Electronic Supplementary Material (ESI) for Molecular Systems Design & Engineering.

Electronic Supplementary Information
Enhanced scavenging of a minor component from mixtures of two immiscible liquids by hollow polymer microgels

Mikhail V. Anakhov,[a, b, c] Rustam A. Gumerov, [a, b, c] and Igor I. Potemkin* [a, b, c, d]

[a]Physics Department, Lomonosov Moscow State University, Moscow 119991, Russian Federation

[b]DWI − Leibniz Institute for Interactive Materials, Aachen 52056, Germany

[c]A. N. Nesmeyanov Institute of Organoelement Compounds, Russian Academy of Sciences, Moscow 119991, Russian Federation

[d]National Research South Ural State University, Chelyabinsk 454080, Russian Federation

*Corresponding author. E-mail: igor@polly.phys.msu.ru

Table S1 Characteristics of microgel models

Subchain Length N_{sub}	**Cavity size** R_c/R_s	**Total number of beads** M	**Crosslinking fraction %**
20	0.5	69492	2.5
15	0.5	70092	3.3
10	0.4	74690	5
	0.5	70184	5
	0.6	62900	5
5	0.5	20498	10
	0 (regular)	23489	10

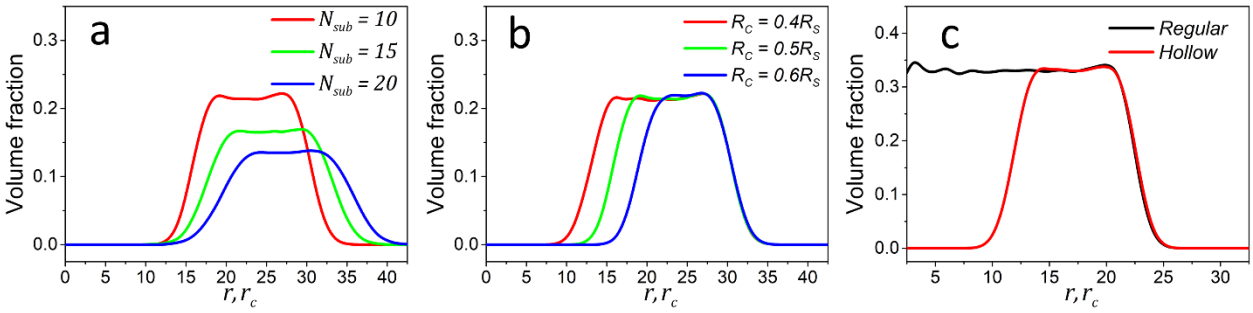

Fig. S1. Radial concentration profiles (volume fractions) for hollow microgels (a) with different subchain lengths and (b) different cavity sizes. Microgel models are based on regular microgel model comprised of ~80000 beads. (c) Radial concentration profiles (volume fractions) for microgels with different architectures. Microgel models are based on regular microgel model comprised of ~50000 beads.

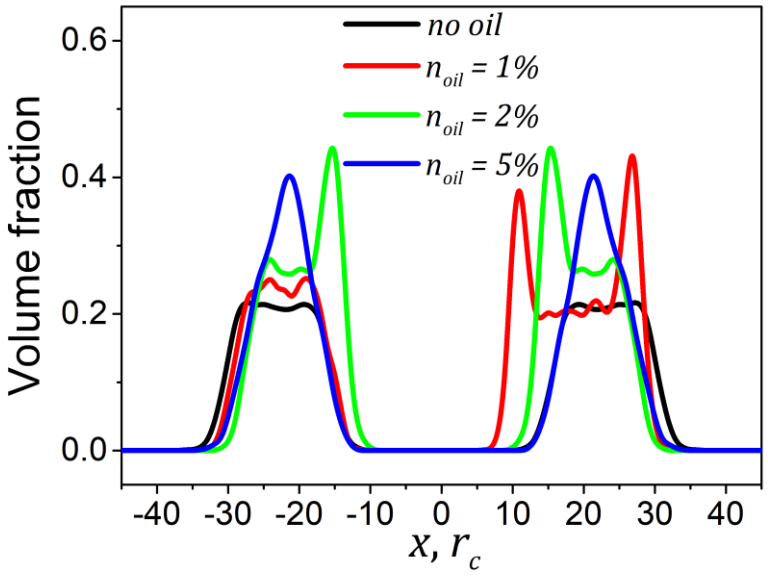

Fig. S2. Concentration profiles (volume fractions) along the axis crossing the microgel center of mass at different values of the average concentration of oil in oil−water mixture. The subchain length is N_{sub} = 10.

