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Self-organization of multivalent counterions in polyelectrolyte brushes

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The structure and interfacial properties of a polyelectrolyte brush (PEB) depend on a broad range of parameters such as the polymer charge and grafting density, counterion valence, salt concentration, and solvent conditions. These properties are of fundamental importance in technological applications of PEBs including colloid stabilization, surface modification and lubrication, and in functioning of biological systems such as genome packaging in single-strand DNA/RNA viruses. Despite intensive studies by experiments, molecular simulations, and myriad analytical methods including scaling analyses, self-consistent-field theory, and most recently density functional theory, the behavior of PEBs in the presence of multivalent counterions remains poorly understood. In this talk, I will present a density functional method for polyelectrolyte brushes and discuss self-organization of multivalent counterions within highly charged polyelectrolyte brushes. The counterion-mediated attraction between polyions leads to a first-order phase transition similar to that for a neutral brush in a poor solvent. The self-organization of multivalent counterions results in a wavelike electrostatic potential and charge density that oscillate between positive and negative values.