Abstract Submitted
for the MAR12 Meeting of
The American Physical Society

How the antimicrobial peptides destroy bacteria cell membrane: Translocations vs. membrane buckling[1]
LEONARDO GOLUBOVIC, West Virginia University, LIANGHUI GAO, LICUI CHEN, WEIHAI FANG, Beijing Normal University —
In this study, coarse grained Dissipative Particle Dynamics simulation with implementation of electrostatic interactions is developed in constant pressure and surface tension ensemble to elucidate how the antimicrobial peptide molecules affect bilayer cell membrane structure and kill bacteria. We find that peptides with different chemical-physical properties exhibit different membrane obstructing mechanisms. Peptide molecules can destroy vital functions of the affected bacteria by translocating across their membranes via worm-holes, or by associating with membrane lipids to form hydrophilic cores trapped inside the hydrophobic domain of the membranes. In the latter scenario, the affected membranes are strongly corrugated (buckled) in accord with very recent experimental observations [G. E. Fantner *et al.*, Nat. Nanotech., 5 (2010), pp. 280-285].

[1]Supported by the National Science Foundation of China (Grant No. 20873007)

Leonardo Golubovic
West Virginia University

Date submitted: 08 Nov 2011 Electronic form version 1.4