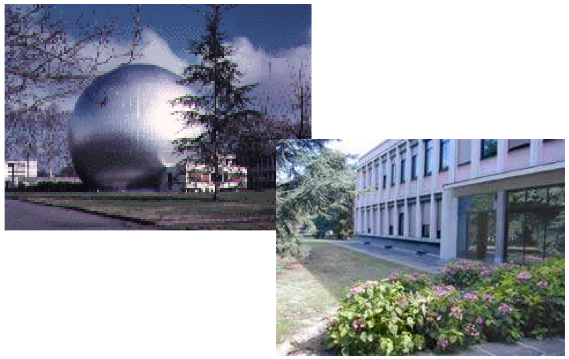


www.cemes.fr/GNS

A controlled quantum SWAP logic gate in a 4-center metal complex

Jacques Bonvoisin

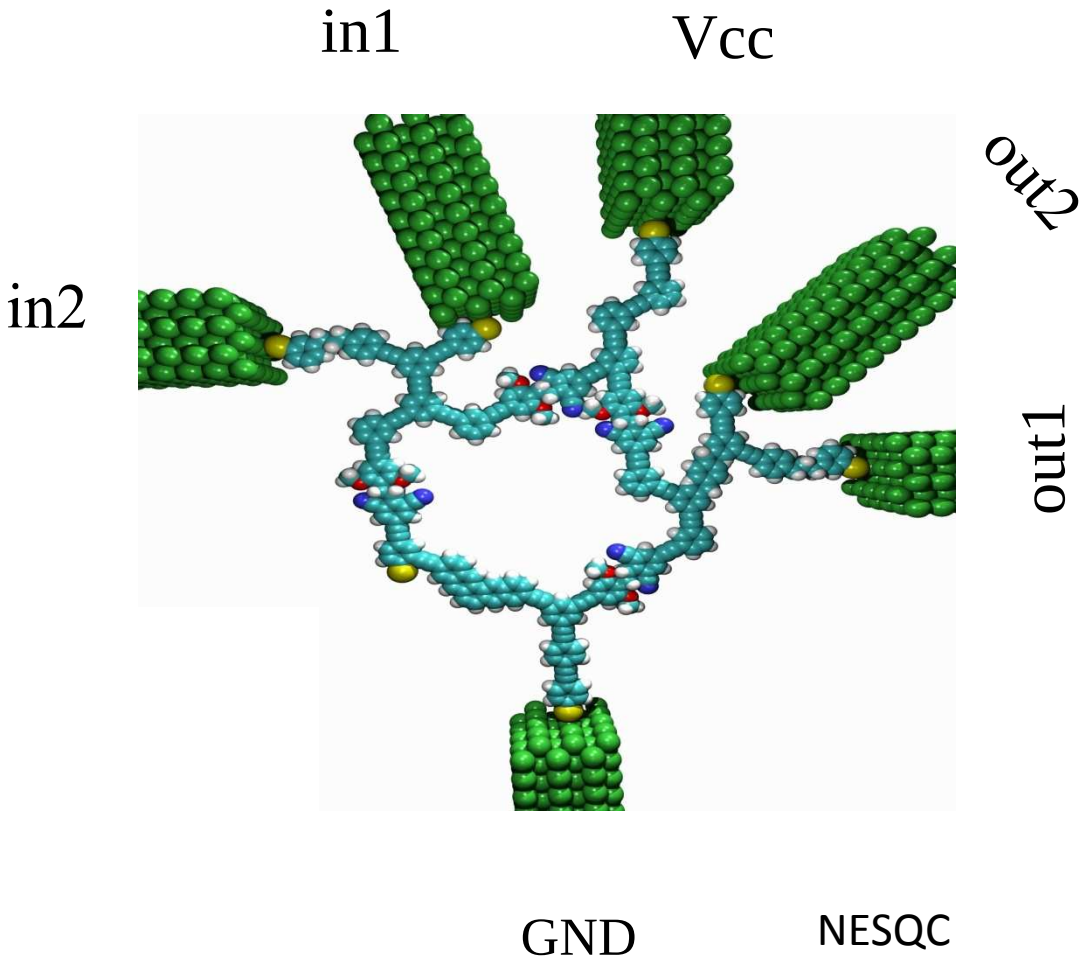
Mohamed Hliwa, Christian Joachim

CEMES – CNRS – UPR 8011

AtMol International Workshop on Architecture & design of Molecule Logic Gates and Atom Circuits
12&13 January 2012 - Barcelona

Calculation on a single molecule ?

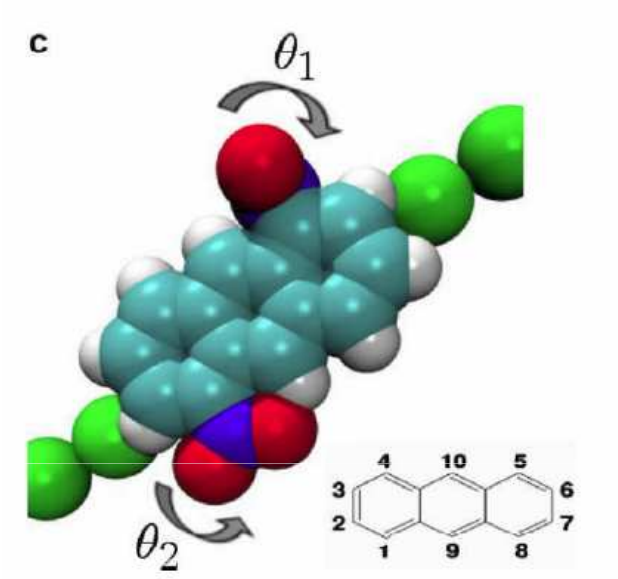
1° To force a molecule to look like a classical electronic circuit…
but integrated inside a single molecule !



S. Ami, M. Hliwa and C. Joachim, Chem. Phys. Lett. 367, 662 (2003)

Calculation on a single molecule ? QHC

2° To use intramolecular dynamical quantum behavior leading to Hamiltonian Quantum Computer !



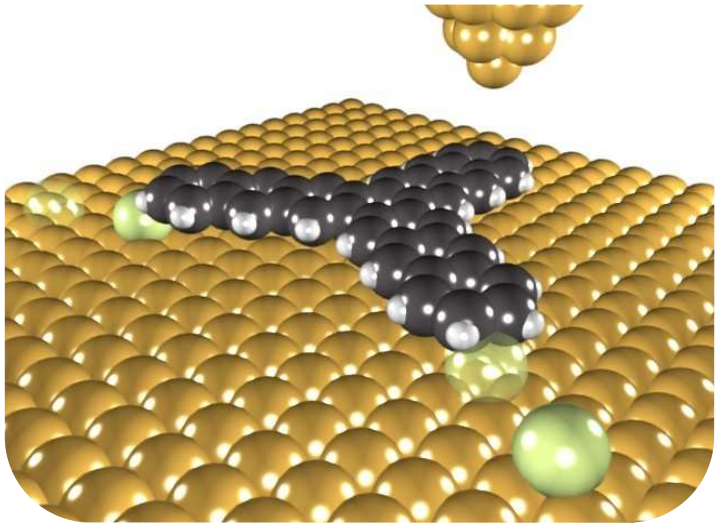
Rotation of functional group

A NOR–AND quantum running gate molecule

N. Renaud [a], M. Ito [b], W. Shangguan [c], M. Saeys [c], M. Hliwa [a,d,*], C. Joachim [a,e]

Inputs (eV)		ω_{ab} (THz)	
α	β	*NOR*	*AND*
0	0	0.3	$5 \cdot 10^{-5}$
0	1	10^{-4}	$2 \cdot 10^{-4}$
1	0	10^{-4}	$2 \cdot 10^{-4}$
1	1	$5 \cdot 10^{-5}$	0.5

CPL 472 (**2009**) 74

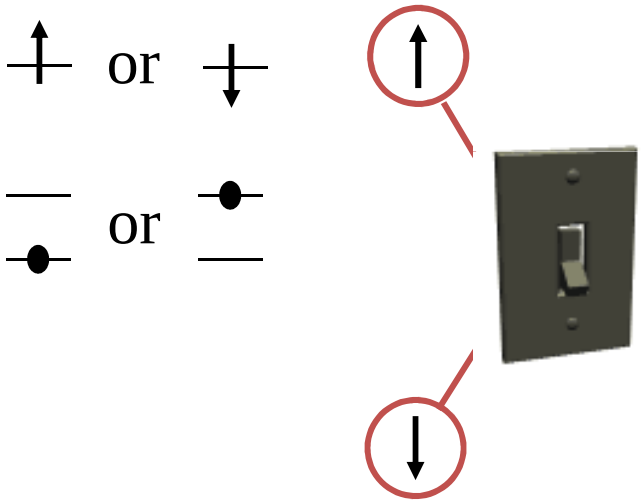


Atoms manipulation on surface

Starphene on Au(111)

