Unravelling the Structure of Silver-Mediated DNA Homopolymers using ab initio Computational Tools

Leonardo Espinosa[1], Alexander Karpenko[1], Steven M. Swasey[2], Elisabeth G. Gwinn[3] and Olga Lopez-Acevedo[1]
[1] COMP Centre of Excellence, Department of Applied Physics, Aalto University, P.O. Box 11100, 00076 Aalto, Finland [2] Department of Chemistry and Biochemistry, University of California, Santa Barbara, Santa Barbara, California 93106, United States [3] Department of Physics, University of California, Santa Barbara, Santa Barbara, California 93106, United States

We present computational and experimental studies of highly stable silver-mediated DNA homopolymers with promising applications for DNA nanotechnology and biomedical sciences[1, 2]. Experiments with base replacements showed the stability of the silver-mediated cytosine (cytosine-Ag+-cytosine) in both parallel[3] and antiparallel[4] duplexes. Using Electrospray Ionization Mass Spectrometry in combination with different ab initio techniques we have found evidence of a novel stable guanine-Ag+-guanine conformation in a non-canonical Watson-Crick pairing[5]. Moreover, a direct comparison between experimental data and calculations of Electronic Circular Dichroism (ECD) spectra within the Time Dependent Density Functional Theory (TDDFT) framework has allowed us to elucidate the representative three-dimensional geometries for both stable mediated homopolymers. Through the analysis of the final structures, we report the presence of a new interplanar type of hydrogen-bond interactions[6].

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