Abstract Submitted
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**Molecular Dynamics Simulations of Protein-Polyelectrolyte Multilayer Assembly**[1] VENKATESWARLU PANCHAGNULA, Department of Chemistry, University of Connecticut, JUNHWAN JEON, ANDREY DOBRYNIN, Polymer Program, Institute of Materials Science, University of Connecticut — Nanoscale assembly of protein-polyelectrolyte multilayer thin films on solid surfaces has tremendous potential in areas such as biomaterials, drug delivery and fabrication of biosensing devices. The ability to control nanoscale structure and order of these films is essential for surface patterning and templating. We performed molecular dynamics simulations of the protein-polyelectrolyte layer-by-layer assembly on a solid planar surface formed by hexagonally packed particles. Spherical-shaped model protein was constructed by utilizing the charged residues of lysozyme, which was obtained from the Protein Data Bank, to model protein charge distribution. Multilayer build-up was achieved through sequential adsorption of proteins and flexible polyelectrolytes in a layer-by-layer fashion from dilute solutions. The effect of the three dimensional structural rigidity of proteins, charge distribution and hydrophobicity on the film structure was studied.

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Junhwan Jeon
Polymer Program, Institute of Materials Science, University of Connecticut

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