

## Biphasic Nano-Domain Model Derived from Molecular Dynamics of Phospholipid-Diacetylene Complex Bilayer for Antimicrobial Detection

정우혁, 황지민, 안동준<sup>†</sup>

고려대학교

(ahn@korea.ac.kr<sup>†</sup>)

Polydiacetylene (PDA), one of the responsive polymers, is an attractive material for sensors, bio-imaging and drug delivery system. By assigning this material, exhibiting blue-to-red color transition due to external stimuli, to supported lipid bilayer platform, it delivers selectivity in bio-molecular detection.

To investigate time-dependent nanoscale phase behavior and color transition after antimicrobial peptide injection on SLB system, we adapted computational chemistry, especially coarse-grained (CG) molecular dynamics simulation. We conducted CG simulation with antimicrobial peptide on phospholipid-diacetylene system to present a crucial role of in regulating the degree of phase coexistence. In this study, we confirmed that the liquid-disordered phase of the system plays a critical role on increased detection capability against peptide.