Biophysical Journal, Volume 96

Supporting Material

Molecular Renormalization Group Coarse-Graining of Polymer Chains: Application to Double-Stranded DNA

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Supplemental Information: Molecular Renormalization Group Coarse-Graining of Polymer Chains: Application to Double-Stranded DNA

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Supplemental Materials

	Intra-strand		*Inter*-strand (*fan*)										
	Bond	**Angle**	**5p**	**4p**	**3p**	**2p**	**1p**	**bp**	**1m**	**2m**	**3m**	**4m**	**5m**
K_1	2.475	10.1	0.29	0.06	0.053	0.0064	0.69	2.68	0.158	0.0005	0.0007	0.0005	0.095
K_2	-0.983	1.99	0.06	-0.012	-0.04	-0.032	-0.137	-0.085	-0.052	-0.032	-0.017	-0.0032	-0.018
K_3	0.126	4.99	0.005	0.0007	0.004	0.0057	0.028	0.025	0.005	0.005	0.0025	0.0013	0.0047

Table 1: Optimized parameters for the coarse-grained DNA Hamiltonian defined by polynomials in Eqs.(2) are shown. Intra-starnd bond and bending angle potentials describe the polymeric interactions within each of the DNA strands. Inter-strand interactions are described by the *fan* potential representing the set of constraints among two polynucleotides to maintain the desired DNA structure (see Fig. 1 in the main text). These include, in particular, base pair interactions (denoted as "bp"), as well as the interactions among the given bead located on one strand and a series of beads located on the other strand (denoted as "1..5p" and "1..5m" and corresponding to beads $[(N \pm 1..5) - i]$ in notations of Fig. 1). Parameters K_1 and K_2 and K_3 for all types of interactions, aside from the bending angle potential, are given in units of [kcal/mol·Å^{-2}], [kcal/mol·Å^{-3}] and [kcal/mol·Å^{-4}], respectively. Analogous parameters for bending angle potential are measured in units of [kcal/mol·rad^{-2}], [kcal/mol·rad^{-3}] and [kcal/mol·rad^{-4}], respectively.