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Modeling phase separation in mixtures of intrinsically-disordered proteins CHAD GU, ANTON ZILMAN, University of Toronto — Phase separation in a pure or mixed solution of intrinsically-disordered proteins (IDPs) and its role in various biological processes has generated interest from the theoretical biophysics community. Phase separation of IDPs has been implicated in the formation of membrane-less organelles such as nucleoli, as well as in a mechanism of selectivity in transport through the nuclear pore complex. Based on a lattice model of polymers, we study the phase diagram of IDPs in a mixture and describe the selective exclusion of soluble proteins from the dense-phase IDP aggregates. The model captures the essential behaviour of phase separation by a minimal set of coarse-grained parameters, corresponding to the average monomer-monomer and monomer-protein attraction strength, as well as the protein-to-monomer size ratio. Contrary to the intuition that strong monomer-monomer interaction increases exclusion of soluble proteins from the dense IDP aggregates, our model predicts that the concentration of soluble proteins in the aggregate phase as a function of monomer-monomer attraction is non-monotonic. We corroborate the predictions of the lattice model using Langevin dynamics simulations of grafted polymers in planar and cylindrical geometries, mimicking various in-vivo and in-vitro conditions.

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