

Abstract Submitted
for the MAR13 Meeting of
The American Physical Society

Exploring the atom-resolution properties of peptoid nanosheets

RANJAN MANNIGE, RONALD ZUCKERMANN, STEPHEN WHITELAM, Molecular Foundry, Lawrence Berkeley National Laboratory, STEVE WHITELAM TEAM¹, RONALD ZUCKERMANN COLLABORATION² — Peptoids are artificial positional isomers of peptides, where the sidechains are attached to the backbone nitrogen in stead of the alpha carbon. Recently, an amphiphilic peptoid was found to form bilayers (nano-sheets) that expand in area to the mesoscopic level but which display uniform thickness of only between 2 to 3 nanometers. While progress in the chemical synthesis of these sheets have witnessed leaps, an atomistic understanding of peptoid nanosheets is lacking. We report recent developments in the atomistic simulation of assembled peptoid nanosheet candidates which resulted in a configurational energy landscape where only specific arrangements of peptoids are energetically feasible. Additionally, we find that while the charged sidechains situated on the exterior of the bilayer describe the general arrangement of the sheet, the exact positions of each peptoid appears to be dominated primarily by the hydrophobic residues that interact in the interior of the bilayer. These results provide a novel picture of the atomistic features of peptoid nanosheets, which serves as a useful platform for the further and rational development of novel peptoid nanosheets.

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Date submitted: 09 Nov 2012

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