

# Quantum Information Processing IRC



Arzhang Ardavan  
Simon Benjamin  
David Britz  
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Mark Jones  
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Gavin Morley  
John Morton  
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David Pettifor  
Alexei Tyryshkin  
Andrew Watt

# QIP IRC postdoctoral opportunities

## Postdoctoral Research Assistant in the Theory of Quantum Information Processing

- Postdoctoral Research Assistant in the Theory of Quantum Information Processing Grade 7 / Salary in the range £25,889 to £27,465 pa / Job Ref: DJ07/021. The closing date for applications is 31 August 2007.

## Theoretical studies of electrically detected magnetic resonance in carbon nanostructures

- Theoretical studies of electrically detected magnetic resonance in carbon nanostructures. Grade 7 / Salary in the range £25,889 to £29,138 pa / Job Ref: DJ07/020. The closing date for applications is 31 August 2007.

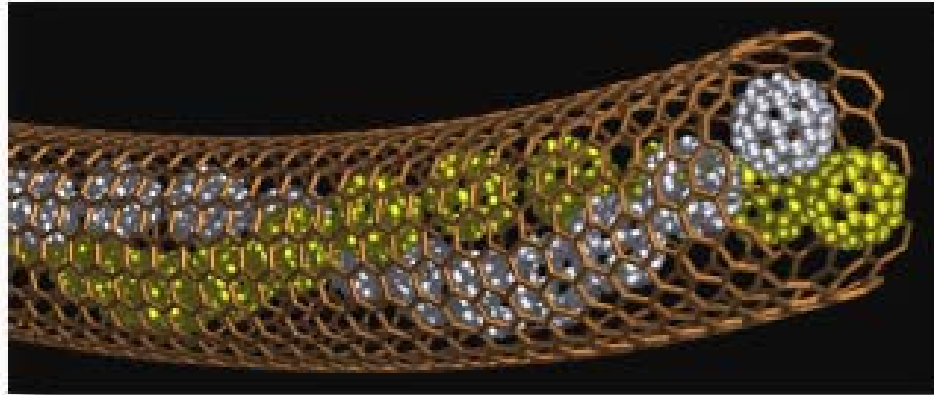
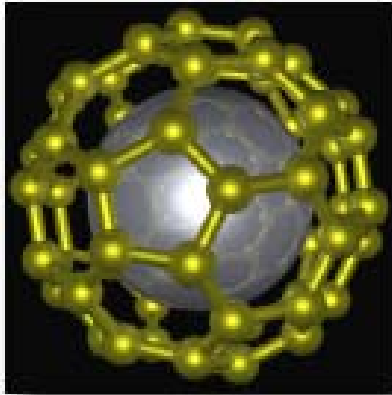
## Carbon Nanomaterials for Quantum Information Processing

- Carbon Nanomaterials for Quantum Information Processing Grade 7 / Salary in the range £26,666 to £29,139 pa / Job Ref: DJ07/022. The closing date for applications is 28 September 2007.

[www.materials.ox.ac.uk/vacancies/index.htm](http://www.materials.ox.ac.uk/vacancies/index.htm)



## Spins in carbon nanomaterials for qubits



*Quantum transport and dynamics in nanostructures*

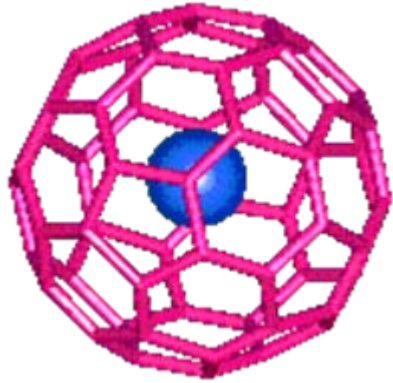
*Windsor*

*11<sup>th</sup> August 2007*

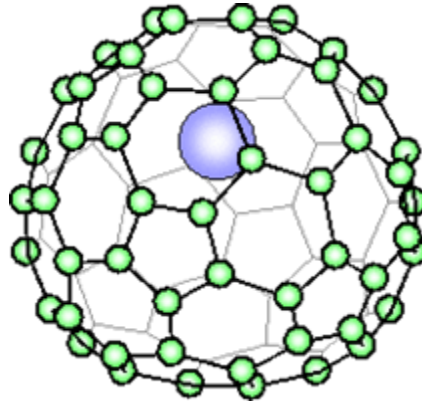
[www.qipirc.org](http://www.qipirc.org)

# Atoms in fullerenes

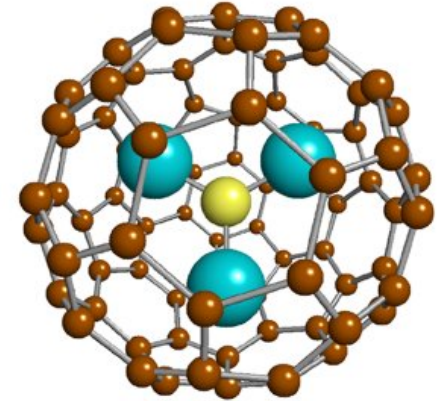
The fullerene cage can encapsulate other species:



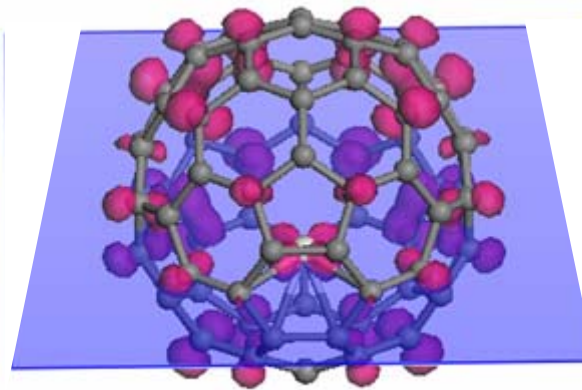
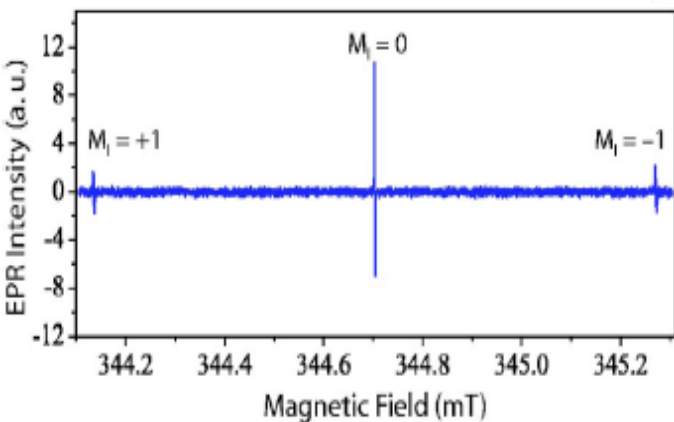
N@C<sub>60</sub>



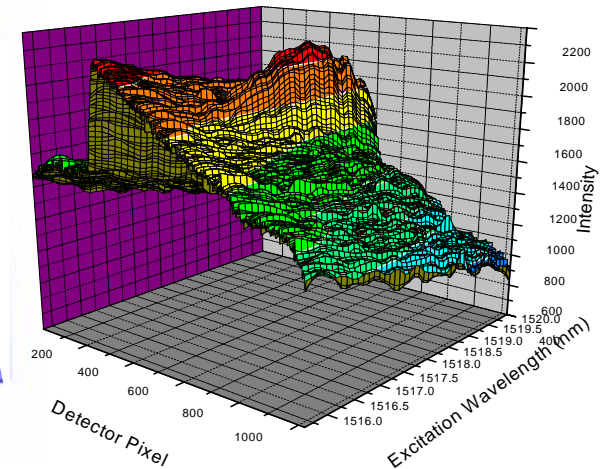
Sc, La, Ce, ... @C<sub>82</sub>



Er<sub>3</sub>N@C<sub>80</sub>

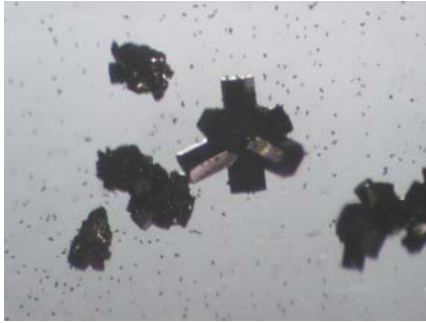


Spin density:  $> 0.01 \mu_B$



# 1-D spin arrays

Gas-Phase Nanotube Filling (300-500°C):



Fullerene

$C_{60}$ ,  $C_{70}$ ,  $C_{82}$ ,  $Sc@C_{82}$ ,  $Ce@C_{82}$ ,  $Nd@C_{82}$   
 $Sc_2@C_{80}$ ,  $Ce_2@C_{80}$ ,  $Er_3N@C_{80}$ ,  $Sc_3N@C_{80}$

+



Nanotubes

(diameters 1.36nm and 1.49nm)



