Abstract Submitted
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A DFT look at transport properties of Graphene nano-ribbons coupled to DNA Base pairs[1] JACOB GAYLES, LUIS AGAPITO, CHRISTIAN WOLOWEIC, NICHOLAS KIOUSSIS, Deparment of Physics and Astronomy, California State University Northridge — This study investigates the electronic structure and transport properties of DNA base pairs coupled to reconstructed zigzag edge Graphene Nano-Ribbons (z-GNRs PRL 101, 115502 (2008)[1]). *Ab initio* electronic structure calculations show reconstructed z-GNR to be more stable compared to the unreconstructed[1]. By cleaving these metallic reconstructed ribbons, we create two graphene electrodes separated by a 5 Å wide gap. The DNA base pair is then coupled to the graphene electrodes and relaxed using density functional theory. Transport properties are calculated in the ATK commercial packages (Atomistix ToolKit version 7.0, QuantumWise A/S). We compare tunneling currents for different base pairs, at finite biases. Understanding transport properties of the base pairs will potentially benefit areas such as DNA sensors and DNA sequencing.

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