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Polyelectrolyte condensation by linear molecules of variable length: a grand-canonical Monte Carlo study CAMILO GUAQUETA, ERIK LUIJTEN, University of Illinois at Urbana-Champaign — The condensation of likecharged polyelectrolytes has been observed to occur under the addition of a variety of oppositely-charged species, such as multivalent counterions, charged globular proteins, and even short chain molecules with monovalent end groups. Inspired by the latter, we study via computer simulations a prototypical polyelectrolyte bundle where condensation is induced by dumbbell-like charged molecules of variable length. We present results from a systematic investigation into the effects of the concentration of bundling agent on the stability of the system. We also consider the effect of changing the length of the dumbbells, as well as the surface charge density of the polyelectrolytes. Recent work<sup>1</sup> has illustrated the important role of the osmotic pressure exerted by the excess solution. In order to take this effect directly into account, we perform simulations in the grand-canonical ensemble, which allows us to equilibrate the bundle with an excess solution of dumbbell molecules at fixed chemical potential.

<sup>1</sup>L. K. Sanders, C. Guáqueta *et al.*, Phys. Rev. Lett.**95**, 108302 (2005).

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