LACNS

Louisiana Consortium for Neutron Scattering

SEMINAR SERIES 2018

Monday, April 23
3:00 pm
1008B Digital Media Center
Louisiana State University

DFT and Force Field Study on the Effect of Ions on Structure and Side-Chain Interactions in Peptoids

Guest Speaker

Dr. Marcel Baer

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The description of peptides and the use of molecular dynamics simulations to refine structures and investigate the dynamics on an atomistic scale are well developed. A consensus in this community over multiple decades has resulted in the availability of parameterized force fields that only require the sequence of amino-acids and an initial guess for the three-dimensional structure. The recent discovery of peptoids, that are designed with functionality attached to the nitrogen instead of the Ca is a significant departure from the standard force fields for peptides and will require a retooling of the currently available interaction potentials in order to have the same level of confidence in the predicted structures and pathways as there is presently in the peptide counterparts. Here we present modeling of peptoids using a combination of *ab initio* molecular dynamics (AIMD), atomistic resolution classical FF and coarse-grained models (CG) to span the relevant time and length scales. To make contact with experiments and identify features of the peptoid monomers that promote formation of stable/ordered nanostructures, both nucleation and aggregation will be explored using CG simulations. To properly account for the dominant forces that stabilize ordered structures of peptoids, namely steric-, electrostatic, and hydrophobic interactions mediated through sidechain-sidechain interactions in the CG model those have to be first mapped out using high fidelity atomistic representations. A key feature here is not only to use gas phase quantum chemistry tools, but also account for solvation effects in the condensed phase through *ab initio* molecular dynamics simulation. One major challenge is to elucidate ion binding to charged or polar regions of the peptoid and its concomitant role in the creation of local order. Here, similar to proteins, a specific ion effect is observed suggesting that both the net charge and the precise chemical nature of the ion will need to be described.

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