

## **Determination of the DNA Deformability Matrix on the Trinucleotide Level which Reveals the Coupling Strength of All the Base Movements**

\*M. Bagherpoor Helabad<sup>1</sup>, D. Norouzi<sup>2</sup>

<sup>1</sup>*Free University of Berlin, Physics, Berlin, Germany*

<sup>2</sup>*Institute for Advanced Studies in Basic Sciences(IASBS), Zanjan, Islamic Republic of Iran*

The mechanical deformability of DNA is sequence-dependent and plays important role in various biological processes such as packaging, gene regulation, and perhaps in all protein-DNA interactions. X-ray crystallography, NMR spectroscopy, and molecular dynamics simulation data confirmed that the mechanical response of DNA to external interactions depends on the sequence content. Here, with using all-atom Molecular Dynamics simulation, we aim to investigate sequence dependent mechanics in trinucleotide level. we derived base-pair step parameters for every trinucleotide step and tested sequence dependent characteristics of base pair step parameters and their relationship to features of DNA structure. Our results show more detailed coupling between inter and intra base-pair parameters. Also Coupling coefficients indicate significant values for adjacent base pairs.