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A Theoretical Study of The Coupling Between Chemical Equilibrium and Physical Interactions That Determine Self-Organization in End-Grafted Polyelectrolytes for Tissue-Material Applications EBTISAM ALDAAIS, MARK ULINE, Univ of South Carolina, ULINE RESEARCH TEAM — Understanding the competition of interactions in highly inhomogeneous environments such as those relevant in tissue engineering nanotechnology, and those responsible for biological cell function is critical to the further development of design platforms for such systems. We use a three dimensional mean-field theory to study the competition between electrostatic, van der Waals and steric interactions in determining the molecular organization of end-grafted polyacids. The polyelectrolyte layers spontaneously form self-assembled aggregates whose morphologies are manipulated by the composition of the solution in contact with the film. These theoretical calculations show that chemical equilibrium and the relevant physical interactions present in responsive polymer layers couple in a highly non-additive manner. We find that charge regulation stabilizes micellar domains over a wide range of pH by reducing the local charge in the aggregate at the cost of chemical free energy and gaining in the van der Waals attractive interactions. The balance of interactions in this highly inhomogeneous environment determines the boundaries between different aggregate morphologies. We predict the formation of domains based on the proper choice of solution pH and salt concentration, and one can use these predictions to provide design guidelines for the creation of responsive polymer layers presenting self-organized patterns with the desired functional properties.

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