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An investigation of the structural transitions between different forms of DNA using the Adaptively Biased (ABMD) and Steered Molecular Dynamics Methods MAHMOUD MORADI, VOLODYMYR BABIN, CHRISTOPHER ROLAND, CHiPS and Department of Physics, North Carolina State University, THOMAS A. DARDEN, National Institute of Environmental Health Sciences (NIEHS), CELESTE SAGUI, CHiPS and Department of Physics, North Carolina State University — Left-handed A-DNA and B-DNA along with right-handed Z-DNA, are believed to be the three main biologically active double-helix structures associated with DNA. The free energy differences associated with the A to B-DNA, and B to Z-DNA transitions in an implicit solvent environment have been investigated using the recently developed Adaptively Biased Molecular Dynamics (ABMD) method, with the RMSD as the collective variable associated with the former transition, and handedness and radius of gyration as the collective variables associated with the latter. The ABMD method belongs to the general category of umbrella sampling methods with a time-dependent potential, and allows for an accurate estimation of the free energy barriers associated with the transitions. The results are compared to those obtained using the Steered Molecular Dynamics method, and ultimately are used in order to gain insight into the microscopics of the DNA transitions.

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