PRB 83 **(2011)** 155443; ACS NANO 5 (**2011**) 1436

3° To divide the molecule into "qubits" …



Qubit

$|0\rangle$, $|1\rangle$, $a|0\rangle + b|1\rangle$ with $a^2 + b^2 = 1$

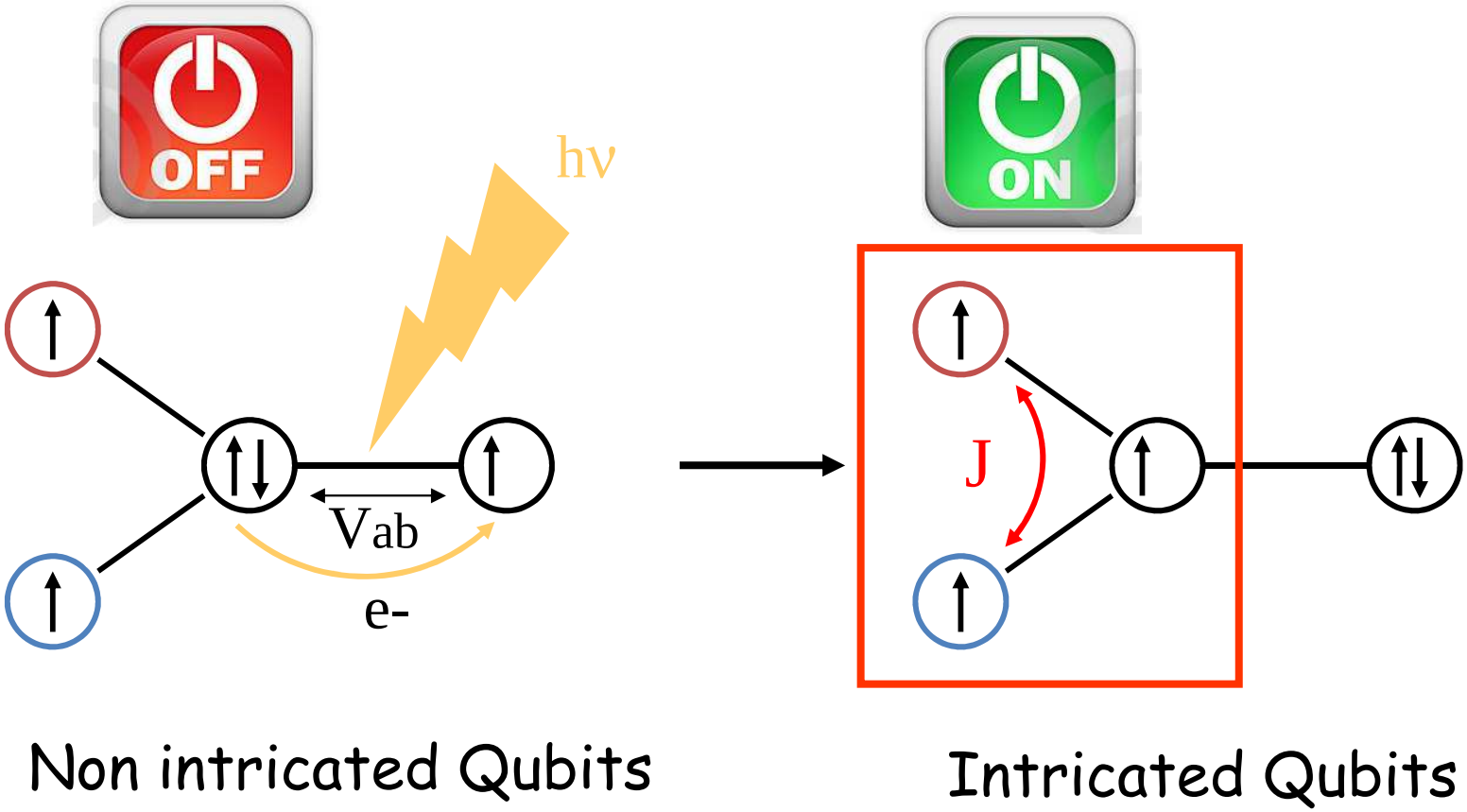
⟶ Intramolecular "temporal" Circuit

Mathematic formulation for the SWAP operation

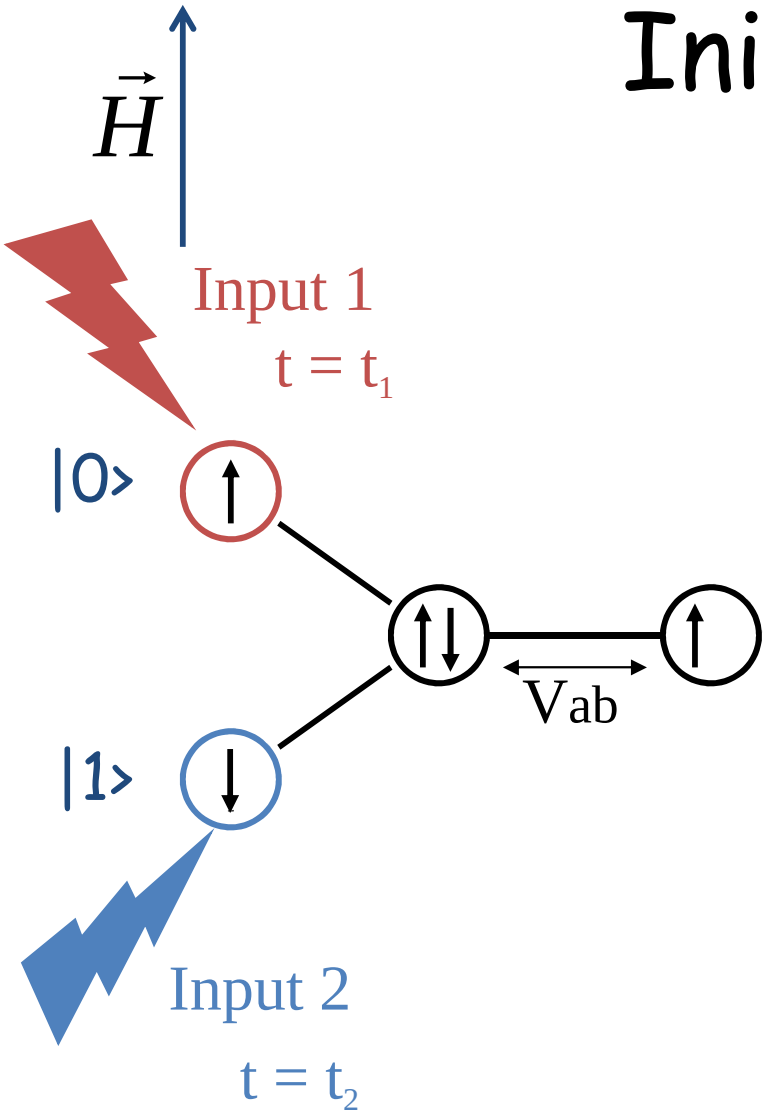
$$U_{DS}\begin{pmatrix} |00\rangle \\ |\mathbf{01}\rangle \\ |\mathbf{10}\rangle \\ |11\rangle \end{pmatrix} = \begin{pmatrix} |00\rangle \\ |\mathbf{10}\rangle \\ |\mathbf{01}\rangle \\ |11\rangle \end{pmatrix} \qquad U_{DS} = \begin{pmatrix} 1\ 0\ 0\ 0 \\ 0\ 0\ 1\ 0 \\ 0\ 1\ 0\ 0 \\ 0\ 0\ 0\ 1 \end{pmatrix}$$

$$\begin{cases} \quad A_0B_0\,|00\rangle + \mathbf{A_0B_1}\,|\mathbf{01}\rangle + \mathbf{A_1B_0}\,|\mathbf{10}\rangle + A_1B_1\,|11\rangle \\ U_{DS} \\ \longrightarrow \quad A_0B_0\,|00\rangle + \mathbf{A_0B_1}\,|\mathbf{10}\rangle + \mathbf{A_1B_0}\,|\mathbf{01}\rangle + A_1B_1\,|11\rangle \end{cases}$$

