Abstract Submitted
for the MAR14 Meeting of
The American Physical Society

Coarse-grained molecular dynamics simulations linking molecular features of polycations to polycation-polyanion complexation for gene delivery ANNA MCLELAND, DANIEL JOHNSON, ARTHI JAYARAMAN, University of Colorado, Boulder — Gene therapy is a method involving transfection or delivery of therapeutic DNA to target cells for expression of proteins that can cure diseases. Polycations have shown tremendous potential as DNA delivery vectors because the positive charges along the polycation interact with the negatively charged DNA backbone to form a polyplex that protects and transfects the DNA. Past work has shown that the structure and chemistry of the polycation affects DNA transfection efficiency. In this work, we use coarse grained models that are mapped from atomistic simulations, along with molecular dynamics simulations to study the binding of polycations and polyanions into polyplexes. We characterize the structure, surface composition and shape of the polyplex, features that impact DNA delivery, as a function of polycation chemistry, architecture (linear versus grafted), and molecular weight. The results from these simulations serve as valuable guidelines for experimentalists on what molecular characteristics they need to incorporate in the polycations to achieve higher transfection efficiency.

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Date submitted: 14 Nov 2013 Electronic form version 1.4