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Research Interests

Our research interests mainly focuses on applying molecular simulations to study soft matter and bio-nanomaterials. Current research have spanned the fields of protein folding and aggregations, self-assembly of nanoparticle and surfactants, and advanced simulation algorithm developments. All the research topics have been closely collaborate with experimentalists and theorists from various disciplines:

A. Characterization of Ion Pair Amphiphile Vesicular Membrane

Ion pair amphiphile (IPA), a lipid-like complex composed of a pair of cationic and anionic surfactants, has been suggested as an inexpensive phospholipid substitute with great potentials in various pharmaceutical applications such as drug or DNA deliveries. Choices of the composing cationic and anionic surfactants give rise to a large flexibility on controlling the IPA complex structure and modulating the IPA membrane properties. In this project, we utilized multi-scale molecular dynamics (MD) simulation to systematically examine the parameters affecting the IPA vesicle stabilities, including the hydrophobic chain lengths, the symmetry of IPAs, the number of hydrophobic chains, and the addition of stabilization compound such as cholesterol. Using all-atom (AA) molecular simulations, we examine the structural, thermodynamic and kinetic properties of the IPA bilayers at the molecular level. Simplified coarse-grained (CG) models are applied to explore the large-scale phase transition behaviors or IPA bilayers and the complex self-assembling behaviors of IPAs. The molecular insights provided by simulations into the IPA bilayer systems can serve as useful reference for fabricating IPA vesicles and future application designs

B. Proteins Folding, Misfolding and Aggregation

The fibril deposits of amyloid proteins are strongly associated with various diseases, including Alzheimer's disease, Parkinson's disease, and type II diabetes. Specifically, the amyloid fibrils of human islet amyloid polypeptide (hIAPP), or human amylin, are closely related to the development of type II diabetes. We utilize molecular dynamics combined with advanced sampling techniques to study the conformations of hIAPP monomers, oligomers, and mature fibrils. Through the combination of experiment, theory, and simulations, we have identified the aggregation mechanism of hIAPP and characterized the important intermediate species during the aggregation process, which provides valuable insights into the future inhibitor designs. The aggregation of hIAPP triggers other non-amyloidogenic peptide to form amyloid deposits, revealing new pathological roles of amyloid proteins.

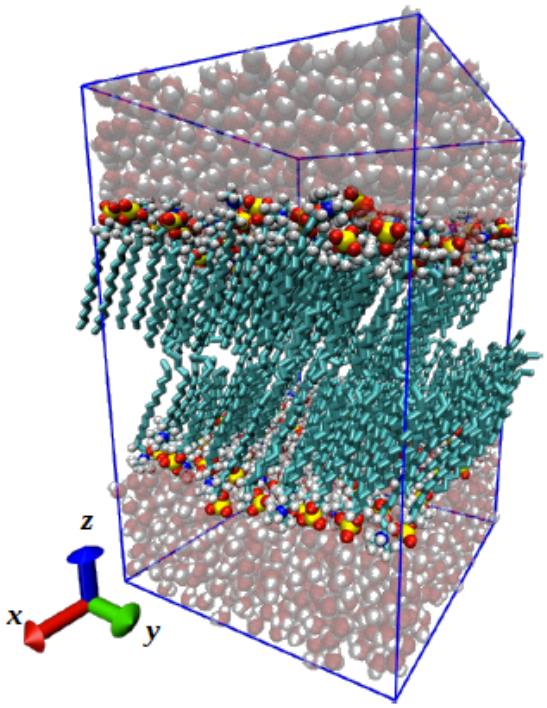
C. Effects of nanoparticles on biological membranes

While nanomaterials receive substantial considerations in various potential applications, a proactive approach is needed to ensure the environmental, health, and safety (EHS) impacts are well understood.
To probe the cytotoxicity of carbon based nanoparticles (CNPs) at the molecular level, we applied multi-scale simulation techniques to study the effects of CNPs on biological. Based on all-atom force fields, we have developed a simplified coarse-grained model, which predicts the correct interfacial energy