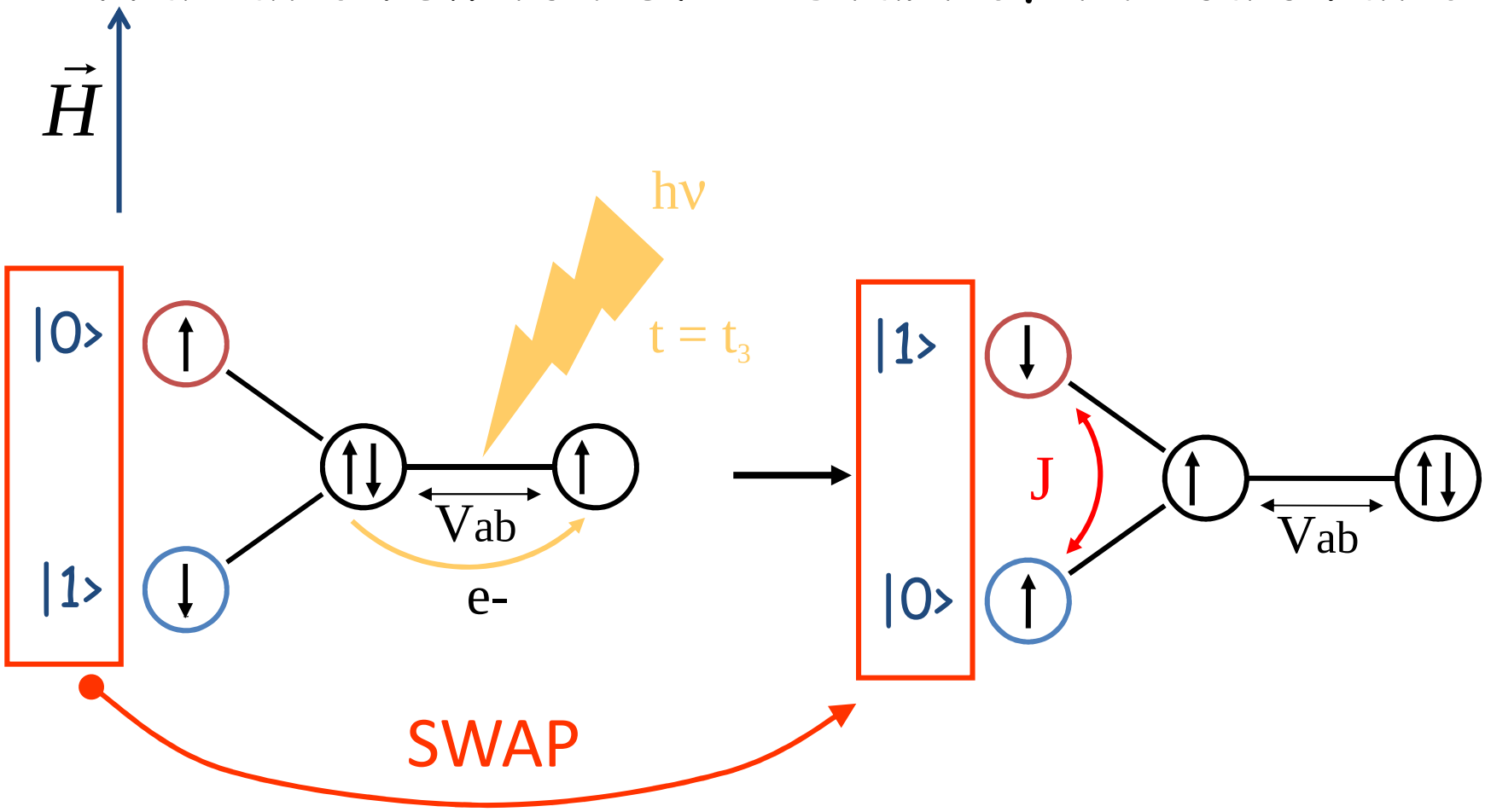
Principle

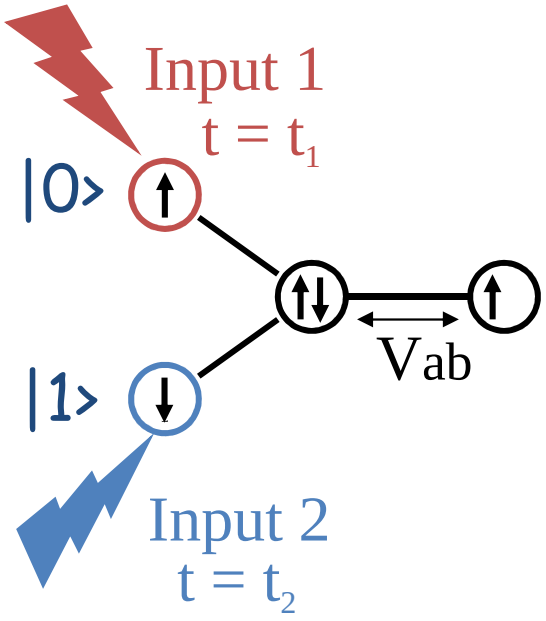


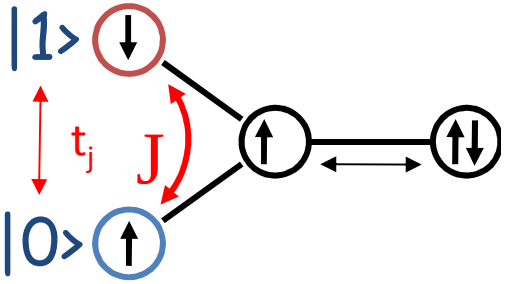
Initialisation

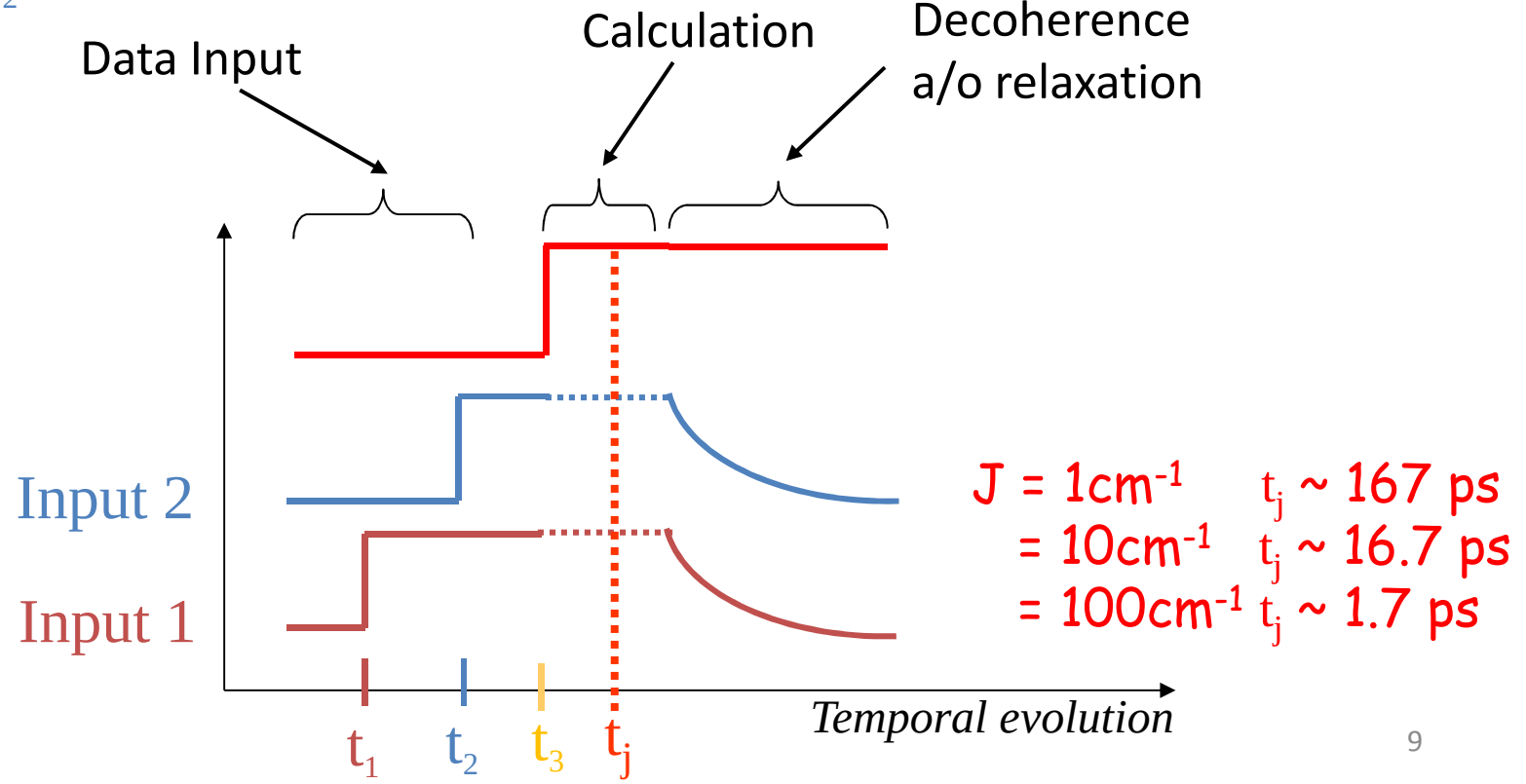


Irradiation switch ON = Start of the calculation



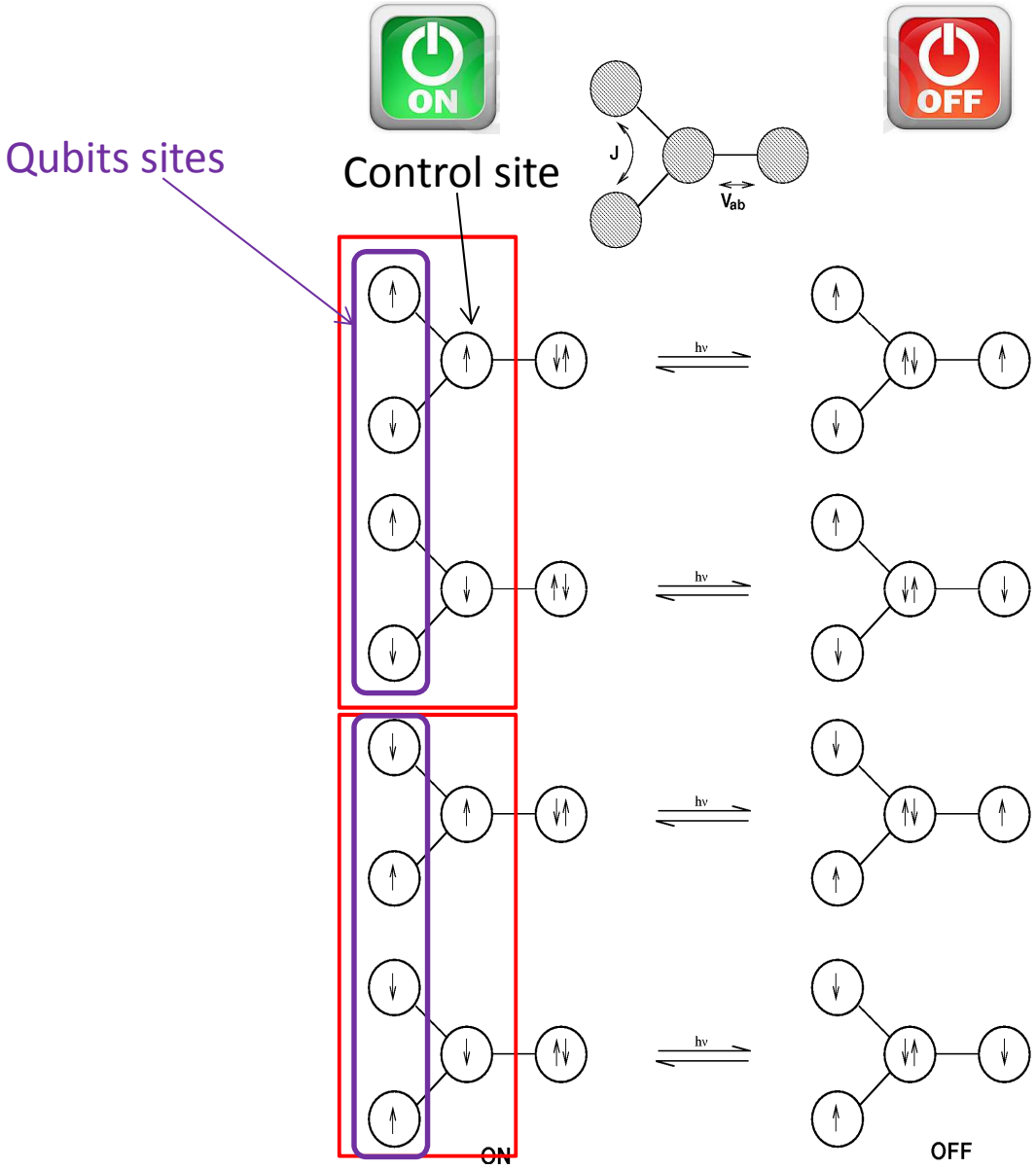




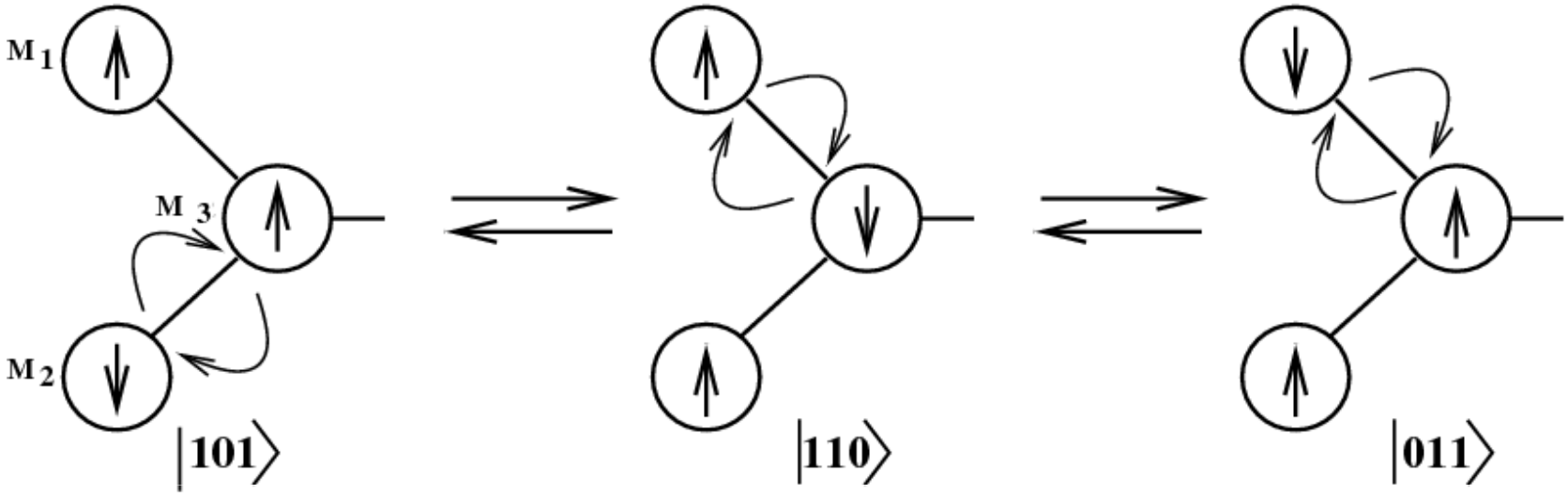


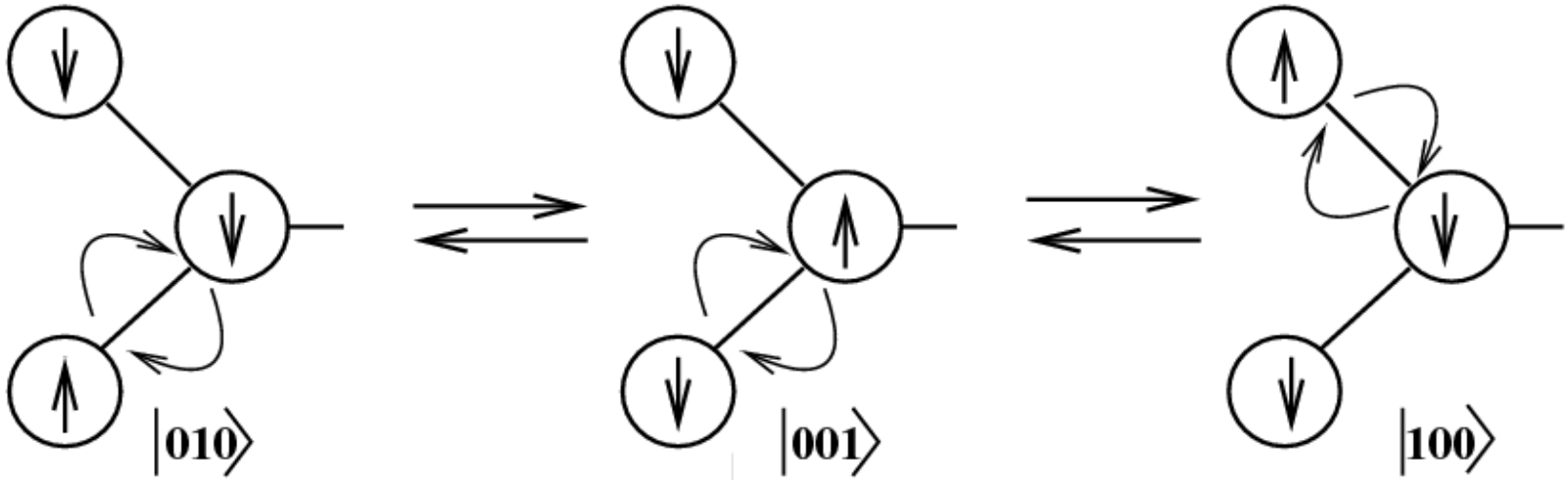
$J = 1cm^{-1}$ $t_j \sim 167$ ps
$= 10cm^{-1}$ $t_j \sim 16.7$ ps
$= 100cm^{-1}$ $t_j \sim 1.7$ ps

Electronic configurations involved in the controlled SWAP process



Schematic representation of the SWAP mecanism





Hamiltonian matrix in the basis of the possible configurations

HDVV spin Hamiltonian

$$\hat{H}_{HDVV} = \sum_{i>j} -J(\overrightarrow{r_{ij}})\hat{\overrightarrow{S_i}}.\hat{\overrightarrow{S_j}}$$

$$\begin{cases} J = J_{13} = J_{23} \\ J_{12} = 0 \end{cases}$$

$$\hat{H}_{HDVV} = -J(\hat{S}_1\hat{S}_3 + \hat{S}_2\hat{S}_3)$$

$$\hat{H}_B = \mu_B \hat{\overrightarrow{B}}_z.\hat{\overrightarrow{S}} = \mu_B \hat{B}_z \hat{S}_z$$
$$= \Lambda_z \hat{S}_z = \Lambda_z(\hat{S}_{1_z} + \hat{S}_{2_z} + \hat{S}_{3_z})$$

[(3x3) bloc matrices : doublets formed by two electrons holding the same spin and the third one with opposite orientation]

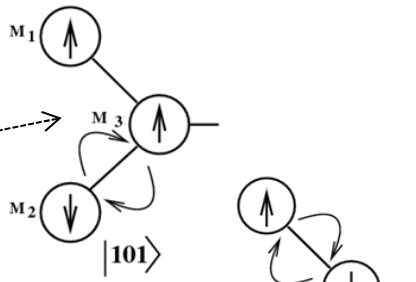
	$\|000\rangle$	$\|001\rangle$	$\|010\rangle$	$\|100\rangle$	$\|011\rangle$	$\|101\rangle$	$\|110\rangle$	$\|111\rangle$
$\|000\rangle$	$-\frac{\mathbf{J-3\Lambda_z}}{\mathbf{2}}$	0	0	0	0	0	0	0
$\|001\rangle$	0	$+\frac{\mathbf{J+\Lambda_z}}{\mathbf{2}}$	$-\frac{\mathbf{J}}{\mathbf{2}}$	$-\frac{\mathbf{J}}{\mathbf{2}}$	0	0	0	0
$\|010\rangle$	0	$-\frac{\mathbf{J}}{\mathbf{2}}$	$\frac{\Lambda_z}{2}$	0	0	0	0	0
$\|100\rangle$	0	$-\frac{\mathbf{J}}{\mathbf{2}}$	0	$\frac{\Lambda_z}{}$	0	0	0	0
$\|011\rangle$	0	0	0	0	$-\frac{\Lambda_z}{2}$	0	$-\frac{\mathbf{J}}{\mathbf{2}}$	0
$\|101\rangle$	0	0	0	0	0	$-\frac{\Lambda_z}{2}$	$-\frac{\mathbf{J}}{\mathbf{2}}$	0
$\|110\rangle$	0	0	0	0	$-\frac{\mathbf{J}}{\mathbf{2}}$	$-\frac{\mathbf{J}}{\mathbf{2}}$	$+\frac{\mathbf{J-\Lambda_z}}{\mathbf{2}}$	0
