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Molecular Dynamics Simulations of Layer-by-Layer Assembly of Charged Macromolecules

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Molecular dynamics simulations of electrostatic assembly of multilayers of flexible polyelectrolytes and charged nanoparticles at a charged surface were performed. The multilayer build-up was achieved through sequential adsorption of oppositely charged macromolecules in a layer-by-layer fashion from dilute solutions. The steady state multilayer growth proceeds through a charge reversal of the adsorbed polymeric film, which leads to a linear increase in the polymer surface coverage after completion of the first few deposition steps. Moreover, substantial intermixing between chains adsorbed during different deposition steps is observed. This intermixing is consistent with the observed requirement for several deposition steps to transpire for completion of a single layer. However, despite chain intermixing, there are almost perfect periodic oscillations of the density difference between monomers belonging to positively and negatively charged macromolecules in the adsorbed film. Weakly charged chains show higher polymer surface coverage than strongly charged ones.