	0.18	0.04	1.5	29.9
4B	-0.463	0.0396	0.86	0.23	2.50	0.40	1.5	33.5
$4\mathrm{C}$	-0.463	0.0396	0.71	0.20	0.80	0.05	2.0	29.7
4D-BIS	-0.463	0.0396	0.69	0.07	2.00	0.01	0.6	29.2
4D-PEGDA	-0.463	0.0396	0.69	0.10	2.50	0.004	0.3	29.2

Table S-4: Material parameters for P(VCL-MEA) microgels with various molar fractions ψ of MEA monomers.

$\overline{\psi}$	χ_0	χ_1	$\chi_{ m max}$	g_1	Q_0	\bar{g}_2	β	β_1	$T_{\rm c}$ °C
0.035	-0.409	0.0382	0.71	0.096	10.3	1.5	0.04	2.5	29.3
0.30	-0.301	0.0277	0.71	0.050	4.6	1.5	0.25	3.0	25.8

Table S-5: Material parameters for poly(vinyl methyl ether) gels.

Figure	χ_0	χ_1	$\chi_{ m max}$	g_1	Q_0	\bar{g}_2	β	$T_{\rm c}~^{\circ}{\rm C}$
5A	0.384	0.0117	0.775	0.080	12.3	0.01	25.0	33.5
5B	0.384	0.0117	0.788	0.080	11.2	0.12	30.0	33.9
$5\mathrm{C}$	0.384	0.0117	0.758	0.081	7.2	0.10	25.0	32.0
5D	0.384	0.0117	0.780	0.147	5.1	0.25	16.0	33.9

Table S-6: Material parameters for poly(N, N-dimethylaminoethyl methacrylate) gels.

Figure	χ_0	χ_1	$\chi_{ m max}$	g_1	Q_0	\bar{g}_2	β	$T_{\rm c}$ °C
6A	-0.3	0.0136	0.310	0.006	0.1	0.400	8.0	44.9
6B	-0.3	0.0136	0.294	0.006	7.8	0.009	10.0	43.7
6C	-0.3	0.0136	0.294	0.005	8.8	0.009	10.0	43.7
6D	-0.3	0.0136	0.304	0.007	9.2	0.006	12.0	44.4

Table S-7: Material parameters for P(DMAEMA-EAAm) and P(DMAEMA-AAm) gels with various molar fractions ψ of comonomers.

Comonomer	ψ	Ϋ́ο	χ_1	$\chi_{\rm max}$	q_1	Q_0	\bar{q}_2	β	$T_c \circ C$
EAAm	Г	7.0	7(1	Amax	91	-00	52	1-	<u> </u>
	0.05	-0.410	0.0129	0.304	0.0067	9.9	0.004	12.0	55.3
	0.10	-0.535	0.0129	0.304	0.0067	7.6	0.004	12.0	65.0
AAm									
	0.20	-0.095	0.0109	0.304	0.0067	7.8	0.008	12.0	36.7
	0.33	0.002	0.0091	0.304	0.0067	8.5	0.008	12.0	31.2

 Table S-8: Material parameters for poly(2-ethyl-2-oxazoline) and poly(2-isopropenyl-2-oxazoline)

 gels.

Figure	χ_1	g_1	Q_0
8A	0.0011	0.0310	7.5
8B	0.0099	0.0972	1.8
$8\mathrm{C}$	0.0082	0.0170	0.3

Table S-9: Material parameters for P(EtOx-HEMA), P(EtOx-HPA) and P(EtOx-MMA) gels with various molar fractions ψ of comonomers.

Comonomer	ψ	χ_0	χ_1	$\chi_{ m max}$	g_1	Q_0	\bar{g}_2	β	$T_{\rm c}$ °C
HEMA									
	0.3	-0.090	0.0077	0.265	0.010	0.1	0.15	4.5	46.2
	0.5	-0.015	0.0055	0.095	0.088	0.1	1.10	4.5	44.7
	0.7	-0.210	0.0033	-0.065	0.481	0.1	4.30	4.5	44.1
HPA									
	0.3	0.057	0.0077	0.425	0.013	0.1	0.80	4.5	47.9
	0.5	0.095	0.0055	0.342	0.027	0.1	1.50	4.5	45.0
	0.7	0.133	0.0033	0.277	0.073	0.1	2.80	4.5	43.8
MMA									
	0.3	0.135	0.0077	0.559	0.255	0.1	0.57	4.5	55.2
	0.5	0.175	0.0055	0.470	0.591	0.1	1.55	4.5	53.8
	0.7	0.315	0.0033	0.465	3.408	0.1	2.00	4.5	45.6

Table S-10: Material parameters for $PMEO_2MA$ macro- and microgels.

Figure	χ_1	g_1	Q_0
10A	0.0316	0.073	1.3
10B	0.0227	0.032	0.1
10C	0.0329	0.048	6.2
10D	0.0139	0.017	1.1

Gel	χ_1	$\chi_{ m max}$	g_1	Q_0	\bar{g}_2	β	$T_{\rm c}$ °C
POEGMA ₃₀₀	0.0067	0.41	0.004	6.3	14.0	0.22	60.0
$POEGMA_{470}$	0.0063	0.55	0.017	7.7	4.0	0.05	87.3
$POEGDMA_{550}$	0.0083	0.45	0.070	1.1	19.0	0.25	54.1

Table S-11: Material parameters for POEGMA and POEGDMA gels.

 Table S-12:
 Material parameters for POEGMA microgels.

Gel	χ_1	g_1	$\chi_{ m max}$	Q_0	\bar{g}_2	β	$T_{\rm c}$ °C
POEGMA ₁₈₈	0.0249	0.033		0.1			
$POEGMA_{232}$	0.0144	0.043		4.1			
POEGMA ₃₀₀	0.0093	0.007	0.57	4.5	10.0	0.4	61.1

Table S-13: Material parameters for (MEA-OEGA) microgels with various molar fractions ψ of OEGA monomers.

ψ	χ_1	g_1	Q_0
0.1	0.0164	0.156	0.1
0.3	0.0165	0.089	0.1