$\|111\rangle$	0	0	0	0	0	0	0	$-\frac{\mathbf{J+3\Lambda_z}}{\mathbf{2}}$

Phenomenological reduction in the qubit basis set

Micro states $\{|101\rangle, |011\rangle, |100\rangle, |010\rangle, |001\rangle, |110\rangle\}$

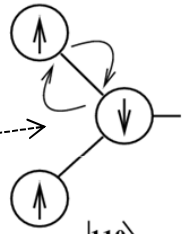
Model subspace $\{|010\rangle, |100\rangle, |011\rangle, |101\rangle\}$

M_1 and M_2 opposite spin signs, M_3 α or β



Intermediate subspace $\{|110\rangle, |001\rangle\}$

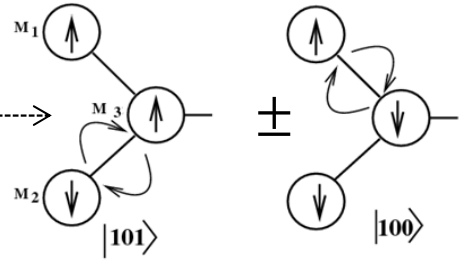
M_1 and M_2 same spin signs, M_3 α or β



Because of degeneracy:

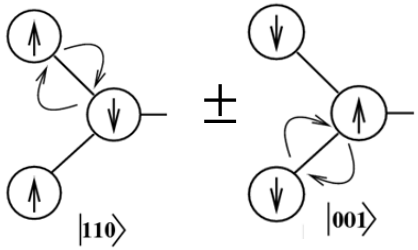
Swaping subspace

$$\begin{cases} \frac{1}{\sqrt{2}}\left[|101\rangle \pm |100\rangle\right] = \left|\Phi^{g,u}_{M_1\bar{M}_2}\right\rangle \\ \frac{1}{\sqrt{2}}\left[|011\rangle \pm |010\rangle\right] = \left|\Phi^{g,u}_{\bar{M}_1 M_2}\right\rangle \end{cases}$$



Control subspace

$$\frac{1}{\sqrt{2}}\left[|110\rangle \pm |001\rangle\right] = \left|\Phi^{g,u}_{M_1 M_2, \bar{M}_1 \bar{M}_2}\right\rangle$$



Electron Indiscernability
& W. Pauli exclusion principle
Antisymmetrisation of the wave function

Description in a base of Slater determinants

$$\left|a\bar{b}c\right| = \left|a(1)b(\bar{2})c(3)\right| = \frac{1}{\sqrt{3!}}\begin{vmatrix} a(1) & a(2) & a(3) \\ \bar{b}(1) & \bar{b}(2) & \bar{b}(3) \\ c(1) & c(2) & c(3) \end{vmatrix}$$

SWAP (3x3) Hamiltonian Matrix in the reduced basis set (in J unit)

$$
\begin{array}{c}
 \\
\left|\Phi^{g}_{M_1\bar{M}_2}\right\rangle \\
\left|\Phi^{g}_{\bar{M}_1 M_2}\right\rangle \\
\left|\Phi^{g}_{M_1 M_2,\bar{M}_1\bar{M}_2}\right\rangle
\end{array}
\begin{array}{c}
\begin{array}{ccc}
\left|\Phi^{g}_{M_1\bar{M}_2}\right\rangle & \left|\Phi^{g}_{\bar{M}_1 M_2}\right\rangle & \left|\Phi^{g}_{M_1 M_2,\bar{M}_1\bar{M}_2}\right\rangle
\end{array} \\
\begin{pmatrix}
\frac{1}{2} & 0 & -\frac{1}{6\sqrt{2}} \\
0 & \frac{1}{2} & -\frac{1}{6\sqrt{2}} \\
-\frac{1}{6\sqrt{2}} & -\frac{1}{6\sqrt{2}} & \frac{5}{16}
\end{pmatrix}
\end{array}
$$

No static magnetic field contribution !

