Molecular Dynamics Simulation of the Layer-by-Layer Assembly Process

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Abstract

The aim of this work is to develop a computational model of the layer-by-layer assembly process using molecular dynamics technique. Layer-by-Layer assembly process is the based on the electrostatic attraction of the oppositely charged particles such as polyelectrolytes and nanoparticles. In this process, a layer of charged species is deposited on top of an oppositely charged substrate; a second layer with a charge opposite to the first layer is then deposited. This process continues until the desired number of layers has been deposited. Layer by layer assembly of polymers on a substrate have many applications in drug delivery, electronic applications and biomedical applications (bioreactors, artificial cells, etc). This work is performed by the Molecular Dynamics (MD) simulations using NAMD (not another molecular dynamics) simulation software. MD is a computer simulation technique based on the solution of the equations of motion for interacting atoms. We simulated the deposition of a bilayer, the stacking consisted on Polymethacrylic acid (PMAA) and Polyacrylic acid (PAA) on top of a silicon dioxide (SiO_2) structure. First the structures of SiO2(4800 atoms), PAA(92 atoms) and PMAA(120 atoms) are built using GAUSSVIEW and DLPOLY visualization tools and from the CONFIG file (contains the Cartesian co-ordinates of the structure) the input files are built using C-language code develop in our group. First the PAA polymers (negatively charged) are deposited on the SiO_2 substrate (positively charged) next the PMAA polymers (positively charged) are deposited on the first layer of PAA polymers. The maximum numbers of PAA polymers that we deposited on SiO_2 are 26 polymers (10 monomers each). Next 20 PMAA polymers are deposited on the first layer of PAA polymers.