Progress towards a single SWAP molecule with Ruthenium complexes: DFT study on a gold surface

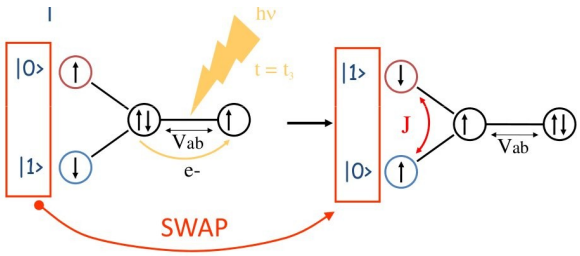
S. García-Gil[1], J. Bonvoisin, X. Bouju

[1]CEMES-CNRS; 29 rue Jeanne-Marvig,F-31055 Toulouse, France
sandra.garcia-gil@cemes.fr

The idea of embedding molecules in between electrodes to make an electronic device that could perform the basic functions of digital electronics begin in the 70's . Due to the intrinsic difficulties of connecting one molecule to another to make complete circuits, it was proposed [1] to use just a single molecule: “mono-molecular electronics” which could integrate the hole circuit.

One possibility to arrive to these “mono molecular circuits” is to divide the molecule in “qubits” in order to exploit the quantum engineering developed for several years around quantum computers [2].

The project to be developped consists in synthetising a molecule which could be able to realize a logical function such an inversor (SWAP).



This molecular logic gate would be made of Ruthenium (III) and (II) metal centers [3,4,5], which magnetic interaction could be turned on/off by changing the oxidation state of the central molecule using an appropiate light radiation.

It is very important to have a good understanding of the behaviour of the building blocks of the target molecule. In particular we present a DFT study of the building blocks (Ru (II) and Ru (III) complexes) on Au(111) in order to understand the magnetic, electronic and geometrical properties of this complexes. Especially how the ligands can affect the magnetism and transport properties of these metal complexes when adsorbed on surfaces. Some recent experimental STM images on these complexes will also be presented.
This work is part of a collaboration between Univ. Zaragoza-INA and CEMES-CNRS within the TRAIN2 project (Trans-Pyrenees Action on Advanced Infrastructures for Nanosciences and Nanotechnology).

References

[1] C. Joachim, J.K. Gimzewski, A. Aviram, Nature, 2000, 408, J41
[2] M.A. Nielsen, I.L. Chiang, Quantum computation & quantum information, Cambridge University Press 2000.
[3] Synthesis and characterization of bis(bipyridine)ruthenium(II) complexes with bromo and protected ethynyl ß-diketonato ligands. S. Munery, J. Jaud & J. Bonvoisin. Inorg. Chem. Commun.(2008)11,975-977
[4] Synthesis and characterization of ß-diketonato ruthenium(II) complexes with two 4-bromo or protected 4-ethynyl-2,2’-bipyridine ligands. C. Viala & J. Bonvoisin. Inorg. chim. Acta (2010) 363, 1409-1414
[5] Synthesis and characterization of a series of ruthenium tris(ß-diketonato) complexes with UHV-STM investigation and numerical calculations. S. Munery, N. Ratel-Ramond, Y. Benjalal, L. Vernisse, O. Guillermet, X. Bouju, R. Coratger & J. Bonvoisin. Eur. J. Inorg. Chem. (2011), 2698–2705
[6]UHV-STM Investigations and Numerical Calculations of a Ruthenium β-Diketonato Complex with Protected Ethynyl Ligand: [Ru(dbm)2(acac-TIPSA)]Loranne Vernisse, Sabrina Munery, Nicolas Ratel-Ramond, Youness Benjalal, Olivier Guillermet, Xavier Bouju, Roland Coratger, and Jacques Jean BonvoisinJ. Phys. Chem. C, Just Accepted ManuscriptDOI: 10.1021/jp304523f