Role of magnetic field : to lift up the degeneracy between the α and β electron spins,

$\longrightarrow$ *no direct influence on the process itself.*

Temporal evolution and effective Hamiltonian

Time-dependent probability to find the system in a final state:

$$\mathcal{P}_f(t) = \left| \left\langle \phi_f \middle| \psi(t) \right\rangle \right|^2, \text{ where } |\psi(t)\rangle = \sum_n C_n(t) \, |\psi_n\rangle$$

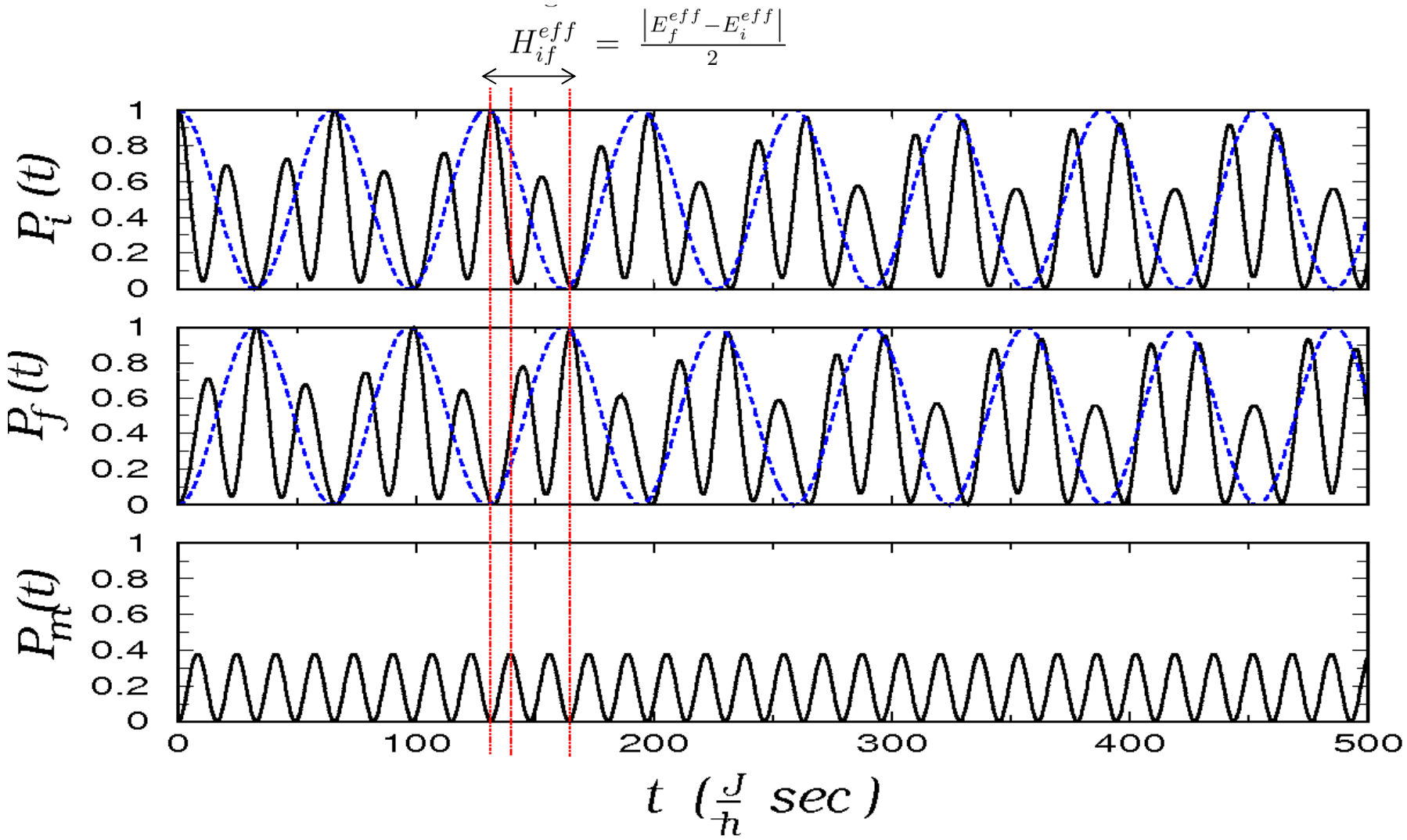
Effective Hamiltonian:

$$H^{eff} = PU^{-1}HUP$$

Effective magnetic coupling between two the 2 qubits through the central atom:

$$H_{if}^{eff} = \frac{\left| E_f^{e\uparrow\uparrow} - E_i^{e\uparrow\uparrow} \right|}{2}$$

Time dependant probability amplitude associated to the controlled SWAP process



Rabi oscillations curves obtained by using H (solid dark lines) or H_{eff} (dashed blue lines)

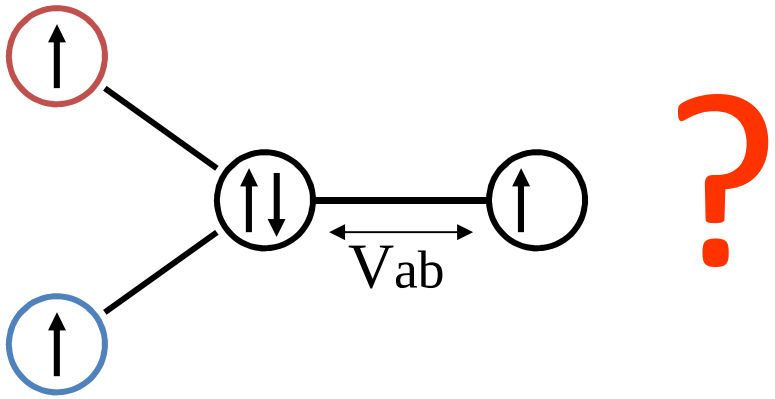
Numerical estimations

$$H_{if}^{eff} = \frac{\left|E_f^{eff} - E_i^{eff}\right|}{2} = 0.050 \text{ (in J unit)}$$

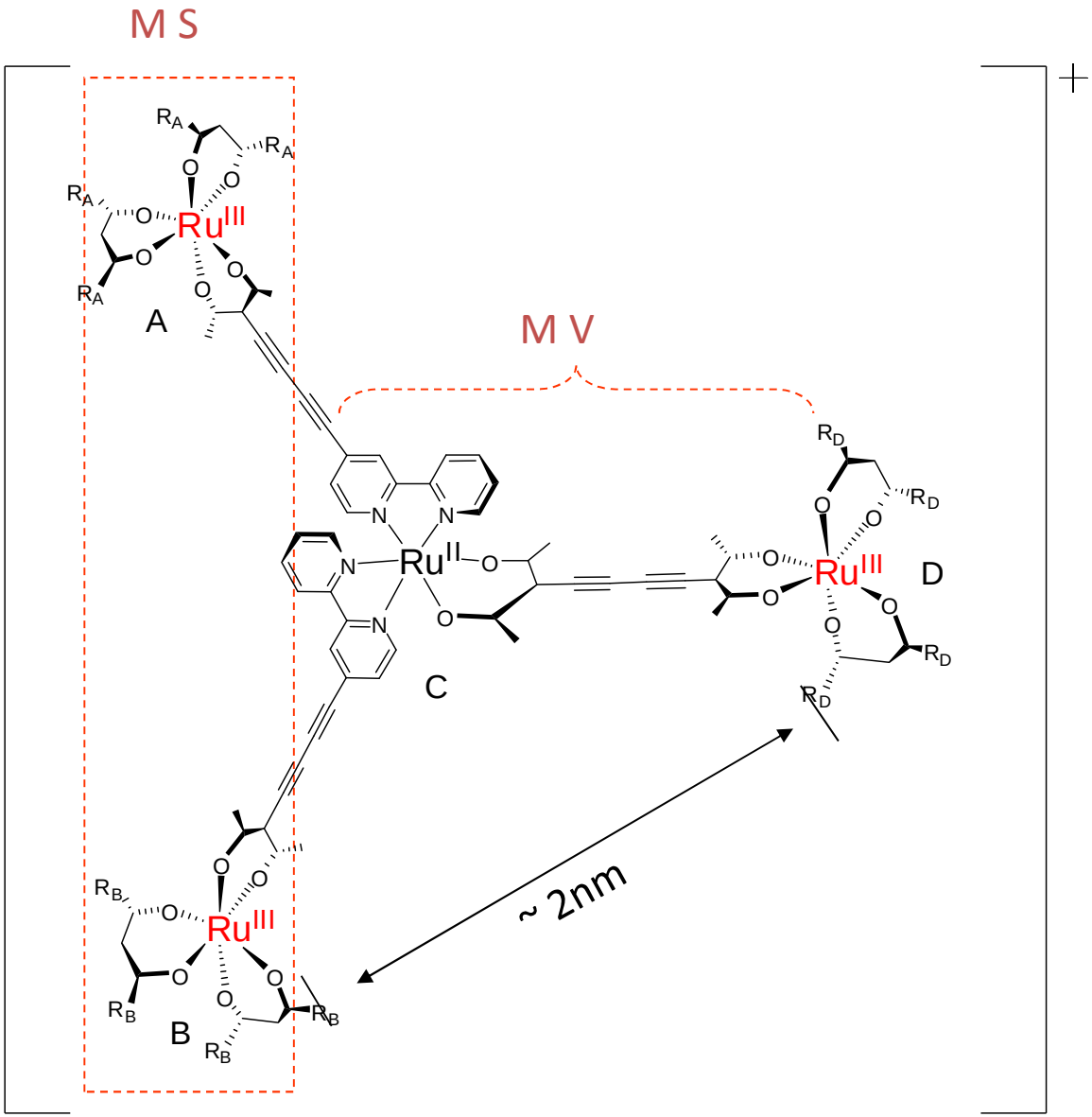
$$t = \frac{\pi\hbar}{2H_{if}^{eff}} = 31.562\frac{\hbar}{J}\,\text{sec}$$

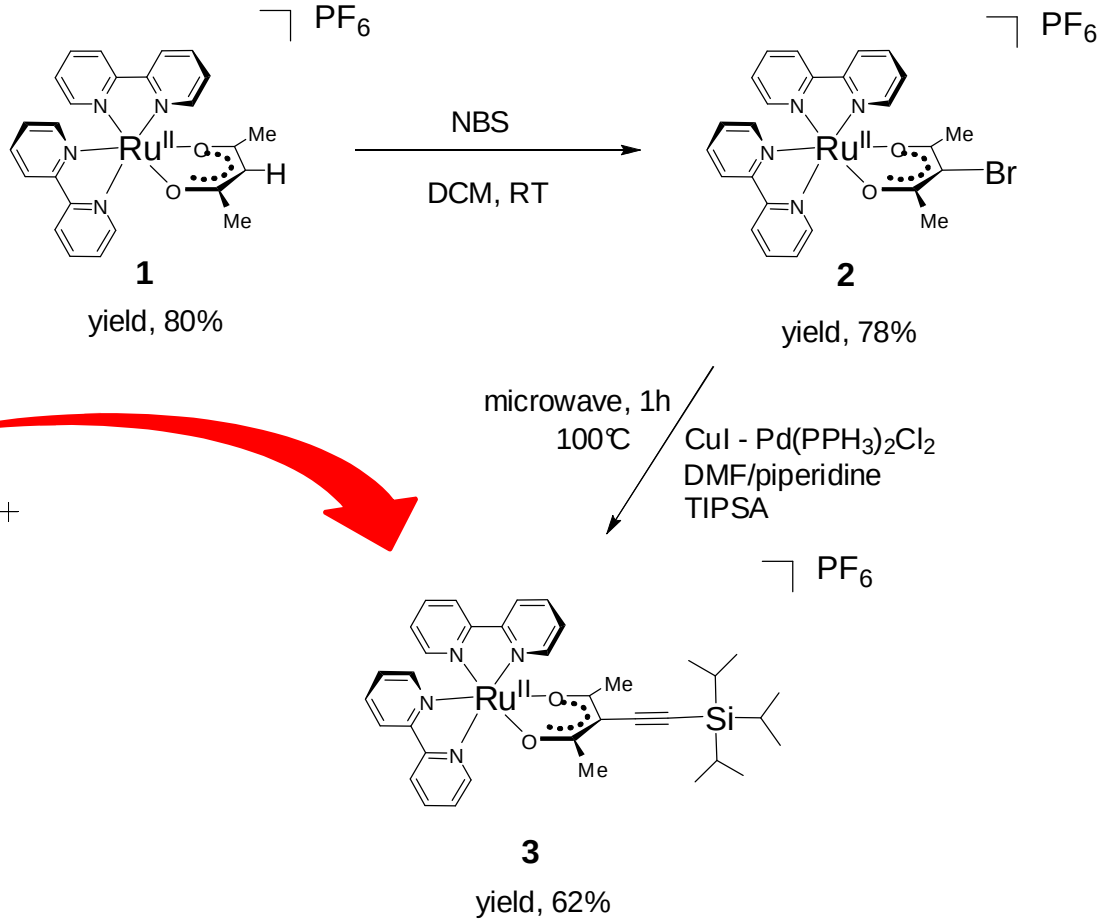
If J = 100 cm^{-1} , t = 1.6 ps and the oscillation frequency is 597 GHz