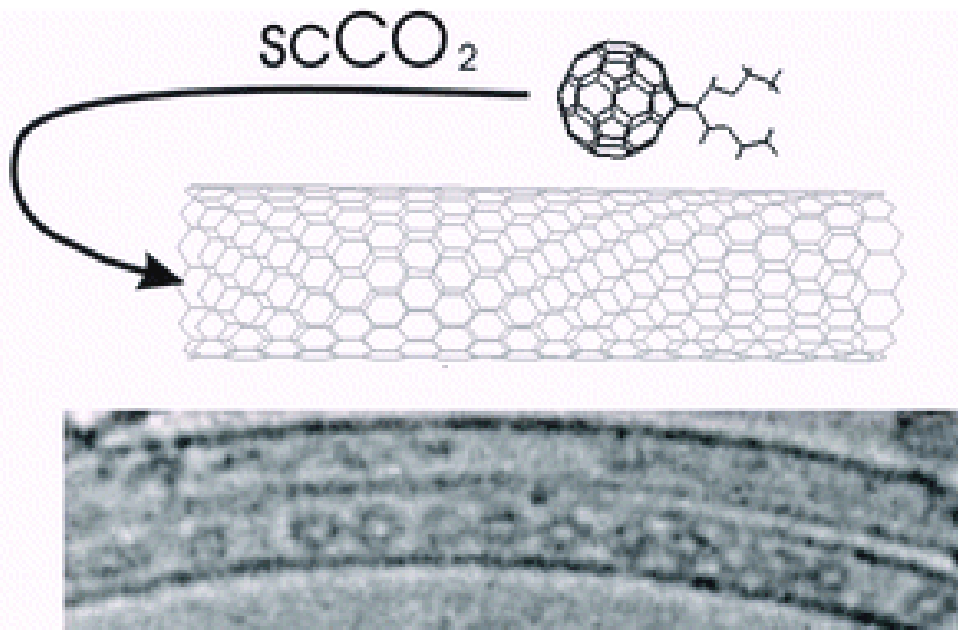
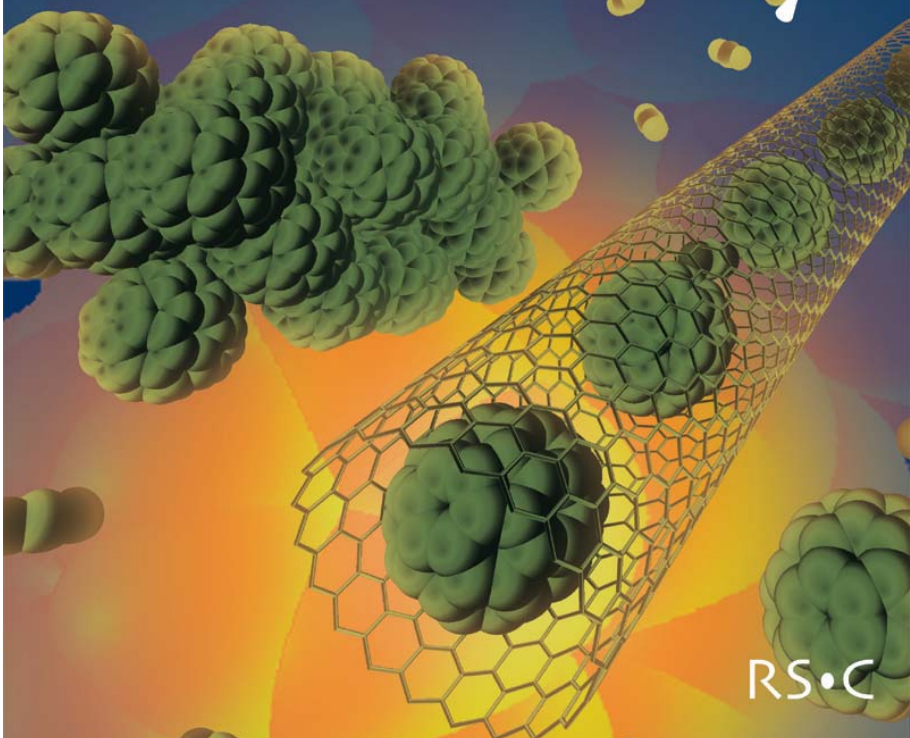
[www.nanotech.org](http://www.nanotech.org)



# Filling nanotubes using supercritical CO<sub>2</sub>

Journal of  
Materials  
Chemistry

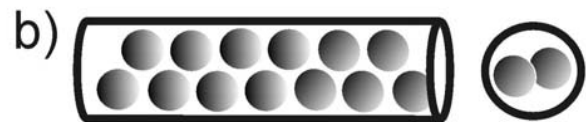
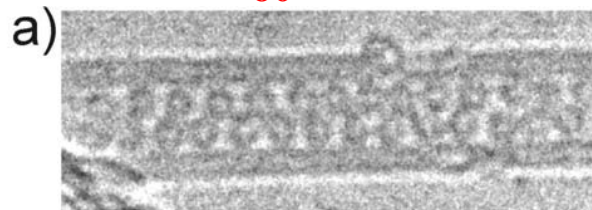
Volume 14 Number 19  
7 October 2004  
Pages 2831–2950  
ISSN 0959-9428  
www.rsc.org/materials



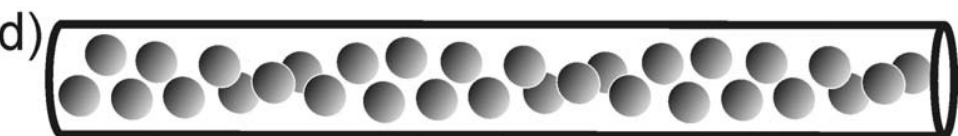
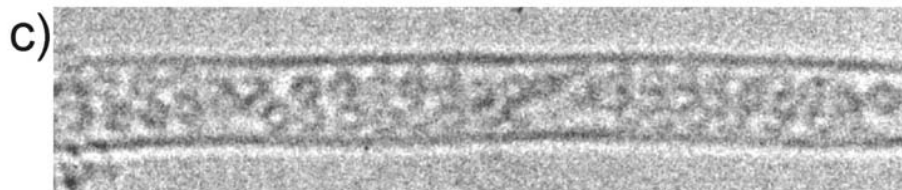
A.N. Khlobystov *et al.*,  
*J. Mater. Chem.* **14**,  
2852-2857 (2004)

# Fullerene molecules in carbon nanotubes

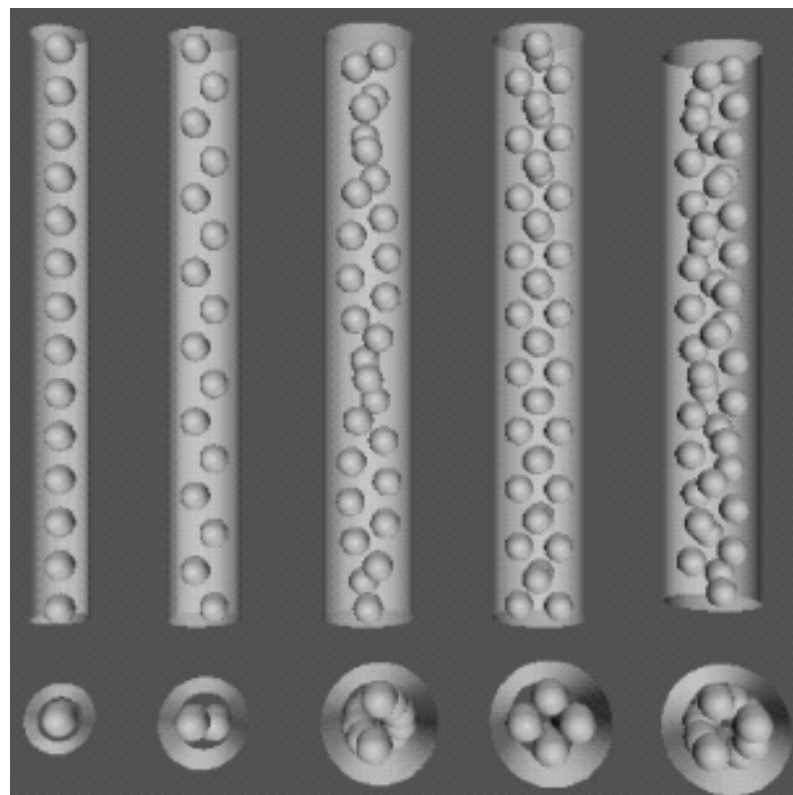
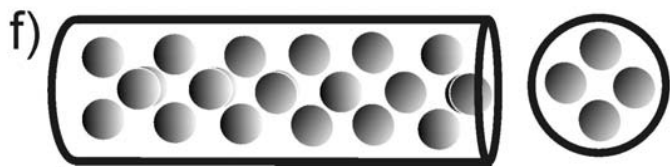
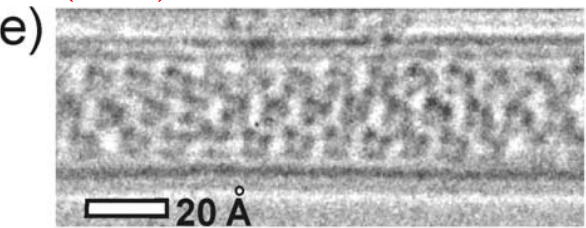
(a, b)  $C_{60}$ @DWNTs zigzag



