Structure and electrostatic properties of polyelectrolyte dendrimer coatings

Pedro A. SANCHEZ - *University of the Balearic Islands, Spain & University of Vienna, Austria*

Surface functionalization with polyelectrolytes (PEs) is a key strategy to create advanced materials and tune their properties. For instance, PE nanocoatings are broadly used to stabilize electrostatically colloids and nanoparticles in suspension. An important application that is currently attracting a large interest is the creation of adsorbing surfaces able to capture ions and charged molecules for separation purposes. For this, the hyperbranched structure of PE dendrimers provides several advantages with respect to conventional linear PEs, including a large and well defined number of tunable functional groups and large internal cavities to host the adsorbed substances. Despite this interest, theoretical studies on PE dendrimer coatings are still much less developed than the ones on linear PEs systems. In this contribution we present an extensive computer simulation study on the equilibrium internal structure and electrostatic properties of PE dendrimer brushes, paving the way to characterize and optimize the performance of these systems as nanosorbent coatings. By means of extensive Langevin dynamics simulations, we analyze the effects of dendrimer grafting density, degree of protonation and surface charge on the equilibrium properties, showing how the interplay between these parameters leads to strong changes in the system. On the basis of the simulation data, the development of an accurate Poisson-Boltzmann theory for this system will be also outlined.