If J = 1 cm^{-1} , t = 160 ps and the oscillation frequency is 5.97 GHz

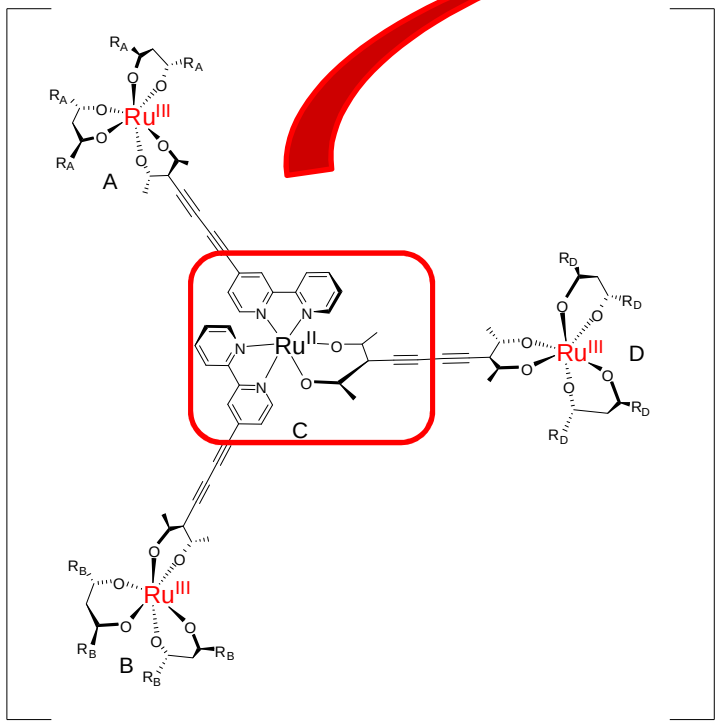

Vab
?

