

Abstract Submitted
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Optical conductivity of wet DNA¹ ARND HUBSCH, UC Davis, ROBERT G. ENDRES, NEC Laboratories, DANIEL L. COX, RAJIV R.P. SINGH, UC Davis — DNA has attracted much attention in view of its possible application to nano-devices, both for device scaffolding and assembly as well as its potential as a molecular electronics component. Despite extensive efforts, however, the experimental and theoretical understandings of the conductivity of DNA are still rather controversial. Motivated by recent experiments [1] we have studied the optical conductivity of DNA in its natural environment containing water molecules and counter ions. Our density functional theory calculations (using SIESTA) for four base pair B-DNA with order 200 surrounding water molecules suggest a thermally activated doping of the DNA by water states which generically leads to an electronic contribution to low-frequency absorption. The main contributions to the doping result from water near DNA ends, breaks, or nicks. [1] E. Helgren, A. Omerzu, G. Gruner, D. Mihailovic, R. Podgornik, and H. Grimm, cond-mat/0111299.

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