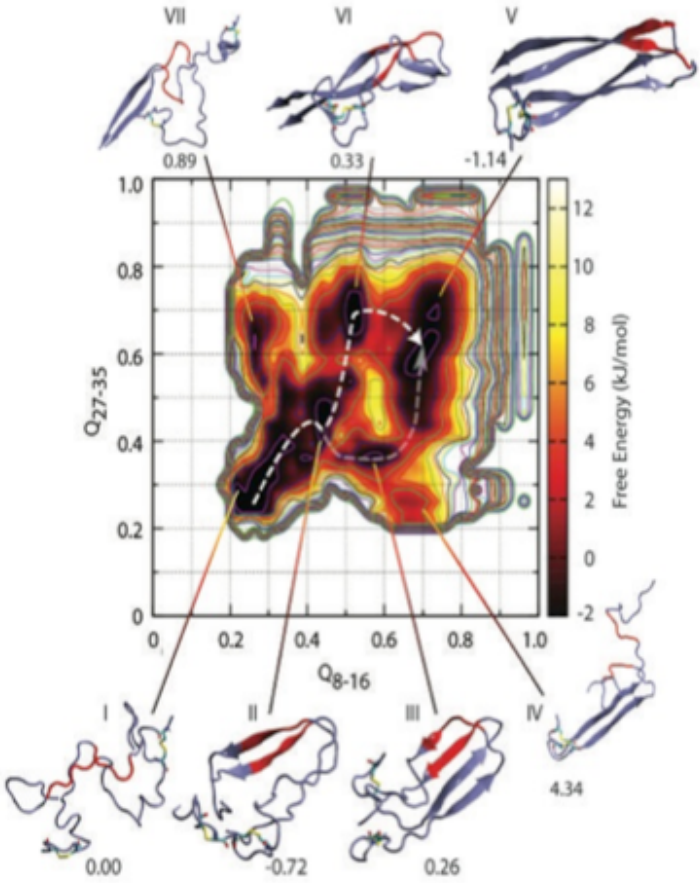
between the nanoparticle and solvent and more accurately describes the interactions within the CNP / bio-membrane systems. Using this model, we examine the self-assembly of CNPs in solution and in the membrane. Furthermore, we also explore the effects of size and compositions of CNPs on the transition between the lipid monolayer and the bilayer. These effects can be correlated with fullerene cytotoxicity toward the lung alveoli through inhalation.

Representative Publications

1. Hoffmann, K. Q., McGovern, M., Chiu, C.-C., & de Pablo, J. J. (2015). PLoS ONE, 10(7), e0134091.
2. Chiu, C.-C., Singh, S., & de Pablo, J. J. (2013). Biophys. J., 105(5), 1227–1235.
3. Buchanan, L. E., Dunkelberger, E. B., Tran, H. Q., Cheng, P.-N., Chiu, C.-C., Cao, P., et al. (2013). Proc. Natl. Acad. Sci., 110(48), 19285–19290.
4. Middleton, C. T., Marek, P., Cao, P., Chiu, C.-C., Singh, S., Woys, A. M., et al. (2012). Nat. Chemistry, 4(5), 355–360.
5. Chiu, C.-C., Shinoda, W., DeVane, R. H., & Nielsen, S. O. (2012). Soft Matter, 1–20.
6. Chiu, C.-C., Maher, M. C., Dieckmann, G. R., & Nielsen, S. O. (2010). ACS Nano, 4(5), 2539–2546.
7. Chiu, C.-C., DeVane, R., Klein, M. L., Shinoda, W., Moore, P. B., & Nielsen, S. O. (2010). J. Phys. Chem. B, 114(19), 6394–6400.



The representative all-atom IPA bilayer structure



The conformational free energy surface for the hIAPP dimer. The important intermediates during the dimerization process and the corresponding free energy values are also given.