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**Molecular dynamics simulations of DNA-polycation complexes**
JESSE ZIEBARTH, YONGMEI WANG, University of Memphis — A necessary step in the preparation of DNA for use in gene therapy is the packaging of DNA with a vector that can condense DNA and provide protection from degrading enzymes. Because of the immunoresponses caused by viral vectors, there has been interest in developing synthetic gene therapy vectors, with polycations emerging as promising candidates. Molecular dynamics simulations of the DNA duplex CGCGAATTCGCG in the presence of 20 monomer long sequences of the polycations, poly-L-lysine (PLL) and polyethyleneimine (PEI), with explicit counterions and TIP3P water, are performed to provide insight into the structure and formation of DNA polyplexes. After an initial separation of approximately 50 Å, the DNA and polycation come together and form a stable complex within 10 ns. The DNA does not undergo any major structural changes upon complexation and remains in the B-form. In the formed complex, the charged amine groups of the polycation mainly interact with DNA phosphate groups, and rarely occupy electronegative sites in either the major or minor grooves. Differences between complexation with PEI and PLL will be discussed.

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