DNA elasticity from coarse-grained simulations: the effect of groove asymmetry

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It is well-established that many physical properties of DNA at sufficiently long length scales can be understood by means of simple polymer models. These models neglect most of the chemical details of DNA and reduce it to a continuous inextensible rod that exhibits resistance to bending and twisting deformations. The simplest such model is the twistable worm-like chain (TWLC) that treats those deformations independently. However, recently it was shown that some discrepancies between experimental results and theoretical predictions obtained with the TWLC can be resolved by introducing a twist-bend coupling into the energy functional of the TWLC. This coupling was predicted to be a direct consequence of a molecular asymmetry of the DNA duplex, but due to the notorious difficulty of its experimental exploration very little information about its strength relative to the more explored bending and torsional stiffnesses is available in the literature. In the present work the origin of this coupling is explicitly explored by means of molecular dynamics simulations of oxDNA, a coarse-grained model of double stranded DNA. It is shown that solely the molecular asymmetry without any further assumptions gives rise to a very substantial contribution of twist-bend coupling in this model. Our analysis is based on the calculation of the covariance matrix of equilibrium deformations, from which the stiffness parameters are obtained. Furthermore, it is shown how the introduction of twist-bend coupling can naturally explain the large variations on experimental estimates of the intrinsic torsional stiffness performed in the past.

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