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The Electronic Structure of Wet DNA RICHARD MARSH, HAO WANG, JAMES LEWIS, Brigham Young University — Currently there is vast interest in the field of nanotechnology. One particularly unique aspect is molecular electronics; the ability to take a single molecule and use it as a device (e.g. transistor). The structure and functionality of DNA make it a great potential for nanowire templates. Previous efforts have yielded the electronic properties of both the poly (A)-poly (T) and poly (G)-poly(C) DNA molecules. We continue this work by calculating the electronic structure of the DNA while taking into account surrounding solvation effects. We consider the electronic structure of DNA with varying solvation layers. This system contains over a thousand atoms and is the first ab initio calculation of wet DNA of this magnitude. Our results for both poly (A)-poly (T) and poly (G)-poly(C) DNA molecules will be presented.

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