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Role of Internal conformation in the coupled deformation of DNA

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The mechanical response of DNA to external forces reveals several anomalous features, including the coupling between twisting and stretching and the unusually large deformation of specific sequence motifs. In this work, I present a theoretical model that incorporates both classical deformation modes of the DNA double helix (stretching, bending and twisting) and an internal conformational degree of freedom associated with sugar ring mobility. It is shown that this internal conformational component plays a key role in the coupled deformation of DNA and can explain the experimentally observed change in the sign of the twist–stretch coupling under applied force. The model also provides a natural interpretation of the unusually large deformation observed in the TATA-box fragment. These results highlight the importance of internal conformational dynamics for understanding anomalous mechanical behavior of DNA.

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