Abstract Submitted
for the OSS17 Meeting of
The American Physical Society

Interplay of electric fields and strain effects on charge transport through DNA molecules YONG JOE, ERIC HEDIN, Ball State University, SADEQ MALAKOOTI, The University of Texas at Dallas — The combination of electric field effect and small mechanical strain perturbations is studied in the electron transport calculations of the poly(G)-poly(C) double-stranded (ds) DNA molecular electronic structure. We use an advanced two-dimensional tight-binding model including hopping integrals of the next nearest-neighbors and the implementation of strain-dependent DNA helix conformation in conjunction with the theories of Slater-Koster and linear elasticity. Determining on-site energies of each base and coupling parameters based on these effects, the transport properties of a 30 base-pair ds-DNA molecule tilted with respect to the inter-contact electric field direction with a mechanical strain are investigated. Specifically, we present single electron transmission spectra and current-voltage characteristics as functions of electron energy and source-drain voltage for both selected tilted angles and percentage strains.

Yong Joe
Ball State University

Date submitted: 06 Apr 2017 Electronic form version 1.4