Abstract Submitted
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A theoretical investigation of the interconversion between B and Z-DNA using the Adaptively Biased and Steered Molecular Dynamics methods MAHMOUD MORADI, CHISTOPHER ROLAND, VOLODYMYR BABIN, CELESTE SAGUI, CHiPS and Department of Physics, North Carolina State University — The transition between right-handed B-DNA and left-handed Z-DNA in an implicit solvent environment was investigated via the free energy landscape of DNA as a function of the collective variables of handedness and radius of gyration, using the recently developed Adaptively Biased Molecular Dynamics (ABMD) method. The ABMD method, which belongs to the general category of umbrella sampling methods with a time-dependent potential, allows for an efficient and accurate estimation of the free energy barriers associated with the transition, especially when combined with multiple-walker and umbrella correction runs. The ABMD results are compared to those obtained using the Steered Molecular Dynamics (SMD) method. The implication of all these free energy results on the microscopics of the B to Z-DNA transition is to be discussed.

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