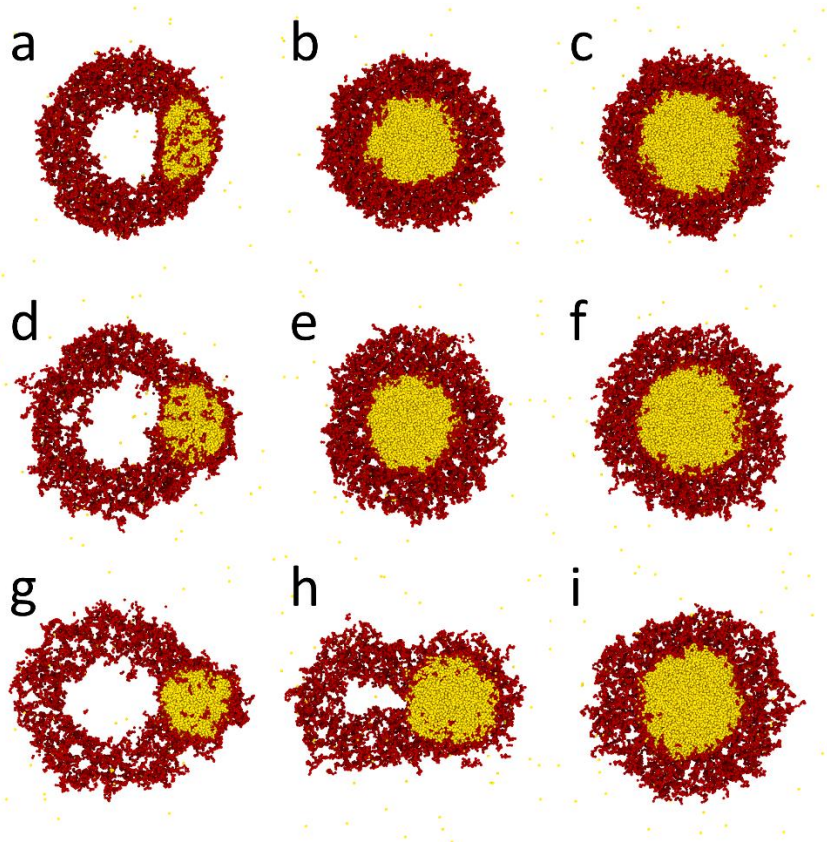

Fig. S3. Snapshots of the microgels (cross-section through the microgel and oil centers of mass) with different subchain length at different values of the average concentration of oil in oil−water mixture: (a-c) N_{sub} = 10, n_{oil} = 1% (a), 2% (b), 3% (c); (d-f) N_{sub} = 15, n_{oil} = 1% (d), 2% (e), 3% (f); (g-i) N_{sub} = 20, n_{oil} = 1% (g), 2% (h), 3% (i). Microgel models are based on regular microgel models comprised of ~80000 beads.

