Focusing the Computational Microscope on Bacterial Cell Envelopes.

Syma Khalid*†[1]

[1]University of Southampton – United Kingdom

Abstract

The cell envelopes the protect Gram-negative bacteria are complex, multicompartment molecular architectures. But in order to defeat harmful, disease-causing bacteria it is imperative that we unravel the structure-dynamics mysteries of these cell envelopes. To this end we have developed atomistic-level models of the two membranes and cell wall that constitute the cell envelope of *E. coli*. Our simulations have begun to provide some insights into the dynamic interplay between the different components and the structural consequences of these dynamics. At a more coarse-grain level, we have recently started looking at how outer membrane vesicles, which are shed by all bacterial studied to date, interact with model plasma membranes. Our large simulations of systems of millions of particles are beginning to provide insights into steps that are important in the process of infection. I will discuss both the atomistic and coarse-grain strands of our work in this presentation.

Keywords: modelling, coarse, grain

*Speaker

†Corresponding author: S.Khalid@soton.ac.uk