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Correction: Transfer matrix theory of polymer complex coacervation

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Correction for 'Transfer matrix theory of polymer complex coacervation' by Tyler K. Lytle et al., *Soft Matter*, 2017, **13**, 7001–7012.

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The authors regret that there is an incorrect equation in ref. 1. Eqn (18) in the manuscript, and the subsequent example, are intended to compute the conditional probability $p(s_i|s_{i-1})$ of observing a state s_i at monomer i given a state s_{i-1} at the previous monomer $i - 1$.¹ The correct expression requires a similar calculation using the frequency n of the transitions from s_{i-1} to s_i :

$$p(s_i|s_{i-1}) = \frac{n(s_i, s_{i-1})}{\sum_{s_i} n(s_i, s_{i-1})} \quad (1)$$

In the original manuscript,¹ the matrix elements \mathbf{M} are taken to be the frequencies, but this is incorrect. Instead, these values of n require that a term be added to the calculation of the partition *via* a factor ζ added to the transfer matrix element of interest (*i.e.*, $\mathbf{M}(s_i, s_{i-1}) \rightarrow \mathbf{M}(s_i, s_{i-1}) \times \zeta$ for s_i, s_{i-1}). The frequency can then be calculated *via* the expression:

$$n(s_i, s_{i-1}) = \lim_{\zeta \rightarrow 1} \left(\frac{\delta \ln(\vec{\psi}^T \mathbf{M}^N \vec{\psi})}{N \delta \ln \zeta} \right) \quad (2)$$

We numerically calculate the new quantities for these conditional probabilities, as a correction to Fig. 3 of the original manuscript,¹ and plot them below against the original simulation values. The same parameters are used here as in the original manuscript. We note that, while possessing quantitative differences from the original (incorrect) values, these theoretical predictions still exhibit similar agreement with simulation values. We thus consider that the original parameters are still appropriate, and therefore the remainder of the manuscript remains quantitatively unchanged and the original conclusions are still valid.

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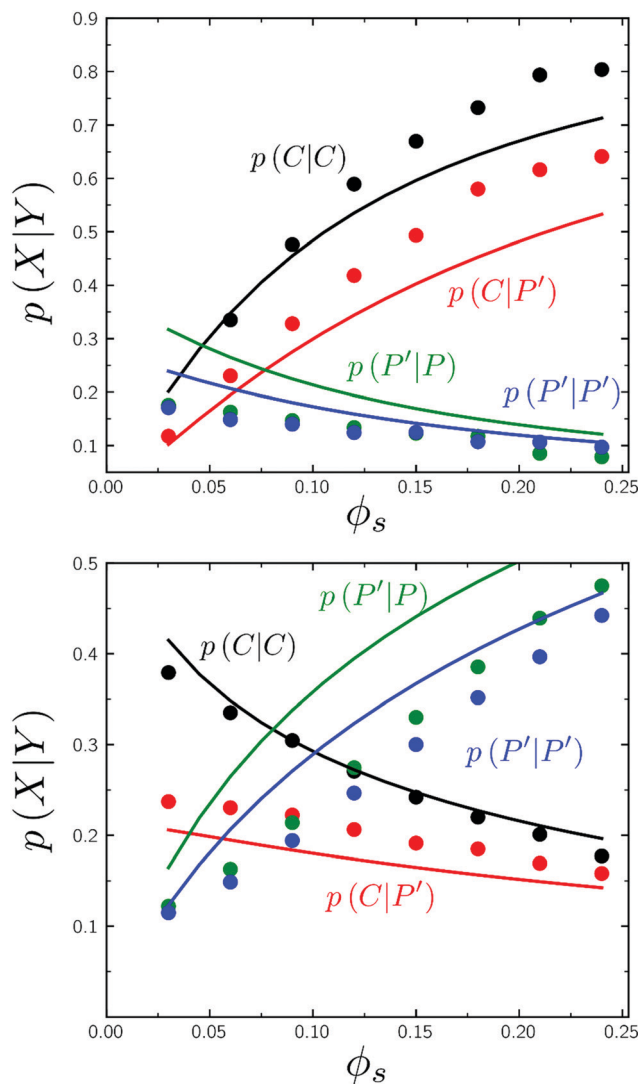


Fig. 3 Simulation (points) and theory (curves) describing the adsorption sequence statistics in various coacervate-forming systems at a number of values of ϕ_p and ϕ_s . (a) The conditional probabilities $p(X|Y)$ of having a monomer with adsorbed state of type X immediately following a monomer with adsorbed state of type Y : $p(C|C)$, $p(C|P')$, $p(P'|P)$, and $p(P'|P')$ as a function of salt concentration ϕ_s at constant $\phi_p = 0.06$. (b) The same conditional probabilities as a function of polymer concentration ϕ_p for constant $\phi_s = 0.06$. For both (a and b) there is near-quantitative fitting between theory and simulation, indicating that this formalism describes the environment surrounding a test chain.

Acknowledgements

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The Royal Society of Chemistry apologises for these errors and any consequent inconvenience to authors and readers.

References

- 1 T. K. Lytle and C. E. Sing, *Soft Matter*, 2017, **13**, 7001–7012.

