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Dynamics of A-B transition of the DNA double helices HAO WANG, THOMAS CHEATHAM, PETER GANNETT, JAMES LEWIS, Department of Physics, West Virginia University, Morgantown, WV 26506 — The conformational transitions of DNA and the sensitivity of DNA structure to the surrounding environment are very relevant to its chemical and biological function and potential applications in nano-technology. Different conformations of DNA, even with the same sequence, exhibit different electronic structures, resulting in different conduction properties. We present theoretical work on the dynamical features of electronic states in the A-B transition of a model DNA duplex of d$(CGCGCGCGCG)_2$ (10 base-pairs, 628 atoms) as the molecule undergoes conformational changes and thermal fluctuations at room temperature. We couple state-of-the art empirical force field molecular dynamics (MD) simulations with an *ab-initio* electronic structure method based on density-functional theory, called FIREBALL. For the A-B transition, we calculated the effects of conformational change on the electronic structure for each snapshot obtained from nanosecond MD simulations.

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