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Abstract for an Invited Paper
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Development and application of coarse-grained models for lipids[1]

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I'll discuss a number of topics that represent our efforts in developing reliable molecular models for describing chemical and physical processes involving biomembranes. This is an exciting yet challenging research area because of the multiple length and time scales that are present in the relevant problems. Accordingly, we attempt to (1) understand the value and limitation of popular coarse-grained (CG) models for lipid membranes with either a particle or continuum representation; (2) develop new CG models that are appropriate for the particular problem of interest. As specific examples, I'll discuss (1) a comparison of atomistic, MARTINI (a particle based CG model) and continuum descriptions of a membrane fusion pore; (2) the development of a modified MARTINI model (BMW-MARTINI) that features a reliable description of membrane/water interfacial electrostatics and its application to cell-penetration peptides and membrane-bending proteins. Motivated specifically by the recent studies of Wong and co-workers, we compare the self-assembly behaviors of lipids with cationic peptides that include either Arg residues or a combination of Lys and hydrophobic residues; in particular, we attempt to reveal factors that stabilize the cubic "double diamond" Pn3m phase over the inverted hexagonal H_{II} phase. For example, to explicitly test the importance of the bidentate hydrogen-bonding capability of Arg to the stabilization of negative Gaussian curvature, we also compare results using variants of the BMW-MARTINI model that treat the side chain of Arg with different levels of details. Collectively, the results suggest that both the bidentate feature of Arg and the overall electrostatic properties of cationic peptides are important to the self-assembly behavior of these peptides with lipids. The results are expected to have general implications to the mechanism of peptides and proteins that stimulate pore formation in biomembranes.

[1]Work in collaboration with Zhe Wu, Leili Zhang and Arun Yethiraj