Possible chemical structure for the SWAP molecule…

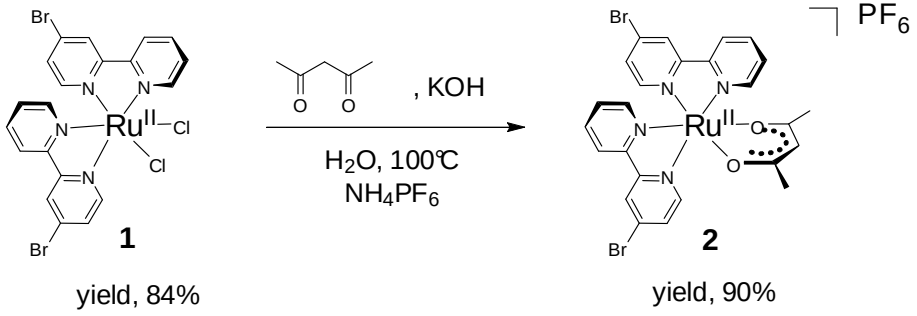




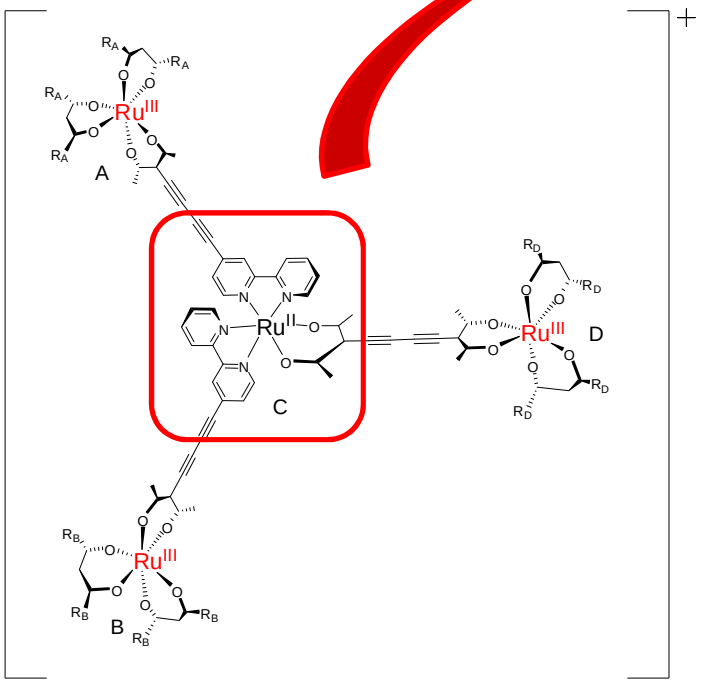
Target molecule

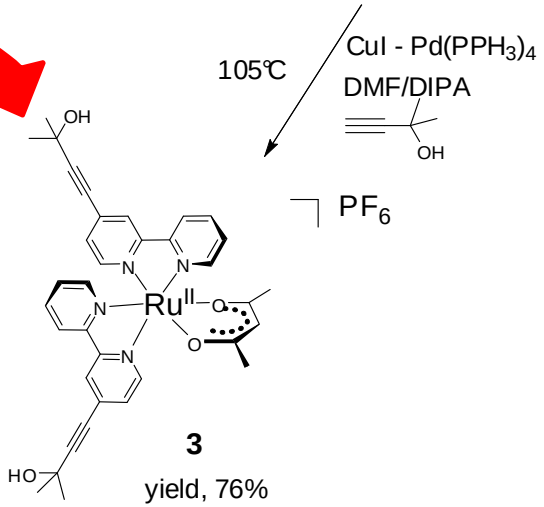


Inorg. Chem. Commun. **2008,** 11, 975



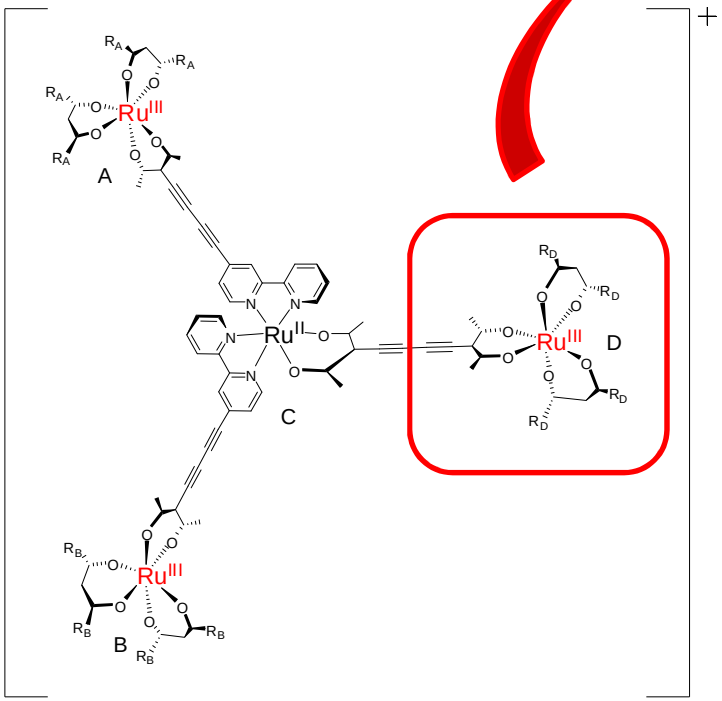
Target molecule

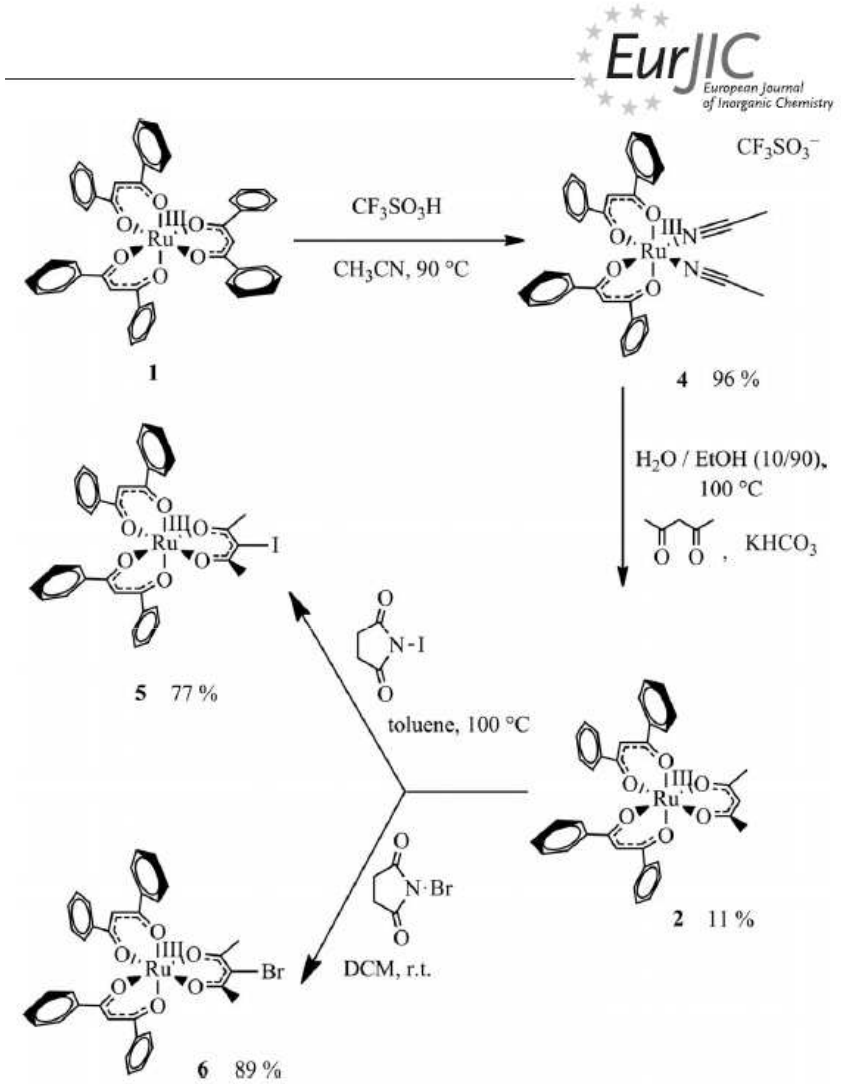




Inorg. chim. Acta **2010**, 363, 1409

Target molecule

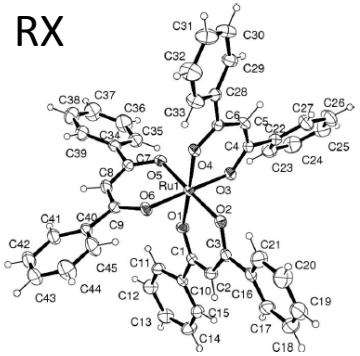




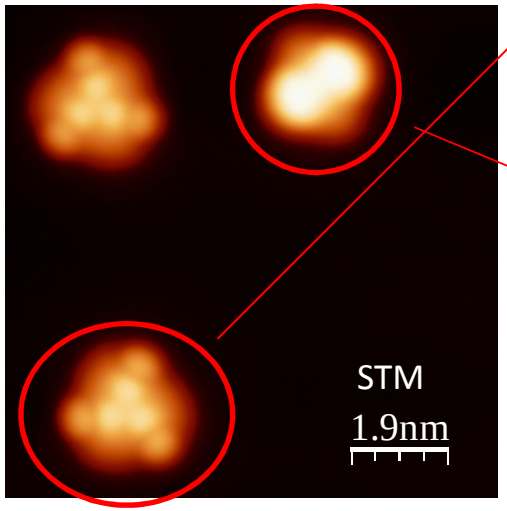
Scheme 2. Synthesis of complexes **2**–**5** and **6**.