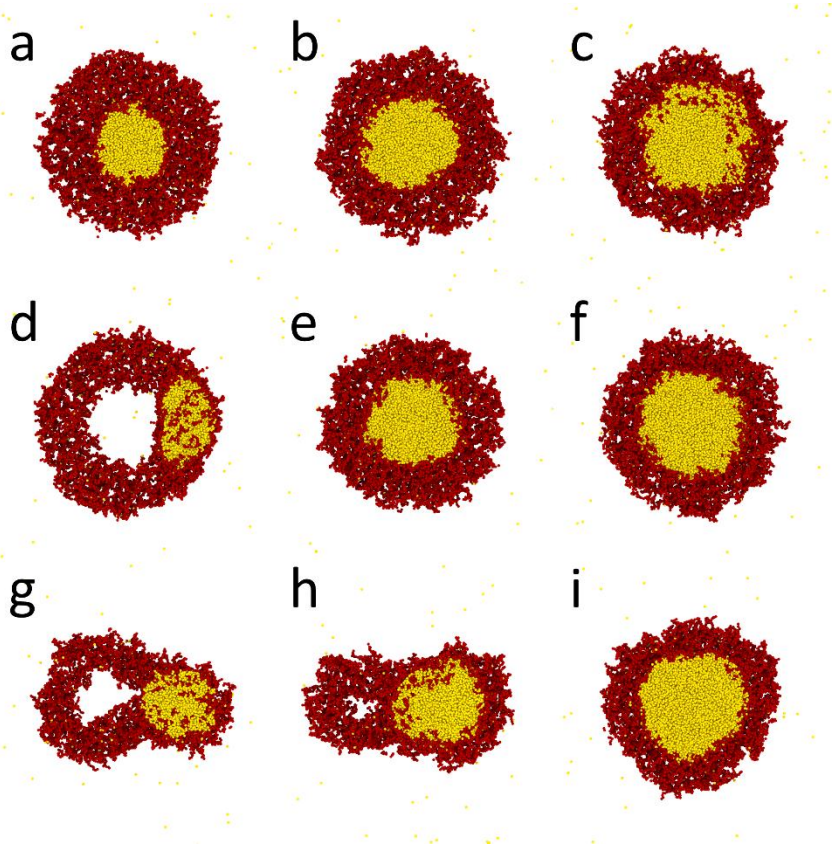

Fig. S4. Snapshots of the microgels (cross-section through the microgel and oil centers of mass) with different cavity sizes at different values of the average concentration of oil in oil−water mixture: (a-c) $R_c = 0.4R_s$, n_{oil} = 1% (a), 2% (b), 3% (c); (d-f) $R_c = 0.5R_s$, n_{oil} = 1% (d), 2% (e), 3% (f); (g-i) $R_c = 0.6R_s$, n_{oil} = 1% (g), 2% (h), 3% (i). Microgel models are based on regular microgel models comprised of 80000 beads.

