THE
CATHOLIC UNIVERSITY
of AMERICA

Department of Physics
Colloquium

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Computer Simulations of Membranes: from Pure Bilayers to Antimicrobial Peptides

Following a brief introduction to the membrane structure, and simulations using the CHARMM lipid force field C36 (J. Phys. Chem. B.,114, 7830, 2010), 3 topics will be presented:

1. *Periodic Boundary Condition in Bilayers.* A generalization of the Saffman-Delbrück model for diffusion in infinite bilayers to bilayers with PBC such as used in computer simulations indicates that protein diffusion constants are underestimated by a factor of 5-10 and for lipids by a factor of 3 in all-atom simulations using the systems sizes currently possible (J. Chem. Phys., 143, 243113, 2015; J. Phys. Chem. B., 121, 3443, 2017).
2. *Calculation of Bending Constants and Spontaneous Curvature.* MD simulations correctly predict that bending moduli obtained from x-ray scattering measurements were systematic underestimates, at least partly because the tilt modulus should be incorporated in the analysis of scattering. Simulations yield good agreement with experiment for spontaneous curvatures in the inverse hexagonal phase, and indicate equivalence with lamellar phases (Biophysical J., 104, 2202, 2013; Chemistry and Physics of Lipids, 192, 60, 2015). Is it also shown that a common assumption regarding the additivity of spontaneous curvatures is incorrect for bilayers with strongly interacting lipids, such as sphingomyelin (Phys. Rev. Lett., 117, 138104, 2016).
3. *Membrane disruption by Antimicrobial Peptides*. A 26 microsecond trajectory and assorted control simulations suggest that antimicrobial activity by piscidin might be via defects, rather than stable pores (Biophysical J., 111, 1248 and 1258, 2016), and point to the importance of lipid composition and experimental conditions.

Wednesday, September 27, 2017
4:00pm
108 Hannan Hall
Refreshments will be served at 3:45

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For more information or if you would like to request disability accommodations, please contact:
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