(c, d)  $C_{60}$ @SWNT chiral



(e, f) two-molecule layer



**Simulated annealing**

Hodak and Girifalco

*Phys Rev B* **67**, 075419 (2003)

A.N. Khlobystov *et al.*

*Phys. Rev. Lett.* **92**, 245507 (2004)

# 10 yoctolitre test tubes

Chemical reactions inside single-walled carbon nano test-tubes. *Chem. Commun.* **2005**, 37-39 (2005)

Hot Paper (19 November 2004)

cover story of Issue 1 of 40<sup>th</sup> Anniversary Year  
*Blueprint* **5**, 3 (18 November 2004)

*New Scientist* (23 November 2004)

BBC News

*Iran Daily Newspaper* (25 November 2004) p. 4

*Financial Times* 35621, 13 (26 November 2004)

*Chemical & Engineering News* **82** (48) 7 (29  
November 2004)

*Chemistry World* **12** (December 2004)

Editor's Choice, *Science* **306**, 1863 (10  
December 2004)

Smallest reactor ever, *Materials Today* **8** (1) 9  
(January 2005)

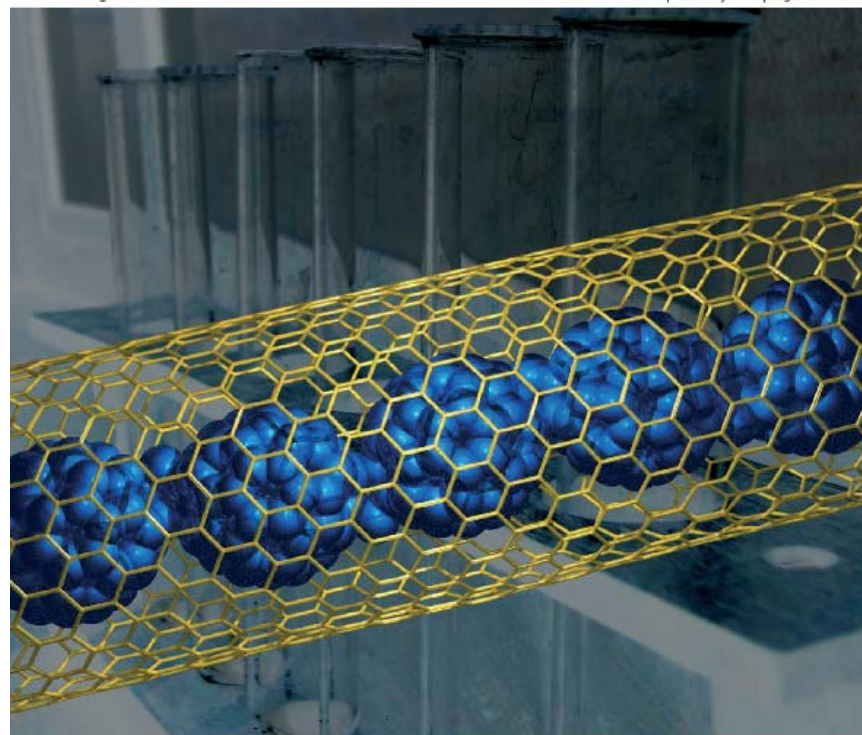
“The smallest test tube” in *The Guinness Book  
of World Records* (2006)

# ChemComm

Chemical Communications

www.rsc.org/chemcomm

Number 1 | 7 January 2005 | Pages 1-140



ESN 1259-7345

COMMUNICATION  
DAVID A. BRITZ, ANDREI N. KHLOBYSTOV, KYRIAKOS PORFYRAKIS,  
ARZHANG ARDAVAN AND G. ANDREW D. BRIGGS  
Chemical reactions inside single-walled carbon nano test-tubes

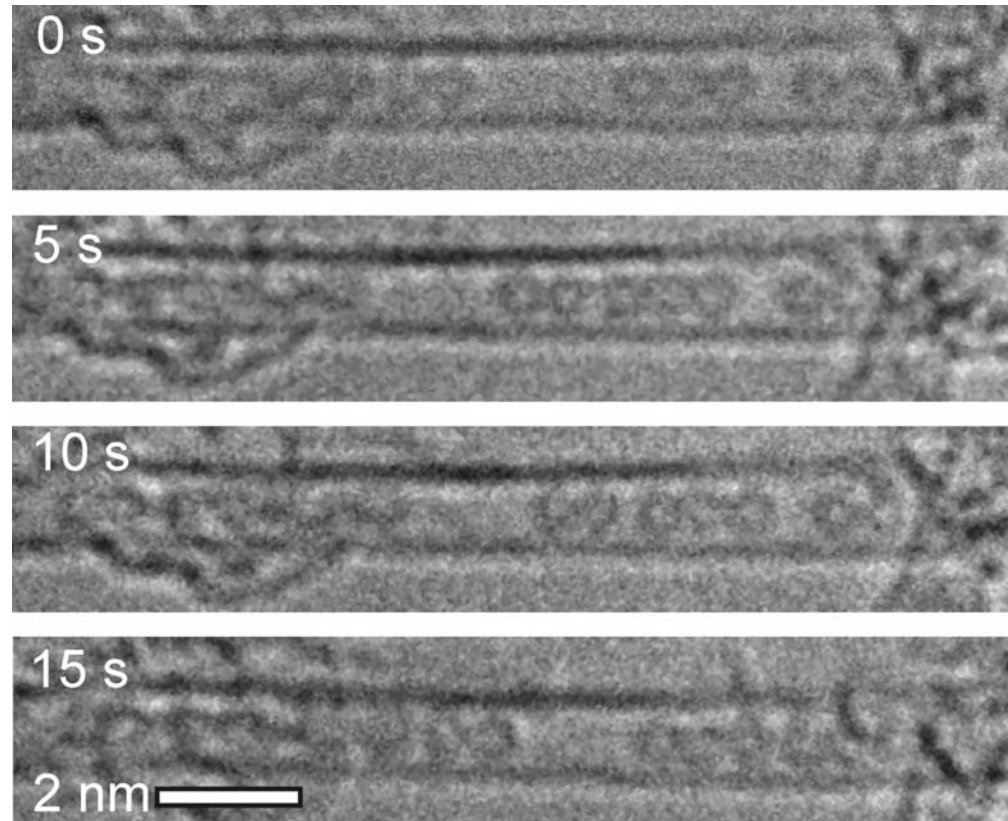
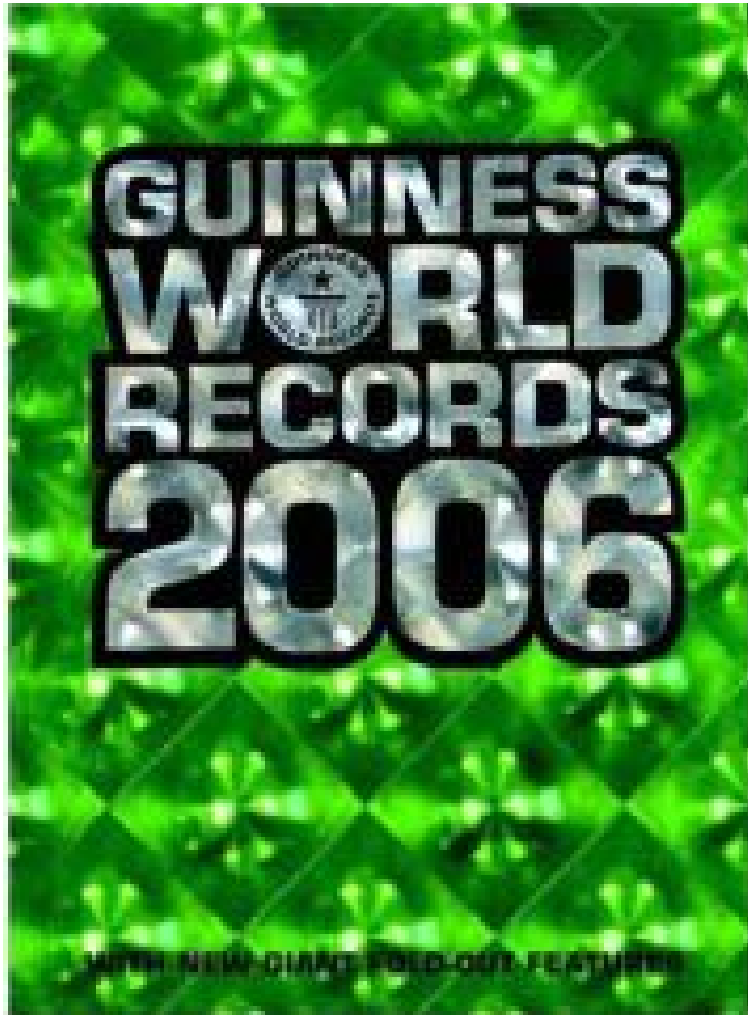
RSC | Advancing the  
Chemical Sciences

