

# Supplementary information for manuscript “Ordering transition in salt–doped diblock copolymers”

Jian Qin<sup>†,‡</sup> and Juan J. de Pablo<sup>\*,†,‡</sup>

*Institute for Molecular Engineering, University of Chicago, Chicago, Illinois 60637, and Argonne National Laboratory, Argonne, Illinois 70439*

E-mail: depablo@uchicago.edu

We performed a different set of simulations with  $\chi_{AC}N = -60$  at  $l_B = 8$ , to show that the reported two competing effects leading to the observed non-monotonic variation of ODT are not specific to the particular choice of  $\chi_{AC}N = -40$ . The dependence of  $(\chi_{AB}N)_{ODT}$  on  $\phi_{salt}$  is shown in Fig. 1(a). The dilution effect still shows up for  $\phi_{salt} > 0.1$ , in agreement with our main results for  $\chi_{AC}N = -40$  (same figure). Increasing the value of  $\chi_{AC}N$  further distorts the system’s morphology, as illustrated in Fig. 1(b), which shows results for  $\chi_{AC}N = -320$ . In that case, we find clusters of “ion–core” micellar structures resulting from the favorable interactions between cations and PEO–like blocks. This is unwanted and is an artefact of using a soft core repulsive potential.

The effects of dilution by a neutral solvent as predicted by our model are illustrated in Fig. 2(a). The curve predicted by the dilution approximation is shown by a dashed line. The results of our simulations, fitted to a power law with exponent -1.22 are shown by a solid line. The effects of ion selectivity are shown in Fig. 2 (b); they indicate that as the PEO-like block becomes more selective to the cations, then the value of  $(\chi_{AB}N)_{ODT}$  decreases monotonically. Fig. 2(c) summarizes the effects of Bjerrum length  $l_B$  on the ODT. The non-monotonic dependence of ODT in the small  $l_B$

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\*To whom correspondence should be addressed

<sup>†</sup>Institute for Molecular Engineering, University of Chicago, Chicago, Illinois 60637

<sup>‡</sup>Argonne National Laboratory, Argonne, Illinois 70439

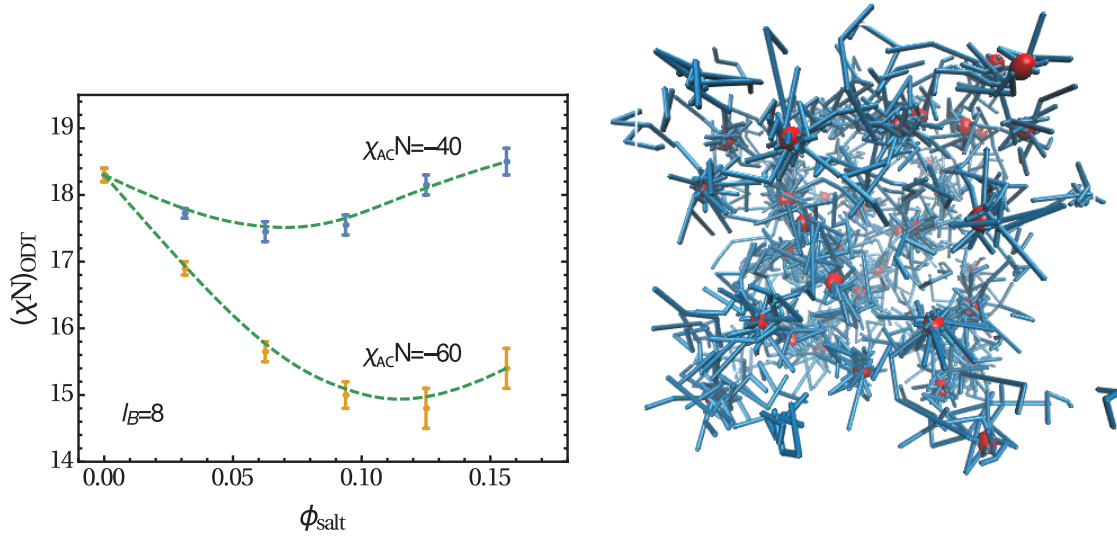


Figure 1: (a) ODT from  $\chi_{\text{AC}}N = -60$  and  $\chi_{\text{AC}}N = -40$ ; (b) Morphology for  $\chi_{\text{AC}}N = -320$ .

regime is attributed to the competition between two effects: entropic gain of delocalizing anions and energetic gain of localizing anions in the PEO rich domain which neutralizes the cations.

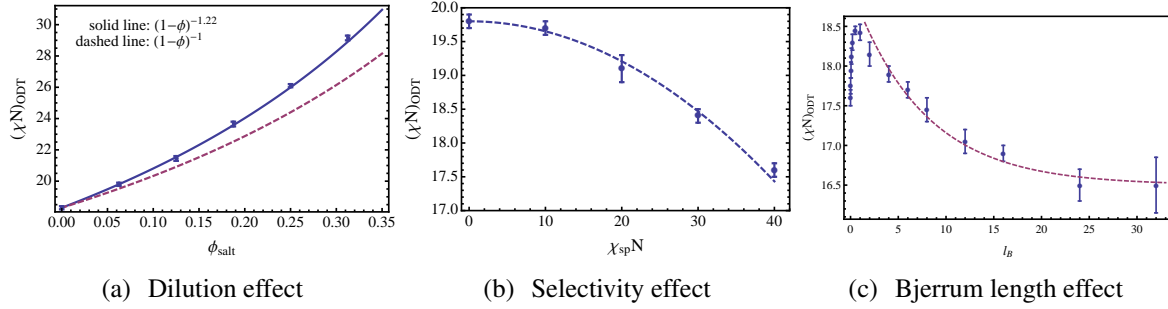


Figure 2: (a) Dependence of ODT on neutral solvent dilution; dashed line is the prediction of dilution approximation;<sup>1</sup> solid line is -1.22 power law fitting. (b) Dependence of ODT on solvent selectivity at  $\phi_{\text{salt}} = 0.0625$ . (c) Dependence of ODT on the electrostatic strength  $l_B$ . All data are obtained at  $\bar{N} = 256$  and  $N = 8$ .

## References

- (1) Fredrickson, G. H.; Leibler, L. *Macromolecules* **1989**, 22, 1238–1250.