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Coarse-grained Simulation of Complexation between Small Interfering RNA and Polycations ZONGHUI WEI, Northwestern University, YONG REN, JOHN-MICHAEL WILLIFORD, HAI-QUAN MAO, Johns Hopkins University, ERIK LUIJTEN, Northwestern University, NORTHWESTERN UNIVERSITY COLLABORATION, JOHNS HOPKINS UNIVERSITY COLLABORATION — Nanoparticles formed through self-assembly of polycations and nucleic acids are promising systems for gene delivery. A full understanding of the behavior of these particles in physiological context requires detailed knowledge of their physical properties. All-atom molecular dynamics simulations can provide insight into the interaction of polymeric carriers with genomic material, but only at limited time and length scales. To overcome these limitations and explore the full complexation process, a reliable coarse-grained model is needed. Here, we systematically develop such a model for a system comprised of small interfering RNA (siRNA) and polyethyleneimine-based carriers, and evaluate the quality of the coarse-grained model through comparison with all-atom simulations. We show that our coarse-grained model provides a reliable description of detailed binding pictures, charge characteristics, and water dynamics, while accelerating the simulations by two orders of magnitude. This makes it possible to quantitatively investigate nanoparticle formation involving multiple siRNA molecules and cationic copolymers.

Zonghui Wei
Northwestern University

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