**D.A. Britz et al., Chem. Commun. 2005, 37-39.**





# 10 yoctolitre test tubes



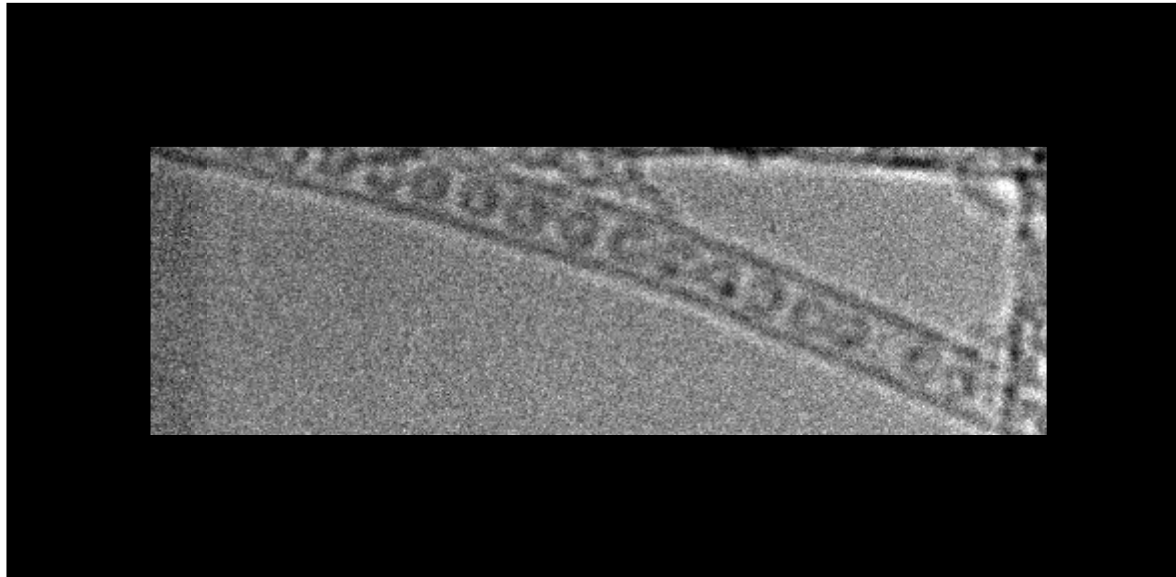
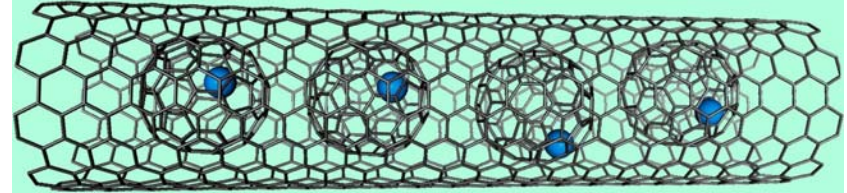
Chemical reactions inside single-walled carbon nano test-tubes.

D.A. Britz *et al.*, *Chem. Commun.* **2005**, 37-39.

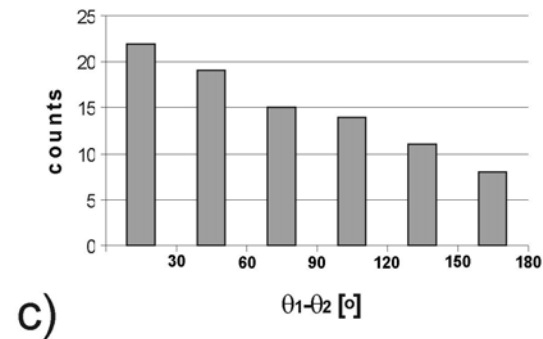
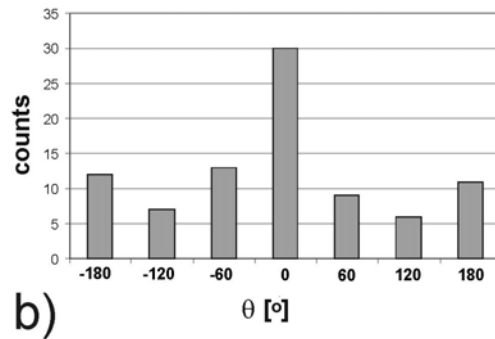
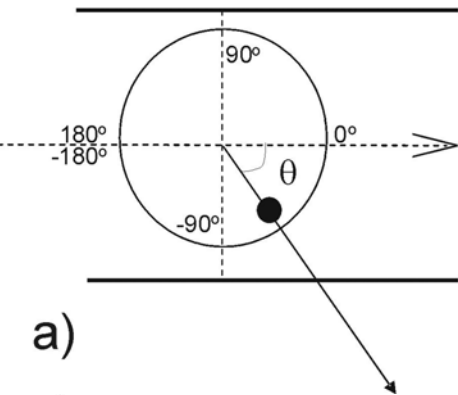


