The Self-assembly of Disk-coil Block Copolymers within 2D Cylinder Confinement with Asymmetric Pair Interactions

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Chlorosomes, the most efficient light-harvesting antenna system in nature, have multi-layered tubular architecture of bacteriochlorophyll molecules with specific molecular arrangement covered by lipid layer. In order to investigate the self-assembly of bacteriochlorophyll molecules on the novel architecture of chlorosomes, self-assembly of a disk-coil block copolymer modeled from porphyrin attached to single alkyl chain of bacteriochlorophyll molecule was investigated. To mimic the self-assembly nature of bacteriochlorophyll molecules covered by lipid layer, disk-coil block copolymers confined in cylinder are systematically studied using molecular dynamics simulation as functions of radius of cylinders, length of coil-like chain and asymmetric pair interaction between disks. Our study is differentiated from the self-assembly behavior of linear block copolymers within cylindrical confinement due to the specific packing structure arising from asymmetric pair interaction between disk part of our modeled molecules. We believe that our study provides physical principles of self-assembled behavior of bacteriochlorophyll molecules to design next generation photoelectronic devices.