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DNA base pairing by noble metal cations: Structure and electronic properties from Density Functional Theory

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Metallo-base 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 with the possibility to design novel DNA-based nanomaterials [1]. Nucleobases and noble metal atoms (Au,Ag) have wide range of possible interacting sites depending on both the metal charge (ion, cation or neutral) and chemical nature [2]. I will overview the electronic properties, both ground state and optical, of metallo-DNA structures obtained by global optimization and Density Functional Theory, discussing the effect of pairing and inclusion of backbone on the metal-base elementary unit.

[1]T. Biver **Coordination Chemistry Reviews** 257 (2013) 27-65
[2]L. Espinosa Leal and O. Lopez-Acevedo, **Nanotechnology Reviews** to appear 2015, arXiv.1403.3494