*Poster*

# SINGLE CHAINS OF A ONE-DIMENSIONAL COORDINATION POLYMER.

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In the search of molecular wires suitable for the construction of nanocircuits several molecules have been considered as feasible candidates with this goal. However, single wall carbon nanotubes (SWCNT) are probably the best option mainly due to their excellent conductor properties. But their difficult synthesis and poor chemistry play against the use of this material. Another candidate that has been extensively studied is the DNA molecule. This stable polymer can be easily handled, produced, modified and its structure properties make it as very appealing molecular wire [1]. DNA seems to be a poor electrical conductor [2], however it is possible that other structures that use DNA bases with incorporated metal ions as building blocks (M-DNA) [3, 4], are suitable for nanoelectronics.

In this context, we have recently focused in the use of one-dimensional polymers containing metal ions and organic fragments. Coordination polymers are infinite aggregates of metal ions bridged by organic ligands. They self-assemble by coordination bonding in one, two or three dimensions (1D, 2D and 3D) [5]. The key to the design of desirable polymer architecture is the selection of the molecular building blocks, which also determine the properties of the resulting materials. Among other properties, these compounds form porous materials and polymer magnets, and they present chromism, nonlinear optical properties, redox properties and electrical conduction [5-7]. However, the application of coordination polymers in many fields is limited by their restricted processability, as a consequence of their lack of solubility, rapid degradation in solution and, in some cases, decomposition upon heating [6]. The studies relative to conduction are very scarce and limited to the macroscopic scale [8]. Coordination polymers have been successfully employed to produce two-dimensional nanoarrays characterized by AFM [9] and STM [10, 11]. 1D coordination polymers are of special interest for nanotechnology because individual chains of these polymers can be used as molecular wires, with a number of advantages over other materials such as carbon nanotubes [12].
The structure of monodimensional nucleobase-coordination polymers may show similarities with that of DNA. The $[Cd(6\text{-}MCP)_2{\cdot}2H_2O]_n$ (6-MCP= 6-mercaptopurinate) is a particularly relevant 1D coordination polymer because it is a simple polymer with important similarities with DNA-based systems. Mercaptopurine is a thiopurine derivative whose structure is closely related to that of oxoderivative guanine, since they differ only in the heteroatom at position 6 and the absence of a $NH_2$ group at position 2 for the mercaptopurine (Fig. 1a). The $[Cd(6\text{-}MCP)_2{\cdot}2H_2O]_n$ polymer is formed as a sequence of mercatopurinate linked by cadmium ions in a self assembly process (see Fig. 1a). This structure, while preserving many of the features of M-DNA nanowires, is much simpler and allows affordable modeling with *ab initio* techniques (Fig. 1b).

This work presents a simple method to obtain individual chains from $[Cd(6\text{-}MCP)_2{\cdot}2H_2O]_n$ which can be suitable for nanotechnology devices. In summary, we have been able to obtain single polymeric chains from crystals of $[Cd(6\text{-}MCP)_2{\cdot}2H_2O]_n$ by simple procedures and we have characterized them extensively by AFM. The mechanical and electrical properties of these single chains have been studied. We have shown that both the Cd and the Zn based

polymers are insulators, suggesting that the inclusion of metals in DNA-based wires does not necessarily imply conductance. The results on this compound, as well as other experiments under progress in our laboratory with different coordination polymers, indicate that the methodology used for making single chains is quite general and could be also employed for other coordination polymers. Furthermore, ongoing calculations, using the same methodology with other metal ions such as $Fe^{III}$, indicate that some of these compounds can be conductors. To the best of our knowledge this is the first time that single chains of a coordination polymer have been isolated and characterized, and it clearly opens a route for future nanotechnological applications of this kind of polymers. The final goal of this research project will be the construction of nanocircuits based on these molecular wires.

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**Figure 1.** (a) Schematic representation of DNA and $[Cd(6\text{-}MCP)_2]_n$. (b) Scheme of the structure and spacefill model of $[Cd(6\text{-}MCP)_2]_n$. (c) First stages of polymer processing after soft centrifugation. (d) Individual polymer chain at the end of the treatment. The size of the individual chain, measured with AFM, is in good agreement with X-ray diffraction data.