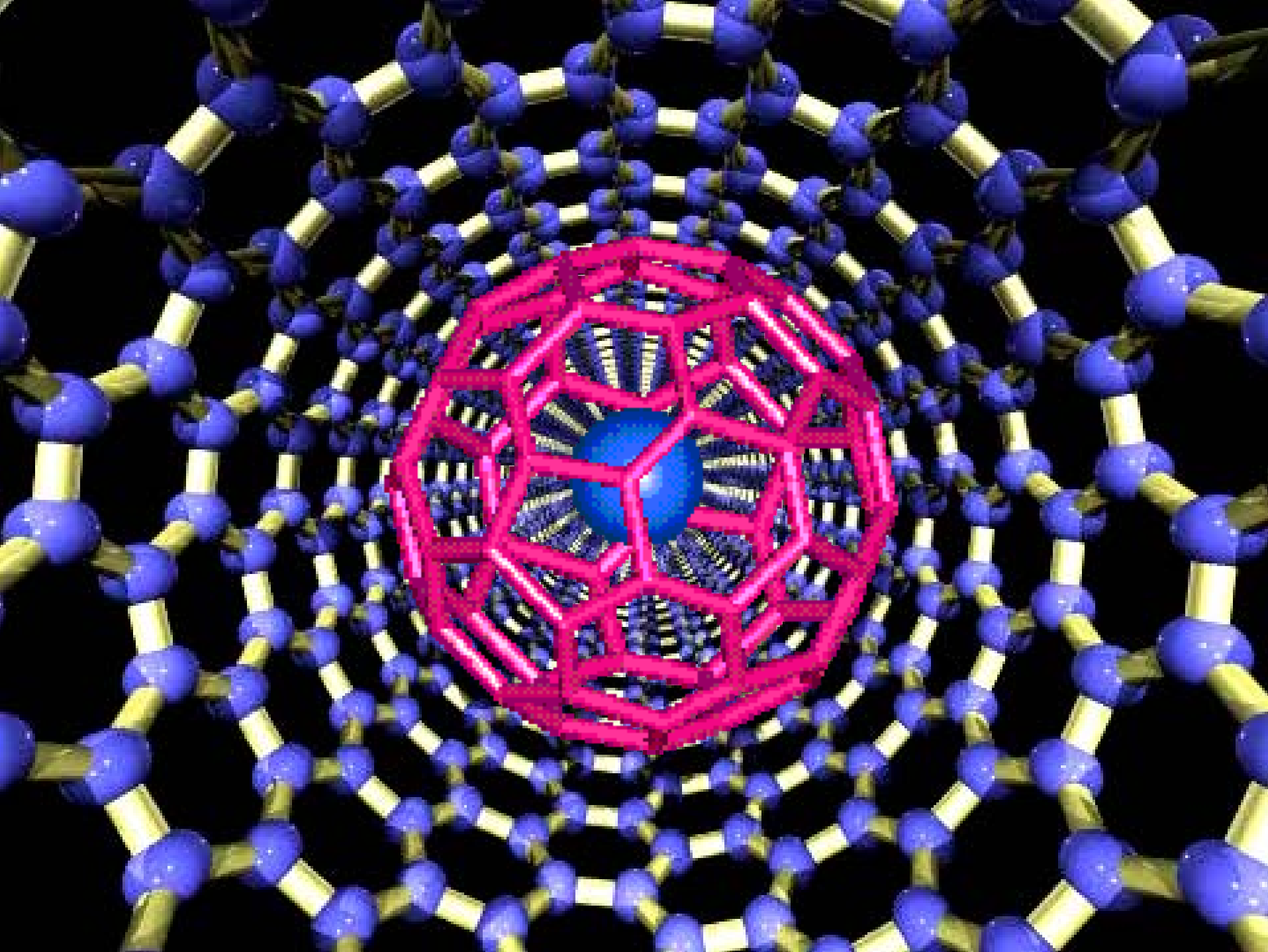
# Ce@C<sub>82</sub> in SWCNT

A. Khlobystov *et al.* *Angewandte Chemie International Edition*  
43, 1386-1389 (2004, “hot paper”)

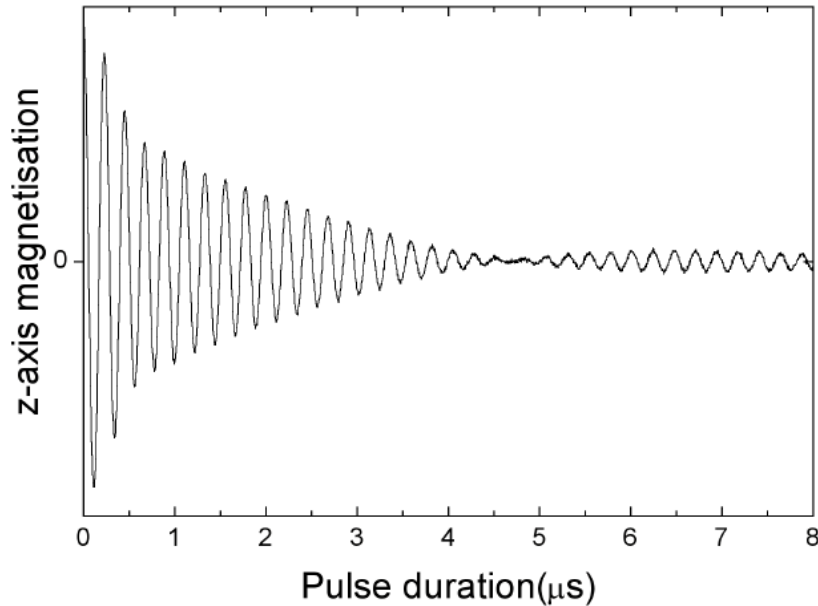


5 nm

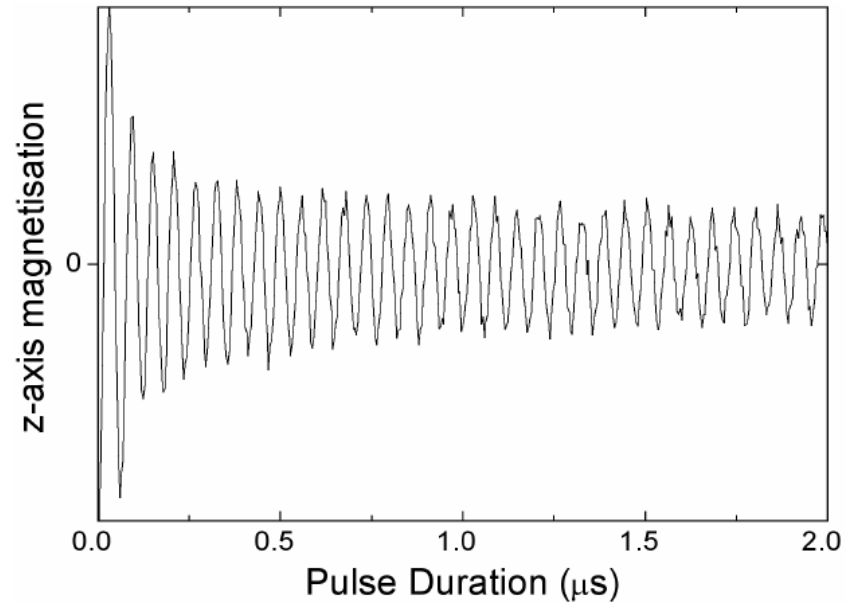




# Imperfect pulses



**The Rabi oscillation envelope is determined by inhomogeneities in the microwave field, not by spin coherence time.**



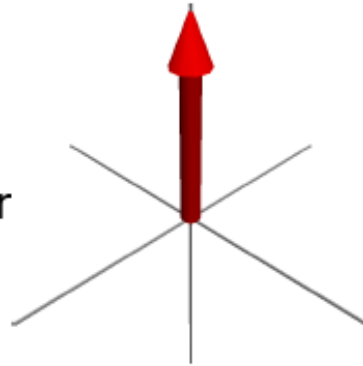
**A smaller sample fares better (note different time scale), but does not eliminate the problem.**



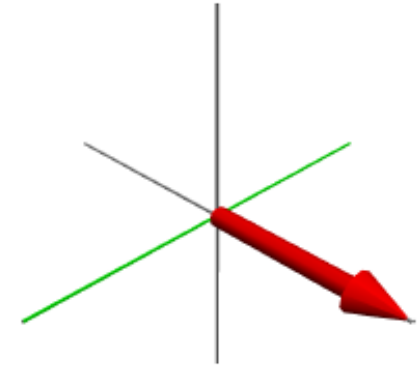
# Imperfect pulses

How well can we perform unitary transformations in an ESR spectrometer?

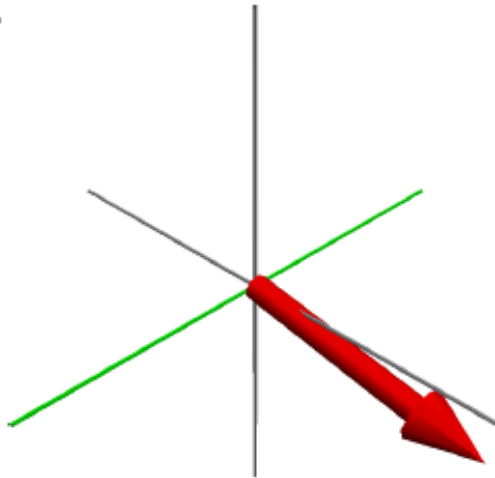
Doing a  $\pi/2$ -pulse or give



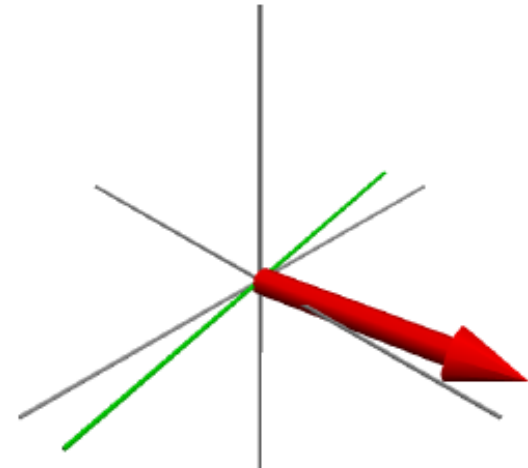
should



But we might get rotation angle errors



or rotation axis errors:



And can we perform complicated pulse sequences?



# BB1 sequence for spin manipulation

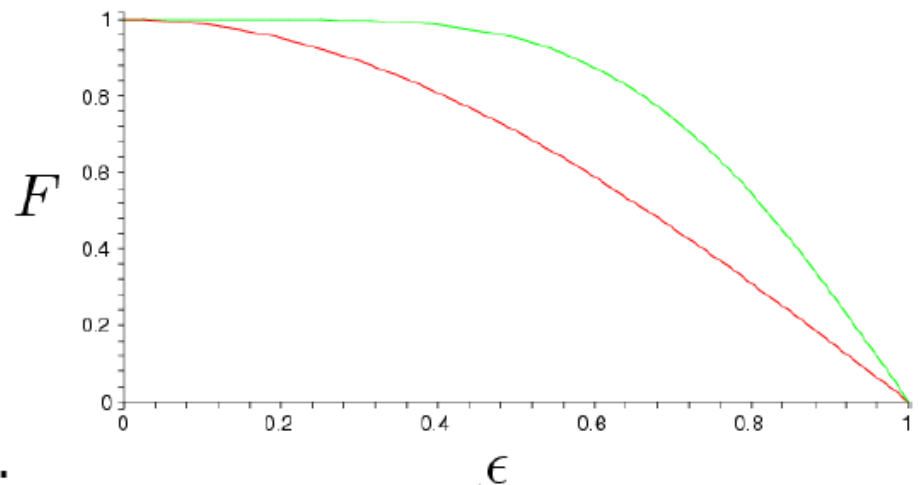
Defining the fidelity of two unitary operators  $A, B$ , as

$$F(A, B) = \frac{1}{2} \text{Tr}(A.B^{-1})$$

expand fidelity of composite operator in powers of the error,

$$F(\mathcal{R}_{\text{composite}}, \mathcal{R}_{\theta}^0) = 1 + F_2\epsilon^2 + F_4\epsilon^4 + \dots$$

