MOLECULAR WIRES WITH NEW PROPERTIES FOR NANO-ELECTRONICS APPLICATIONS

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Abstract:

Molecular junctions (MJ) with molecular self-assembled monolayers (SAM) (Figure 1a) may bring a tangible response to the achievement of electronic system miniaturization with specific molecular design[1].

Although, the conductance of MJ is in principle controlled by the frontier orbitals (FO) correlated to the molecular scaffold, FO pinning to electrodes levels-off the orbital energy levels and results in similar conductance values for SAM of electron rich or poor molecules in a given series[2]. In this first part we present our molecular design and the synthesis of molecules that will allow us to study in depth the pinning effect in SAM by varying the anchoring group of the molecule with its FO energy levels (Figure 1b).

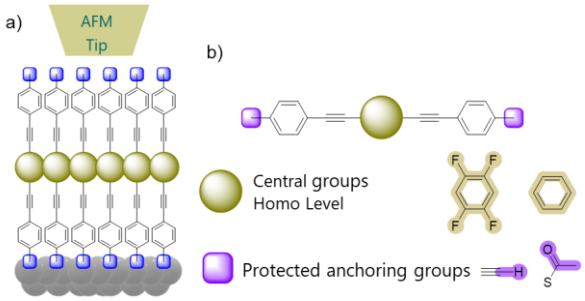

Figure 1 : a) SAM representation. b) New molecular wires for pinning effect investigation.

Importantly, it is well-known that MJ cannot currently compete in terms of electrical conductance with silicon-based technologies. However, *via* dedicated organic molecular systems, new original functionalities could be introduced like thermoelectric behaviour or negative differential resistance (NDR) [3], the latter being characterized by a decrease of intensity with voltage increase at some point.

Theoretical calculations indicated that insertion of silicon atoms within the conjugated path of a molecular wire may result in pronounced NDR effect, through silicon hyperconjugation. Therefore, we choose to add silane and disilane functions to an organic molecular wire in order to break the π-conjugation by allowing hyperconjugation of the silicon with the π-conjugated part. It is anticipated that the second one will increase conductivity with respect to the first one while maintaining the NDR properties of the molecular wires (Figure 2) which synthesis will be described.

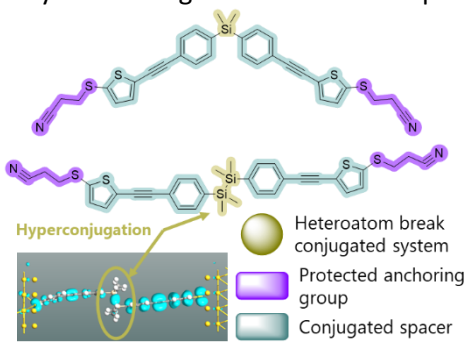

Figure 2 : Molecular wire for NDR effect.

References

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