Theoretical Study of Interaction Mechanism of Bacterial Cell Membrane and Polymer Coated Nanopillar via Coarse-Grained Molecular Dynamics

신은혜, 고은민, 염민선[1], 곽상규[†]
울산과학기술원; [1]KISTI
(skkwak@unist.ac.kr[†])

Nanopatterned surfaces, which were originated from bactericidal effect of dragonfly or cicada wings, have been studied for antibacterial functioning. However, previous nanopatterned surfaces developed were effective only gram-negative or gram-positive bacteria. In this study, nanopatterned surface, effective for both gram-negative and gram-positive bacteria, was investigated via coarse-grained molecular dynamics. Nanopatterned surface was constructed using silicon nanopillar coated with polyarginine as a cell penetrating polymer. Bacterial cell membranes were modeled for gram-negative bacteria (inner membrane, peptidoglycan, and outer membrane) and for gram-positive bacteria (peptidoglycan and inner membrane), respectively. We investigated cell membrane destruction depending on the nanopillar spacing (i.e., 10.7 and 21 nm) and found that wide spacing nanopillar was effective for its destruction. The membrane destruction was more easily occurred as contact area increased between membrane and nanopatterned surface. Specifically, LPS core of gram-negative bacteria and POPG of gram-positive bacteria were interacted with positively charged side chain of polyarginine, respectively.