where  $F_i = F_i(\theta, \alpha, \beta)$



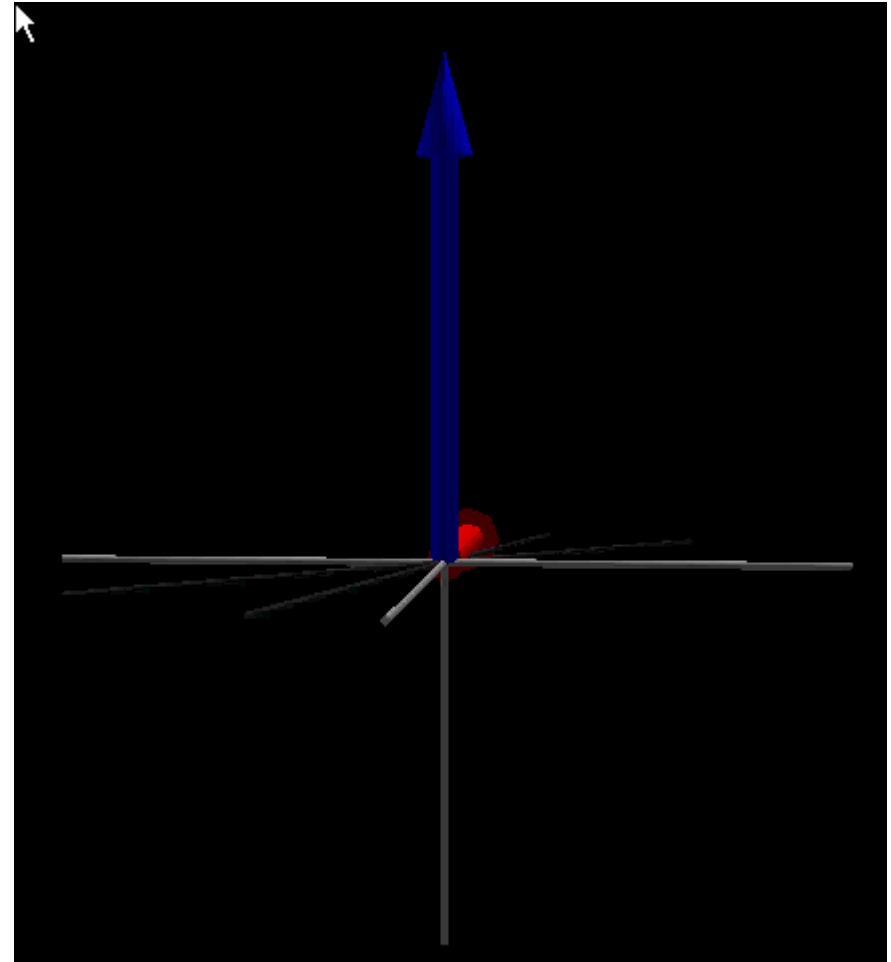
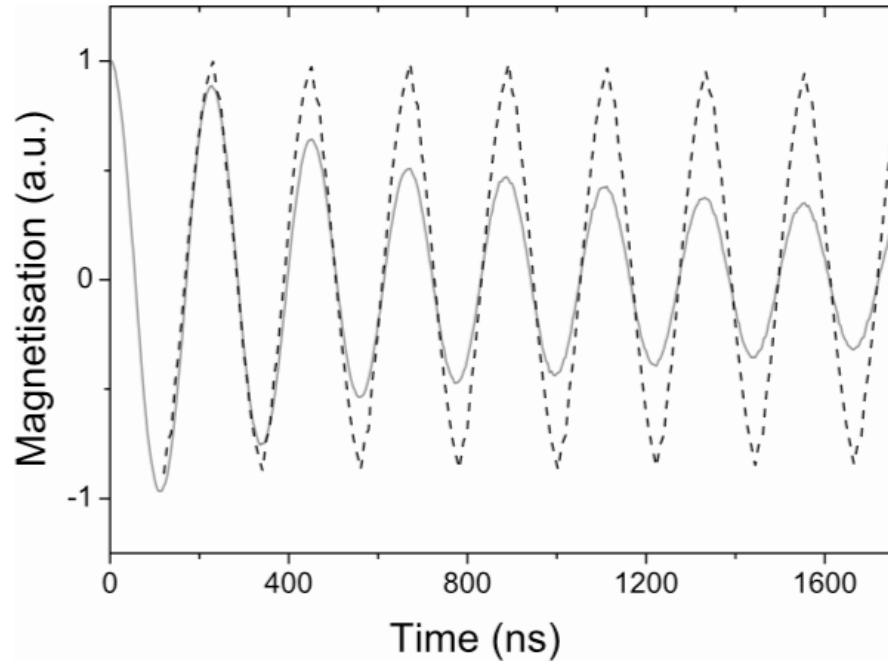
The BB1 composite sequence:

$$(1+\epsilon)\pi_x - (1+\epsilon)\pi_{104.5^\circ} - (1+\epsilon)2\pi_{313.4^\circ} - (1+\epsilon)\pi_{104.5^\circ}$$

is a better  $\pi_x$  rotation.



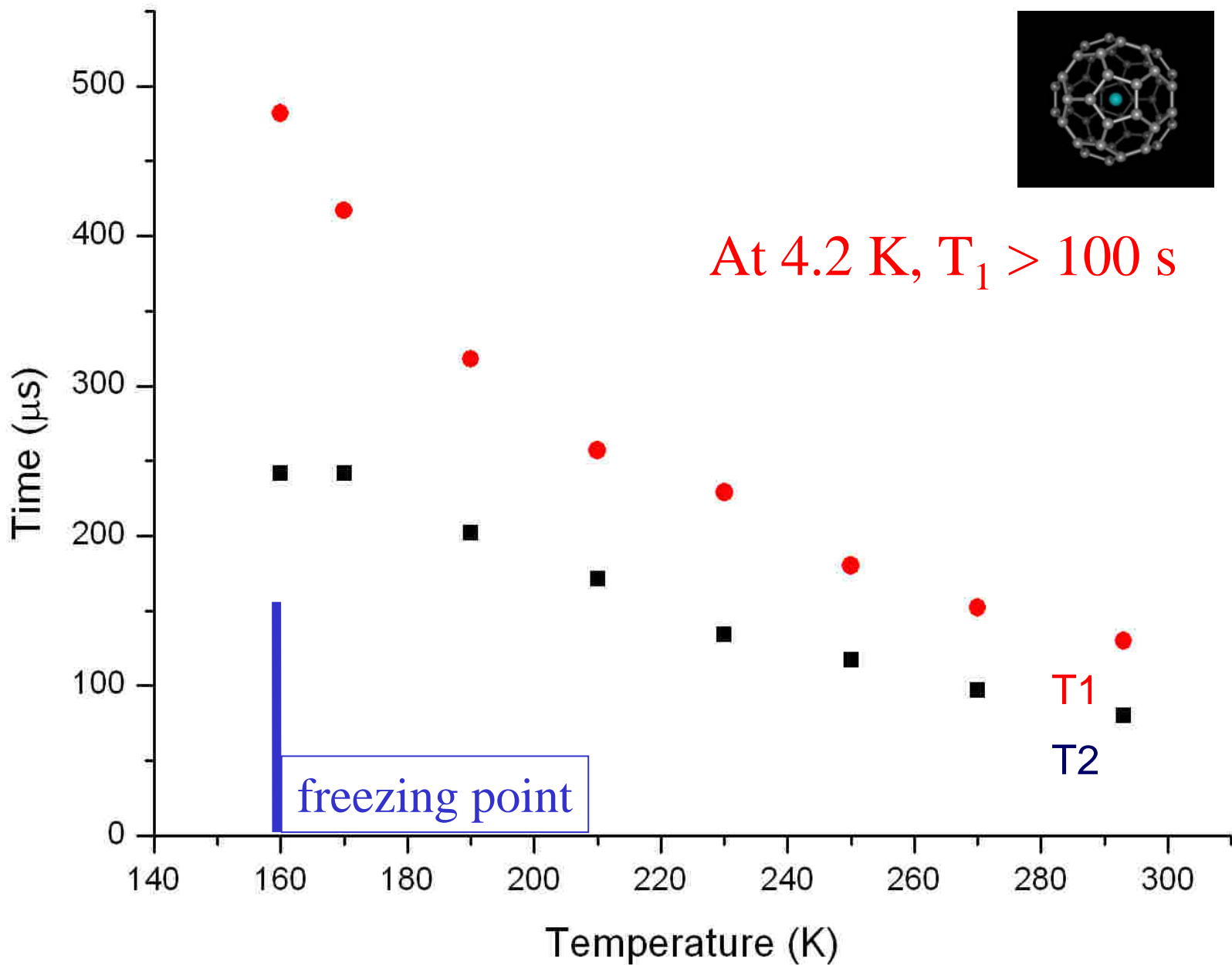
# BB1 sequence for spin manipulation



J.J.L. Morton *et al.*, *Phys. Rev. Lett.* **95**, 200501 (2005)

