Abstract Submitted
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On the electrostatic properties of the phase-separating protein, Gamma-B crystallin[1] K. MICHAEL MARTINI, DAWN HOLLENBECK, ANDREAS LANGNER, DAVID ROSS, ANTHONY HARKIN, EDWARD NELSON, GEORGE THURSTON, Rochester Institute of Technology — Solutions of the eye lens protein Gamma-B crystallin exhibit liquid-liquid phase separation that we find to have interesting pH and ionic strength dependences. To work towards a model for the data, we construct a grand-canonical partition function that incorporates the free energies of proton occupancy patterns on a protein and its neighboring proteins. We evaluate the work of charging numerically in a coarse-grained Debye-Huckel type model. We validate the computations by comparison to analytically tractable configurations. With use of relevant data on proton affinities, we use Monte-Carlo simulation to study the charging statistics of interacting charge networks of Gamma-B crystallin. Application of this model to a single Gamma-B crystallin molecule is in reasonable agreement with currently available potentiometric titration data for dilute solutions. This model can now be applied to study the mutual charging pattern statistics and consequent interactions of closely neighboring Gamma-B crystallin molecules.

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