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Predicting interactions of polymers with cellular matter

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Combining synthetic polymers with biological matter such as proteins or DNA is a cornerstone technique in nanomedicine and biotechnology. For example, antibody formulations can be stabilized through the addition of low molecular weight polymers or nucleic acid delivered by combining them with ionic polymers to form polyplexes. Exploiting the vast chemical composition space spanned by synthetic polymers holds great promise for designing application-specific sequences to overcome problems such as cell-type targeting in nucleic acid-based gene therapy. However, the interactions of these polymers with biological matter are little understood, sequence dependent data scarce, and the system complexity high. In this talk, I will present our recent advances in creating a multiscale simulation framework to simulate, analyze, and ultimately predict the interactions of polymers with cellular matter. Using chemically specific coarse-grained simulation in combination with machine learning and atomistic simulations we aim to create digital twins of near to realistic resolution, which can be used to understand and optimize these systems.

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