Abstract Submitted
for the MAR10 Meeting of
The American Physical Society

Energetics and electronic structure of M-DNA[1] SIMONE ALEXANDRE, Depto de Física - UFMG - Brazil, JOSÉ SOLER, UAM - Madrid, FÉLIX ZAMORA, Depto Química - UAM - Madrid — Charge transport in DNA is currently an open issue, that has defied both theory and experiments. An important possibility is the introduction of a transition metal atom into the DNA structure, forming the so-called M-DNA, in attempt to produce a DNA with a metallic bandstructure. In the present work we investigate the incorporation of zinc into the DNA, at three different sites: (i) in the major groove in the crosslink position; (ii) in the minor groove in the crosslink position; (iii) bound to the N(7) of the guanine. We find that the most stable position is the third altrenative, where the Zn atom is bound to the guanine. For the electronic structure, we find that while the most stable position presents the larger band gap (∼2.2 eV within GGA-DFT). No such trend is found between band gap and stability for the other alternatives: the crosslink positon in the major groove is a more favorable site than in in the minor groove, but with a smaller band gap. These results corroborate our previous finding of a strong metal-site dependence of the electronic and magnetic properties of M-DNA [1].

[1] S. S. Alexandre *et* al., PRB 73, 205112 (2006).

[1]Support from CNPq and Fapemig.

Simone Alexandre
Depto de Física - UFMG - Brazil

Date submitted: 14 Dec 2009 Electronic form version 1.4