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Ab initio modeling of electronic properties of DNA: Comparison to experiments JIANQING QI, University of Washington, SURANGA EDIRISINGHE, Georgia State University, ANANT ANANTRAM, University of Washington — In this work, we model the zero-bias conductance for four DNA strands that were used in Ref. [1]. Our approach consists of three elements: (i) experimental data, (ii) ab initio calculations of DNA and (iii) two parameters to determine the decoherence rates. We find that the coherent conductance is much smaller than the experiments [2]. To understand the reason, we look at the effect of decoherence. By including decoherence, we show that our model can rationalize the measured conductance of the four strands. We find that decoherence on $G:C$ base pairs is crucial in getting agreement with the experiments. However, the decoherence on $G:C$ base pairs alone does not explain the experimentally determined dependence of conductance in strands containing a number of $A:T$base pairs. Including decoherence on $A:T$ base pairs is also essential. By fitting the experimental magnitudes of the conductance for the four DNA molecules, we estimate for the first time that the deocherence rate is 6 meV for $G:C$ and 1.5 meV for $A:T$ base pairs. [1] Ajit K Mahapatro, et al., Nanotechnology, **18**, 195202 (2007) [2] Jianqing Qi, et al. http://www.ee.washington.edu/faculty/anant/publications/JianqingQiPaper.pdf.

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