Abstract Submitted
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Layer-by-Layer Assembly of Polyelectrolyte Chains and Nanoparticles on Porous Substrates: Molecular Dynamics Simulations[1] JAN-MICHAEL CARRILLO, ANDREY DOBRYNIN, Institute of Materials Science and Department of Physics, University of Connecticut — We performed molecular dynamics simulations of a multilayer assembly of oppositely charged polyelectrolyte chains and nanoparticles on porous substrates with cylindrical pores. The film was constructed by sequential adsorption of oppositely charged species in a layer-by-layer fashion from dilute solutions. The multilayer assembly proceeds through surface overcharging after completion of each deposition step. The substrate overcharging fraction fluctuates around 0.5 for nanoparticles-polyelectrolytes systems and around 0.4 for polyelectrolytes-polyelectrolytes systems. The surface coverage increases linearly with the number of deposition steps. The rate of surface coverage increase as a function of the number of deposition steps changes when the pore is closed. The closing of the pore occurs from the pore entrance for nanoparticles-polyelectrolytes systems. In the case of polyelectrolytes-polyelectrolytes systems the pore plug is formed inside the pore and then spreads towards the pore ends.

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