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Kinetics of (un)binding between DNA-functionalized particles using a coarse-grained model with explicit nucleotide representation[1] TIARA MAULA, JEETAIN MITTAL, Department of Chemical and Biomolecular Engineering, Lehigh University — Advances in technology have made necessary the manufacture of materials at increasingly precise scales. However, developing materials with finely ordered structures up to the nanometer scale is infeasible using traditional top-down methods. This has prompted interest in self-assembling materials like DNA-functionalized particles (DFPs). In this research, we use a coarse-grained DFP model which preserves key chemical and structural properties of DNA while explicitly representing nucleotide bases in order to study the kinetics between two complementary particles. Specifically, we explore the effect of temperature, DNA grafting density, and length of the linker sequence on the rates binding and unbinding, with a particular focus on how these factors could be used as tuning parameters for the design of materials which can assemble into desired ordered structures. Our results should help tune assembly conditions and obtain desired crystal lattices unhindered by kinetically arrested amorphous or undesired structures.

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