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# Progress towards SWAP single molecule – A chemical approach

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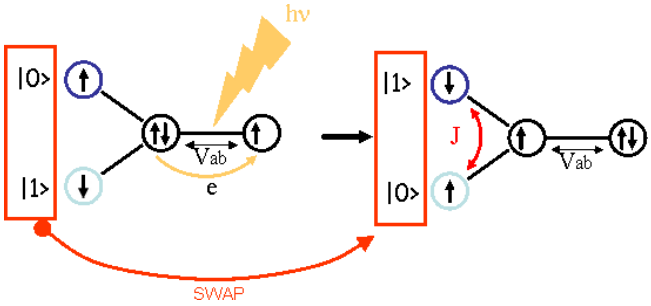
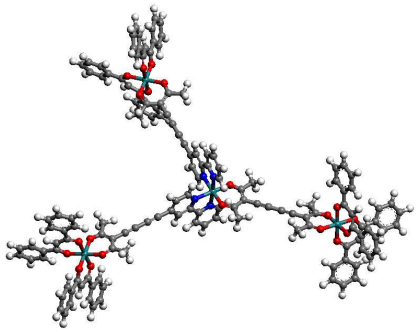
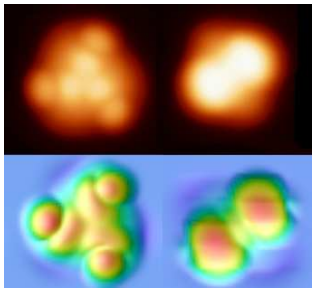
Integrating a logical function in a single molecule should allow reaching the ultimate size of a material based calculator. Several concepts are now under development to make a calculation using a single molecule. [1] One of them is to divide the molecule into "qubits" in order to exploit the quantum engineering developed since several years around quantum computers. [2]




The project developed here consists of synthesizing a molecule which would be able to realize a logical function such as an inversor (SWAP). This molecular logical gate with an optical reset would be made of an IN/OUT ruthenium(III) bimetallic centers. These two ruthenium(III) ions would be in magnetic interaction through bonds, via conjugated organic backbones, with a third ruthenium ion. The magnetic interaction is switched ON and OFF depending on the oxidation state of the central ruthenium atom which can be changed by light by using the special properties of mixed-valent system. Therefore the light will trigger the calculation by adding/removing an extra electron on the central ruthenium atom. The special feature of this target molecule constituted of four metallic centers is that coordination spheres around ruthenium atoms can be different by chosen substituents and then one can have optical access to selected ruthenium atoms.

In this contribution, one will see which steps have been made towards the target molecule[3] In particular, we will show some recent results on STM images concerning ruthenium complexes on gold surfaces. [4]





*Experimental (top) and EHMO-ESQC calculated (bottom) STM image of $Ru(dbm)_3$ adsorbed on Ag(111) surface at liquid helium temperature*

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