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5-Methylation of Cytosine in CG:CG Base-Pair Steps: A Physicochemical Mechanism for the Epigenetic Control of DNA Nanomechanics
TAHIR YUSUFALY, WILMA OLSON, Rutgers University, YUN LI, Delaware Valley College — Van der Waals density functional theory is integrated with analysis of a non-redundant set of protein-DNA crystal structures from the Nucleic Acid Database to study the stacking energetics of CG:CG base-pair steps, specifically the role of cytosine 5-methylation. Principal component analysis of the steps reveals the dominant collective motions to correspond to a tensile "opening" mode and two shear "sliding" and "tearing" modes in the orthogonal plane. The stacking interactions of the methyl groups are observed to globally inhibit CG:CG step overtwisting while simultaneously softening the modes locally via potential energy modulations that create metastable states. The results have implications for the epigenetic control of DNA mechanics.

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