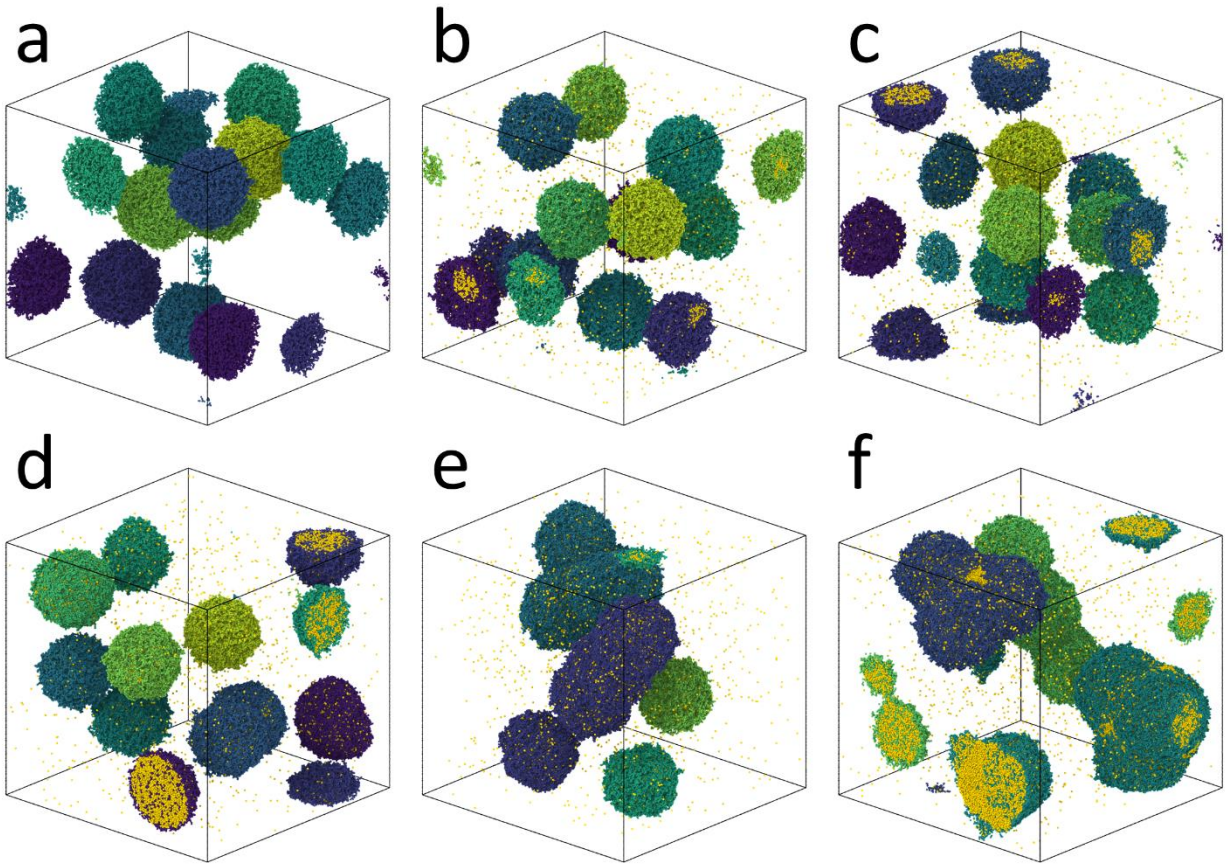

Fig. S5. Simulation snapshots of the ensemble of regular microgels with subchain length N_{sub} = 5 in water/oil mixture at different oil concentrations: n_{oil} = 0% (a), 1% (b), 2% (c), 5% (d), 7% (e), and 10% (f). For clarity, each microgel or microgel cluster is coloured differently.

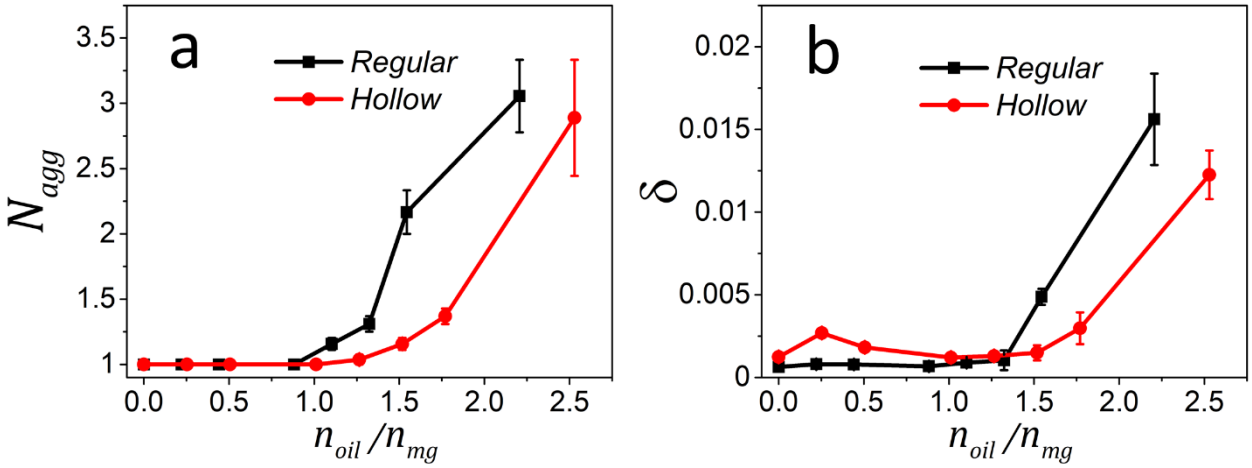

Fig. S6. (a) Mean aggregation number N_{agg} and (b) mean-ensemble relative shape anisotropy δ as functions of oil concentration divided by microgels concentration for the ensembles of microgels of different architectures.