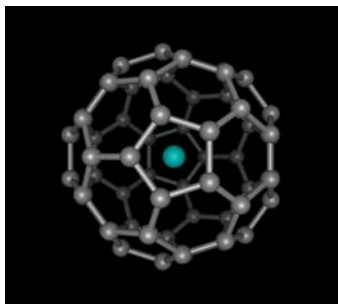
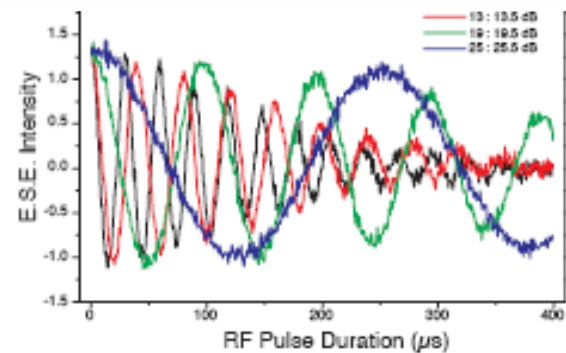
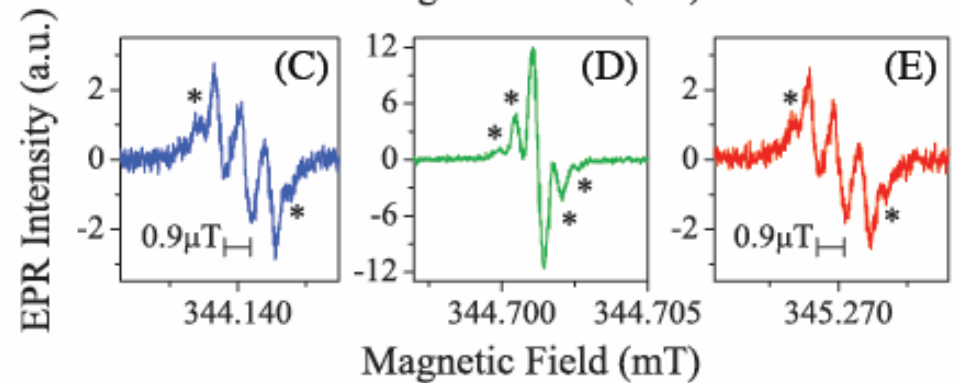
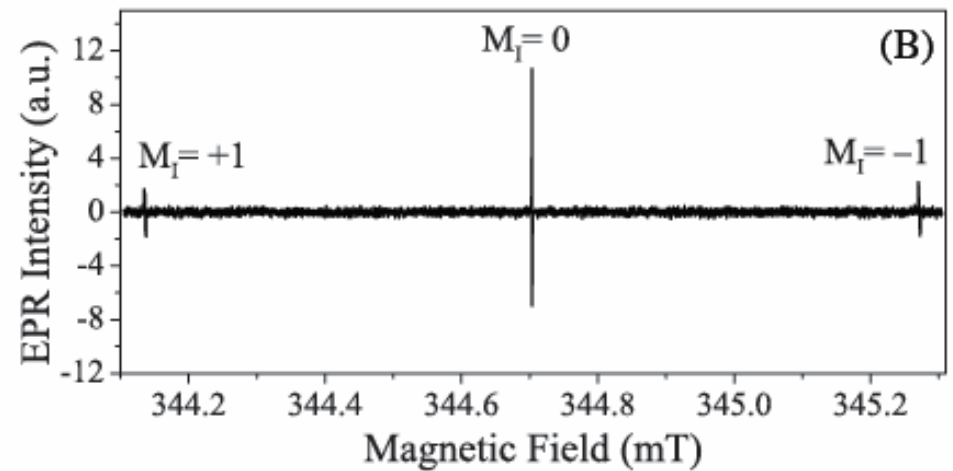
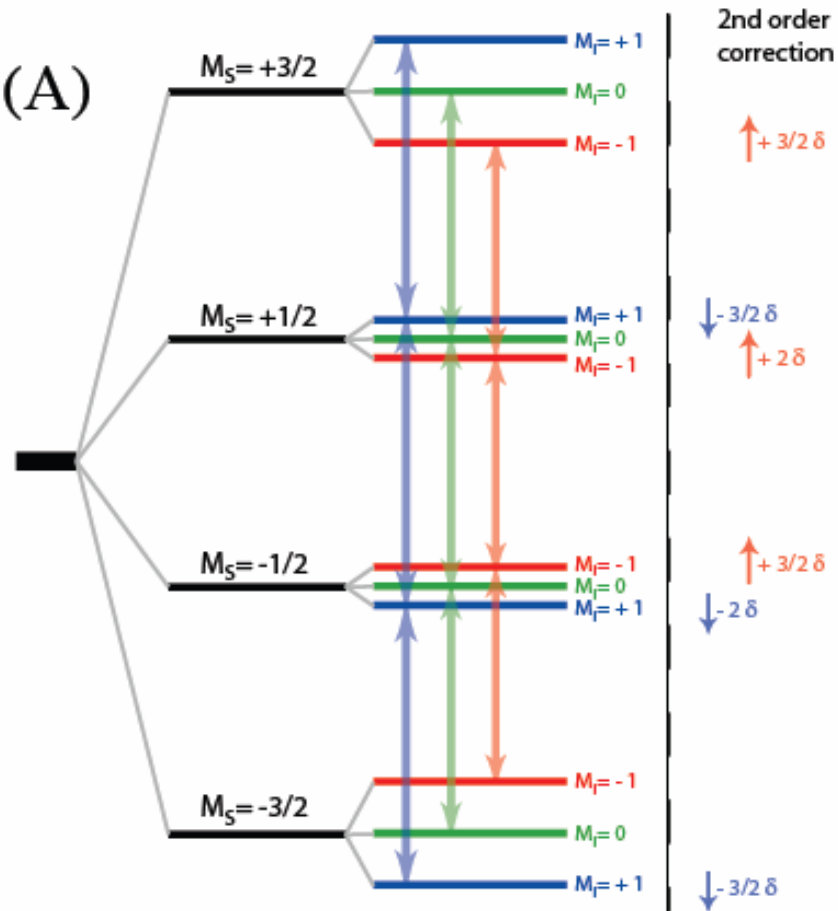


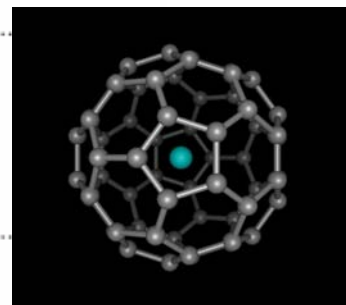
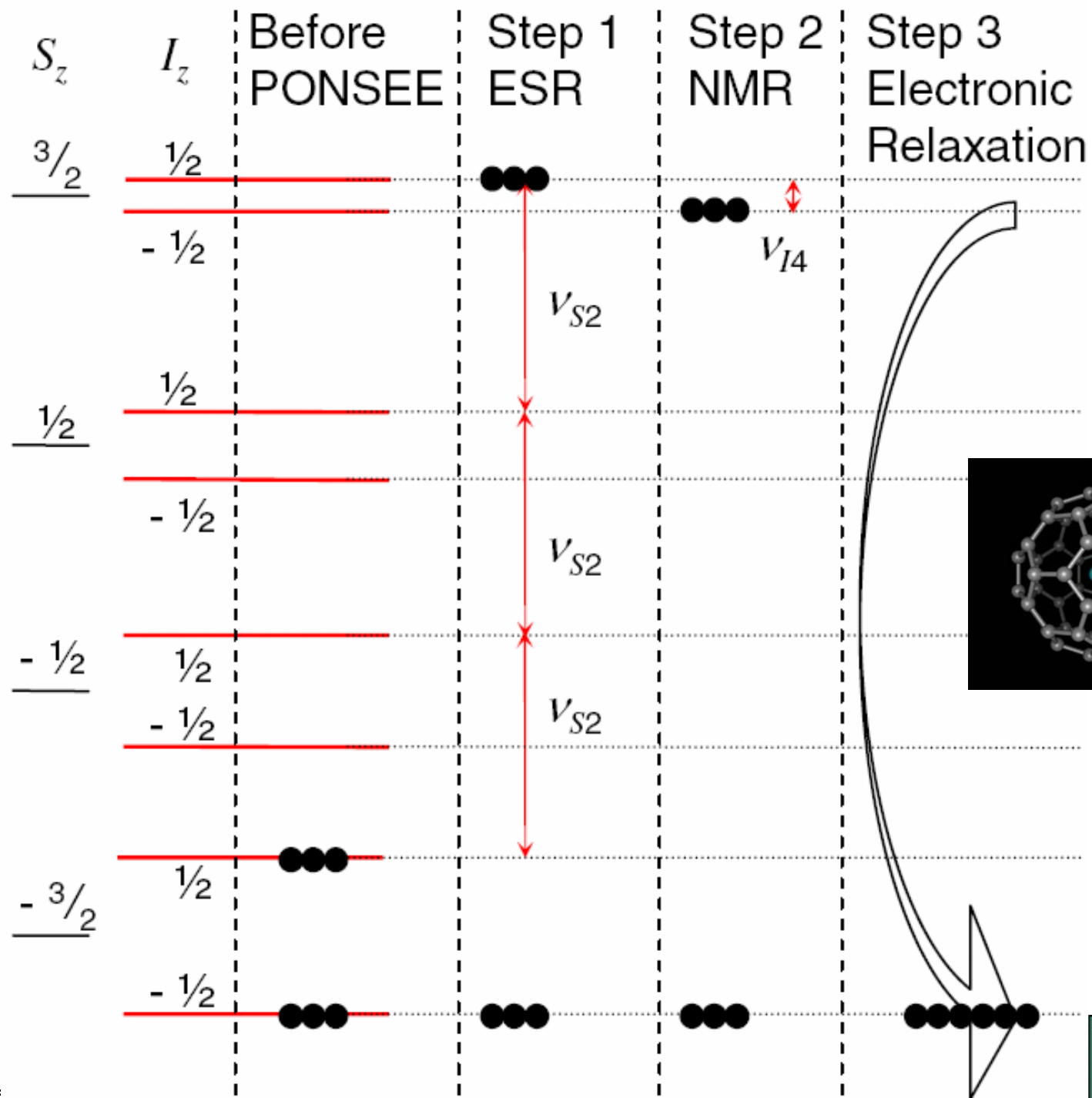
# Electron spin resonance of $^{14}\text{N}@C_{60}$



