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Layer-by-Layer Assembly of Charged 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 multilayer assembly of oppositely charged nanoparticles on porous substrates with cylindrical pores. The film was constructed by sequential adsorption of oppositely charged nanoparticles in layer-by-layer fashion from dilute solutions. The multilayer assembly proceeds through surface overcharging after completion of each deposition step. There is almost linear growth in the surface coverage and film thickness during the deposition process. The multilayer assembly also occurs inside cylindrical pores. The adsorption of nanoparticles inside pores is hindered by the electrostatic interactions of newly adsorbing nanoparticles with the multilayer film forming inside the pores and on the substrate. This is manifested in saturation of the average thickness of the nanoparticle layers formed on the pore walls with increasing number of deposition steps. The distribution of nanoparticles inside cylindrical pore was nonuniform with significant excess of nanoparticles at the pore entrance.

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