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Electric Double Layer electrostatics of spherical polyelectrolyte brushes with pH-dependent charge density HAO LI, GUANG CHEN, SHAYANDEV SINHA, SIDDHARTHA DAS, Univ of Maryland-College Park, SOFT MATTER, INTERFACES, AND ENERGY LABORATORY (SMIEL) TEAM — Understanding the electric double layer (EDL) electrostatics of spherical polyelectrolyte (PE) brushes, which are spherical particles grafted with PE layers, is essential for appropriate use of PE-grafted micro-nanoparticles for targeted drug delivery, oil recovery, water harvesting, emulsion stabilization, emulsion breaking, etc. Here we elucidate the EDL electrostatics of spherical PE brushes for the case where the PE exhibits pH-dependent charge density. This pH-dependence necessitates the consideration of explicit hydrogen ion concentration, which in turn dictates the distribution of monomers along the length of the grafted PE. This monomer distribution is shown to be a function of the nature of the sphere (metallic or a charged or uncharged dielectric or a liquid-filled sphere). All the calculations are performed for the case where the PE electrostatics can be decoupled from the PE elastic and excluded volume effects. Initial predictions are also provided for the case where such decoupling is not possible.

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