

Abstract Submitted
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DNA-DNA interaction inside bacteriophage modulated by multivalent counterions TOAN NGUYEN, SEIL LEE, TUNG LE, Georgia Institute of Technology — The problem of inhibiting viral DNA ejection from bacteriophages by multivalent counterions, especially Mg^{+2} counterions, is studied. Experimentally, it is known that MgSO_4 salt has a strong and non-monotonic effect on the amount of DNA ejected. There exists an optimal concentration at which the least DNA is ejected from the virus. At lower or higher concentrations, more DNA is ejected from the capsid. We propose that this phenomenon is the result of DNA overcharging by Mg^{+2} multivalent counterions. As Mg^{+2} concentration increases from zero, DNA net charge changes from negative to positive. The optimal inhibition corresponds to the Mg^{+2} concentration where DNA is neutral. At lower/higher concentrations, DNA genome is charged. It prefers to be in solution to lower its electrostatic self-energy, which consequently leads to an increase in DNA ejection. Our theory fits experimental data well. The strength of DNA - DNA short range attraction, mediated by Mg^{+2} , is found to be - 0.003 kBT per nucleotide base. Results from expanded ensemble Monte-Carlo simulation of hexagonal DNA bundles are discussed and are shown to be in good agreement with theoretical results.

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