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rntary Material for Core-shell nanogels: the effects of morphology, electro- and magnetostatic interactions †

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In Fig. S1 the density profiles of charged core-shell nanogels with a non-cross-linked shell, $\varepsilon_Y = 4$, $N^{sh} = 1500$, are presented. They look qualitatively similar to those for $N^{sh} = 2000$ provided in the main text, only that the effects are less pronounced. The monomers of the shell are only partially located within the core.

In Fig. S2 signed difference $(R_g^{Yuk} - R_g^{neurt})/R_g^{neurt}$ versus the charge repulsion strength ε_y , the gyration radii are calculated for the entire nanogels with $N^{sh} = 1500$. They confirm that the number of polymers in a shell have a monotonic impact on the swelling, as the curves here show the effects between those in the main text.

Fig. S3 confirms the statement in the main text that the value of λ does not affect the density profiles.



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Fig. S1 Density profiles of charged core-shell nanogels with an noncross-linked shell, $\varepsilon_Y = 4$, $N^{sh} = 1500$: (a) – charged core and shell; (b) – charged core; (c) – charged shell. With solid lines the the results for nanogels with length $M_{sh} = 10$ are plotted; dashed lines correspond to $M_{sh} = 20$. Within each line type, the density profiles for all monomers are plotted with grey; monomer density in the core – blue; monomer density of the shell is plotted with green.





Fig. S2 (a), (c), (e) Signed difference $\left(R_{g}^{Yuk}-R_{g}^{neurt}\right)/R_{g}^{neurt}$ versus the charge repulsion strength \mathcal{E}_y , the gyration radii are calculated for the entire nanogels, filled symbols. (b), (d), (f) Signed difference $\left(R_g^{Yuk,c}-R_g^{neur,c}\right)/R_g^{neur,c}$ versus the charge repulsion strength ε_y calculated for the gyration radii of the nanogel cores, open symbols. (a), (b): all monomers in the nanogels are charged; (c), (d): only monomers in the core are charged; (e), (f): only monomers in the shell are charged. $N^{sh} = 1500$. The shape of the symbol is preserved for a fixed shell polymer length. Circles and solid lines: $M^{sh} = 10$; squares and dashed lines: $M^{sh} = 20$. The type of line: dashed or solid is the same as in Fig. S1.

Fig. S3 Density profiles for magnetic core-shell MNGs with MNPs (a) in the core only and (b),(c) both in the core and in the shell. $K_{sh} = 100$. (a) $M_{sh} = 10, \lambda = 6$; (b) $M_{sh} = 20, \lambda = 3$, (c) $M_{sh} = 20, \lambda = 5$. The grey colour corresponds to all particles in the nanogel, the blue colour is chosen for particles in a core, and the green colour is used for particles in a shell.

1.5

r/R_g

(c)

2.0 2.5 3.0

2.0 2.5 3.0

0.5 1.0

(b)