Eur. J. Inorg. Chem. ***2011****, 2698*

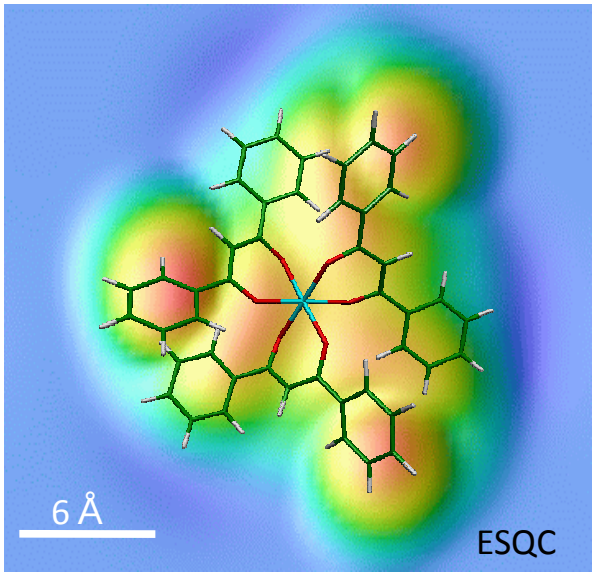
RX

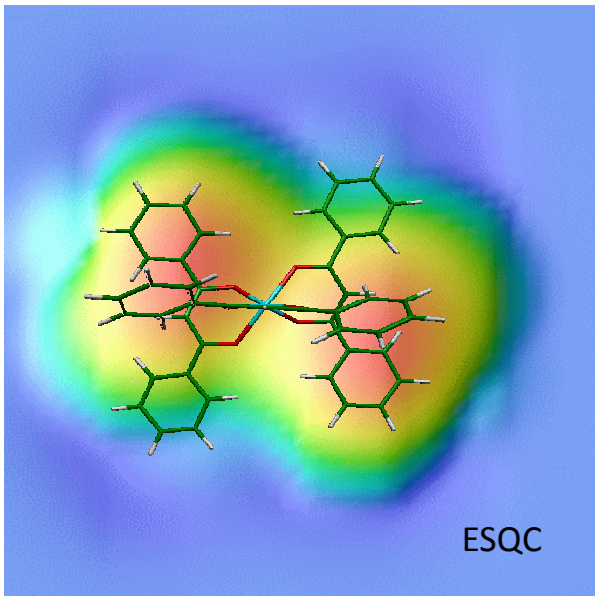


STM

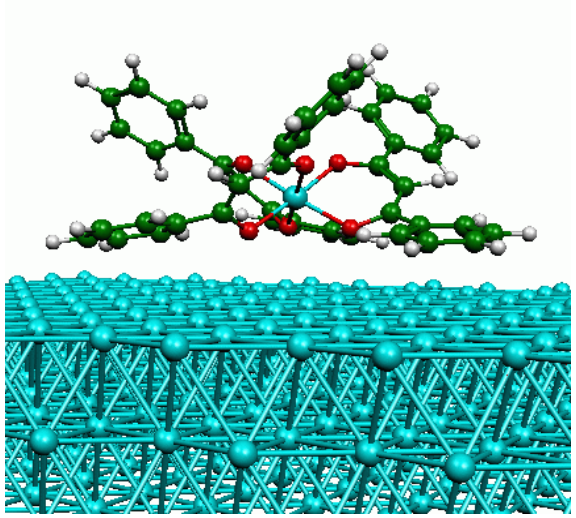


Ru(dbm)$_3$@Ag(111) at He liq

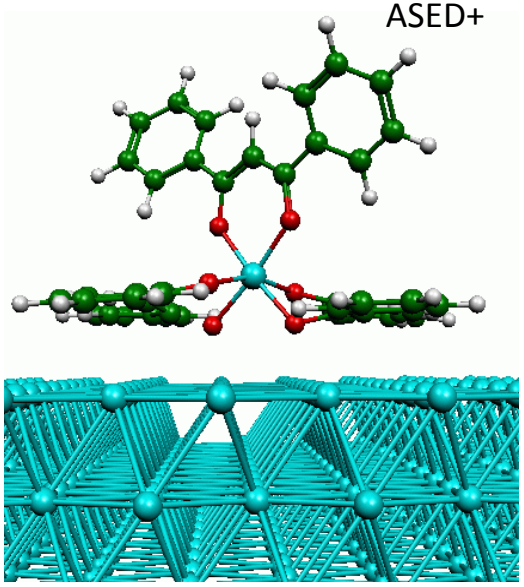




ASED+

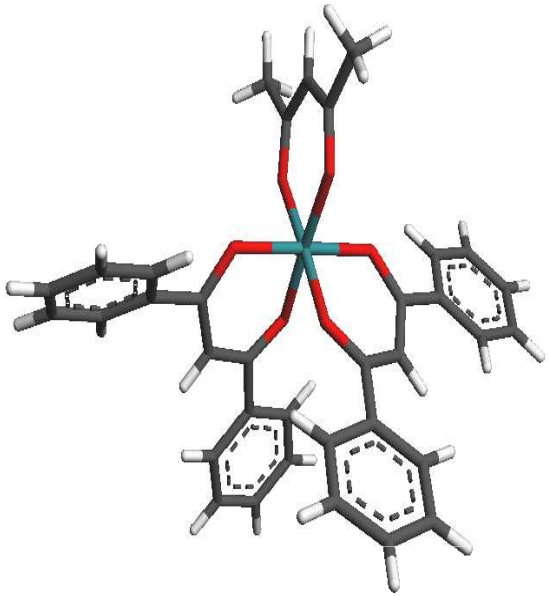


ASED+

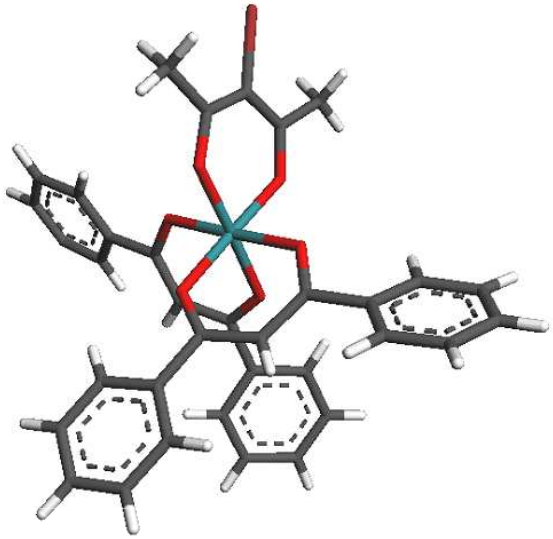


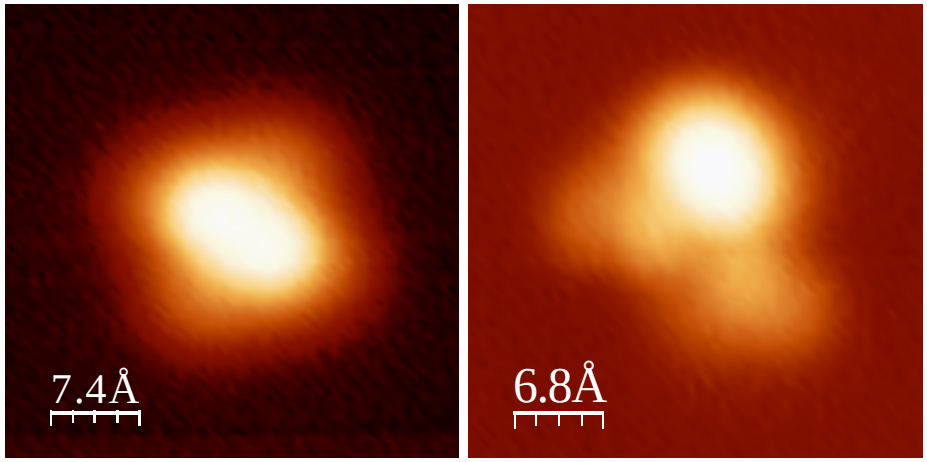
Eur. J. Inorg. Chem. ***2011****, 2698*

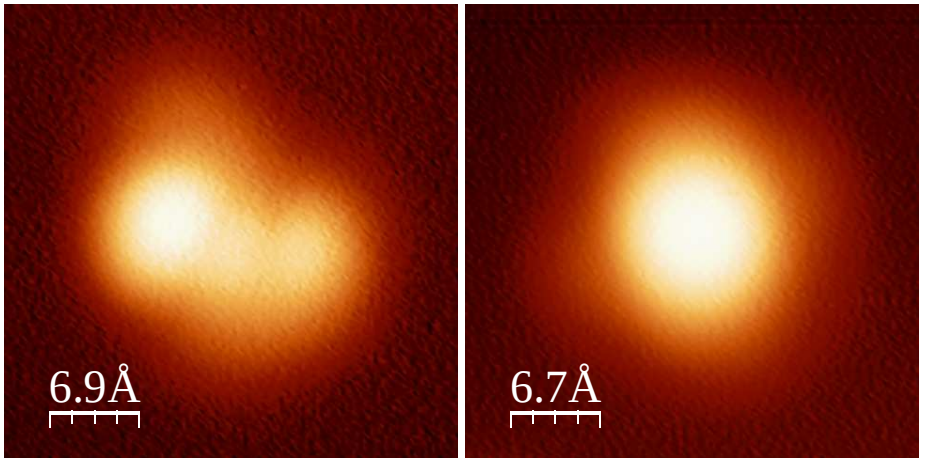
$Ru(dbm)_2Acac$



$Ru(dbm)_2Acac$-Br

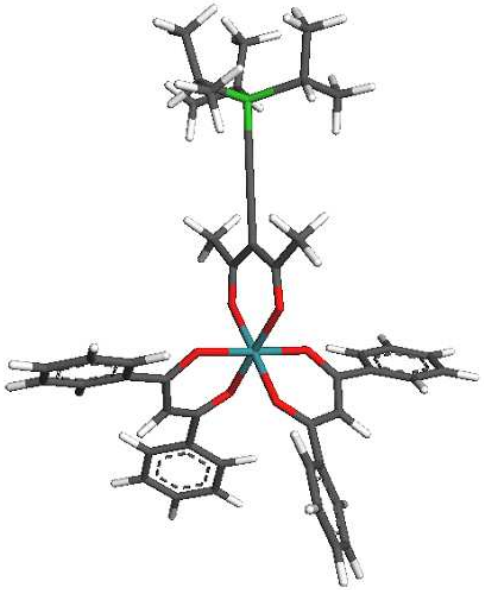


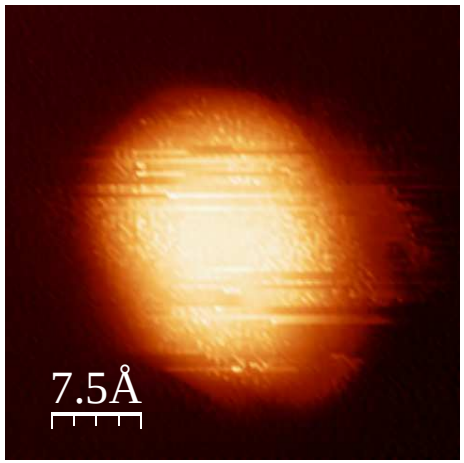


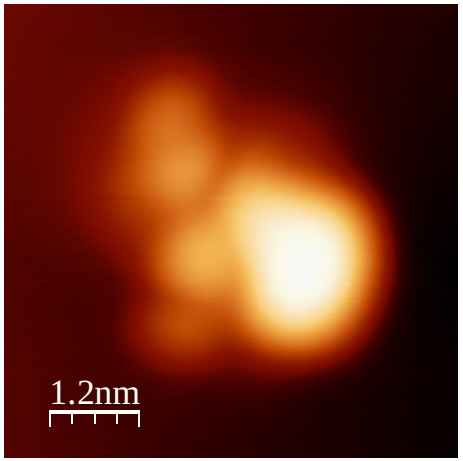


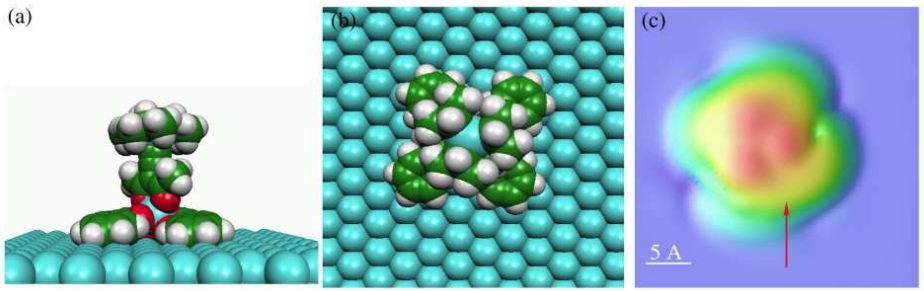
Preliminary results…

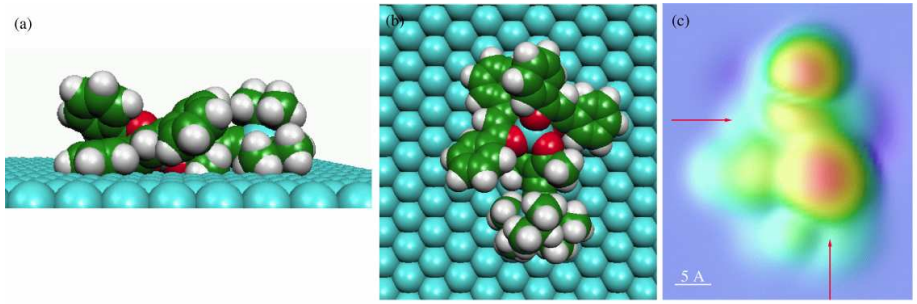
$Ru(dbm)_2(Acac\text{-}TIPSA)$



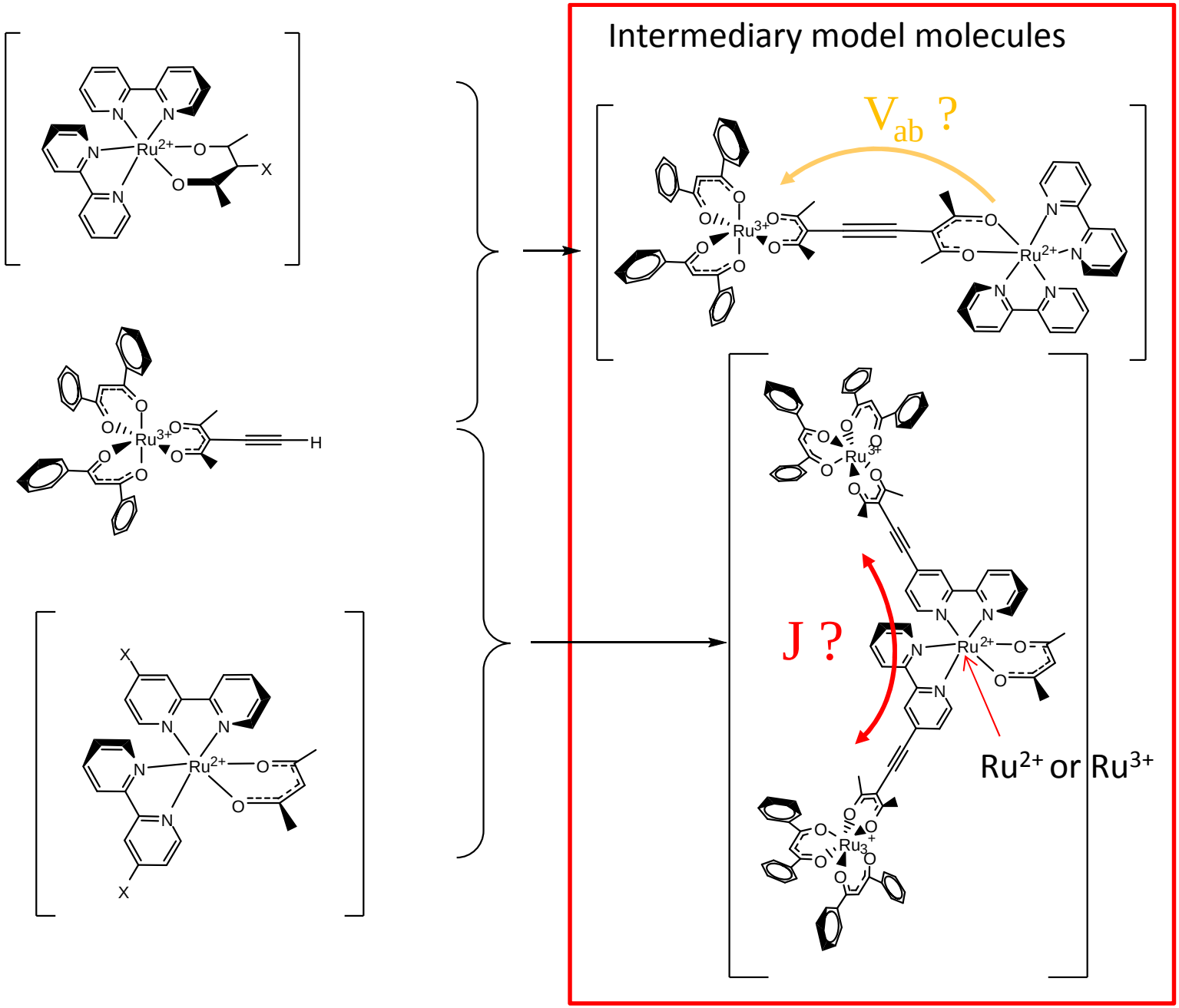




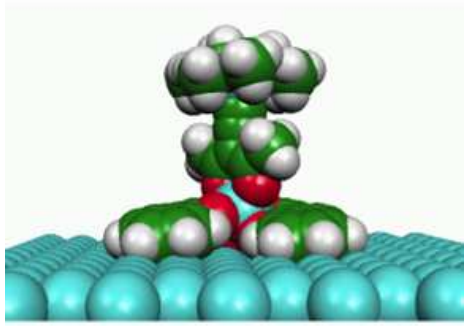




Next necessary step…



Summary and perspectives



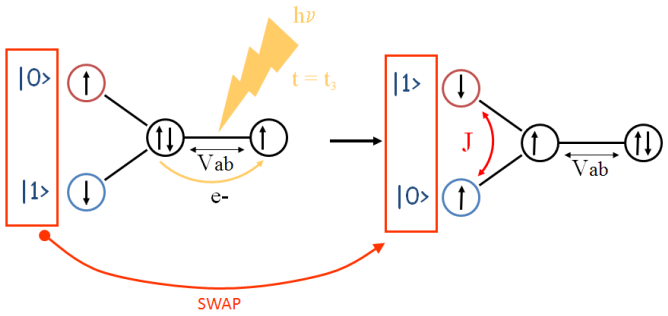
✓ Design of a SWAP molecule logic gate:

- Proposition of a molecule & a model to implement a quantum controlled swap molecule logic gate:
  - Three paramagnetic adjacents centers (two qubits and one control sites)
  - Activation by appropriate light radiation (IVCT)
  - Initiation of the active qubits by applying a static magnetic field and/or appropriate light radiation
  - Field independent swapping time

Manipulation of information inside a single molecule
→ Towards molecular quantum computer !

✓ Atom based technology (STM, SP-STM, AFM, MRFM…) *required* !

Aknowledgements



- *Molécule a calcul*
  - **Concept & Theorie**: Mohamed Hliwa & Christian Joachim
  - **Synthesis** : Cédric Michel (M2R); Sabrina Munery (IE CDD) & Christine Viala (AI)
  - **XR:** Nicolas Ratel-Ramond (IR)
  - **STM** : Loranne Vernisse (PhD); Olivier Guillermet & Roland Coratger
  - **Modelisation & STM image calculation (ESQC, ASED+)**: Youness Benjalal (Postdoc) & Xavier Bouju

And thank you…