

Abstract Submitted
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Molecular dynamics simulations of electrostatics and hydration distributions around RNA and DNA motifs ASHLEY E. MARLOWE, ABHISHEK SINGH, ANDREY V. SEMICHAEVSKY, YAROSLAVA G. YINGLING, North Carolina State University, MATERIALS SCIENCE AND ENGINEERING TEAM — Nucleic acid nanoparticles can self-assemble through the formation of complementary loop-loop interactions or stem-stem interactions. Presence and concentration of ions can significantly affect the self-assembly process and the stability of the nanostructure. In this presentation we use explicit molecular dynamics simulations to examine the variations in cationic distributions and hydration environment around DNA and RNA helices and loop-loop interactions. Our simulations show that the potassium and sodium ionic distributions are different around RNA and DNA motifs which could be indicative of ion mediated relative stability of loop-loop complexes. Moreover in RNA loop-loop motifs ions are consistently present and exchanged through a distinct electronegative channel. We will also show how we used the specific RNA loop-loop motif to design a RNA hexagonal nanoparticle.

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