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A Density Functional Theory Examination of the Local Conformational Energetics of Normal and Epigenetically Modified Duplex DNA
TAHIR YUSUFALY, Department of Physics and Astronomy, Rutgers University, Piscataway, NJ, WILMA OLSON, Department of Chemistry, Rutgers University, Piscataway, NJ — We report density functional theory calculations of various local regions of duplex DNA, including hydrogen bonded base pairs, stacked nearest-neighbor bases, and sugar-phosphate backbones. Special attention is given to the methylation of 5-cytosine, an epigenetic modification believed to play a key role in eukaryotic gene regulation. Energetically stable molecular conformations are identified and their elastic properties analyzed. Our results are compared with previous ab initio studies and high-resolution crystalline structural data.

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