Silver ions are recognized biocidal agents that are able to kill bacteria with long-term mechanisms [1]. There are presently many open questions related to the complex formed by interacting silver ions and biomolecules. The research questions range from the basic geometries to the health risks such nanotechnology pose. Determining the structure of silver mediated DNA complexes will help the collective effort to answer these questions.

Silver-nucleobase pair interactions are two to three times larger than the conventional hydrogen-bond pair interaction. Such high stability can drive the formation of helices and higher-order structures driving also the possibility to design novel DNA-based nanomaterials. Indeed, nucleobases and noble metal atoms (Au,Ag) have a wide range of possible interacting sites depending on both the metal charge (ion, cation or neutral) and chemical nature [2]. We found that silver cations are able to drive the formation of duplexes from DNA homobase strands in configurations away from the expected Watson-Crick ones [3] and through novel interplanar hydrogen bonds [4]. I will overview the solvent and size-dependent electronic and optical properties of these silver-DNA structures obtained by Density Functional Theory and I will discuss the accuracy of the different computational methods used in our studies.

Figure 1: Solvated Ag⁺-bridged cytosine tetramers. The interplanar H-bonds are highlighted with a green dashed line