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Modeling of biomimetic peptoid polymers DINA MIRIJANIAN, STEVE WHITELAM, Lawrence Berkeley National Laboratory — Peptoids are sequence-specific, oligo-N-substituted glycine polymers that can mimic the structural motifs and functionalities of proteins. Recently, novel sheet-like nanostructured materials have been self-assembled from peptoids under physiological conditions. These structures are biocompatible and may be selectively functionalized. We have constructed atomistic models of peptoids using high level ab initio calculations to guide the parameterization of a classical force field based on the CHARMM22 peptide force field. Atomistic molecular dynamics simulations show the accessible configurations of peptoids in water to be markedly different from those of peptides. We have also used our parameterized force field to study the molecular structure of peptoid sheet-like nanostructures.

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