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Langevin Dynamics Simulation of DNA Condensation Induced by Nanoparticles in Confinement GUO-JUN LIAO, Department of Physics, National Taiwan University, Taipei, 10087, Taiwan, R.O.C, YENG-LONG CHEN, Institute of Physics, Academia Sinica, Taipei, 11529, Taiwan, R.O.C. — We study nanoparticle-induced DNA condensation in a confined suspension of dilute DNA molecules and ideal nanoparticles (NPs) with Langevin dynamics simulation. DNA condensation has been observed in a solution of dilute DNA molecules (persistence length $P \approx 50$ nm) and high concentration of electrostatically neutral NPs (diameter $d \approx 5$ to 35 nm) in recent experimental measurements. It is believed that NPs entropically induce an attraction between DNA segments. For NPs much smaller than P, a DNA molecule can be considered as a chain of connected rods, and the NP-induced depletion attraction between DNA segments can be regarded as rod-rod attraction. Thus, the strength of the depletion attraction is proportional to the number of persistence length in a DNA chain, $N = L/P$, the depletion volume NP^2d, and the NP density ρ, where L is the DNA contour length. In slit confinement, DNA conformation changes are much different from in an unconfined environment. The height of the slit relative to the NPs size (H/d) strongly influences the DNA conformation. For $H/d \approx 1$, DNA size decreases monotonically as ρ increases, while non-monotonic dependence happens for $H/d \approx 5$, due to the competition between DNA-DNA, DNA-NP, and NP-wall interactions.

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