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Abstract for an Invited Paper
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Using multi-scale molecular simulations to guide experimental design of biomaterials for drug and DNA delivery

ARTHI JAYARAMAN, University of Delaware

In this talk I will present molecular simulations studies that guide experimental synthesis of polymers for efficient DNA delivery. Viruses, while effective at delivery and transfection of DNA, can elicit harmful immunogenic responses, thus motivating design of non-viral transfection agents. Polycations are a promising class of non-viral vectors that bind to the negatively charged DNA backbone to form a complex (polyplex) that is then internalized into the target cell. Combinatorial approaches have generated various polycations with differing DNA transfection efficacies, but there is a need for general design guidelines that can relate the molecular features of the polycation to its DNA transfection efficiency. Using atomistic and coarse-grained molecular dynamics simulations we connect the thermodynamics of polycation-DNA binding and polyplex structure to experimentally observed transfection efficiency as a function of polycation chemistry and architecture.