A new Monte Carlo method for investigating geometrical structures of lipid membranes with atomistic detail SARA CHENG, UC Berkeley, LIMING QIU, K. CHENG, MARK VAUGHN, Texas Tech University — The distribution statistics of the surface area, volume and voids of lipid molecules are important parameters to characterize the structures of self-assembling lipid membranes. Traditional methods are mostly based on various assumptions of the thickness of the lipid membrane and the volumes of certain types of lipid molecules. However, those methods usually lead to an over- or underestimation of the average surface area of lipid molecules when compared to the experimental results of the pure lipid systems. We developed a new Monte Carlo method that is able to estimate the distributions and averages of surface area, volume and void space of the lipid molecules in the absence and presence of proteins of the MD simulation results of lipid membranes at the atomistic scale. We successfully validated our new method on an ordered hard-sphere system and on a phospholipid/cholesterol binary lipid system, all with known structural parameters. Using this new method, the structural perturbation of the conformal annular lipids in close proximity to the embedded protein in a lipid/protein system will also be presented.

Sara Cheng
UC Berkeley