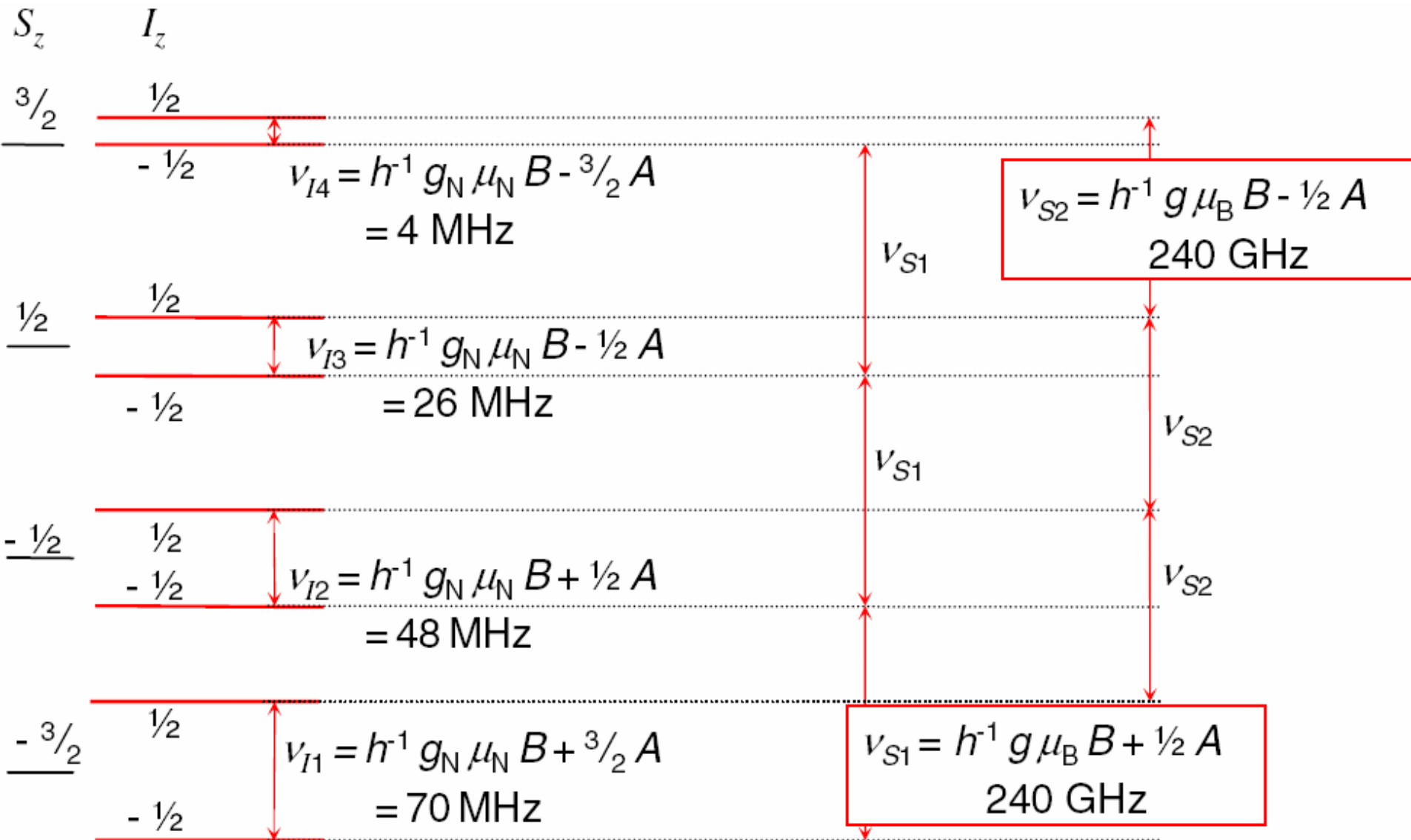


# $^{14}\text{N}@C_{60}$





# Dynamic nuclear polarisation of $^{15}\text{N}@C_{60}$



G. Morley *et al.*, *Phys. Rev. Lett.* **98**, 220501 (2007)

# Dynamic nuclear polarisation of $^{15}\text{N}@C_{60}$

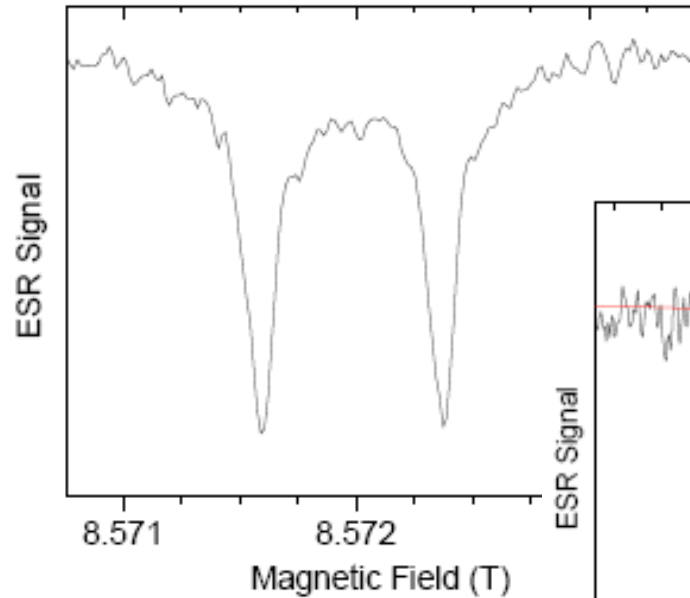


Figure 6.3: CW ESR scan of  $^{15}\text{N}@C_{60}$  in deuterated decalin; unusual lineshape is due to saturation.

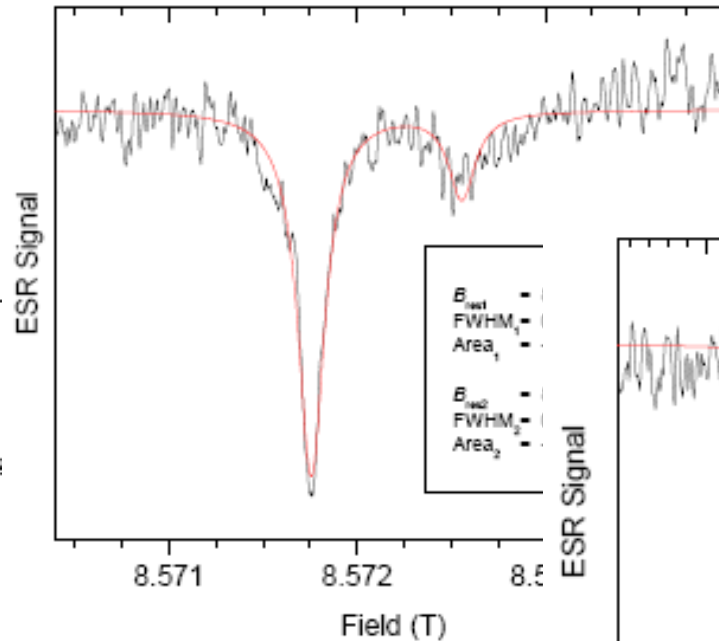


Figure 6.6: Averaged CW ESR scan of  $^{15}\text{N}@C_{60}$  at 3 K. red line is the bi-Lorentzian best fit with the parameters of the two peaks was set to be the same.

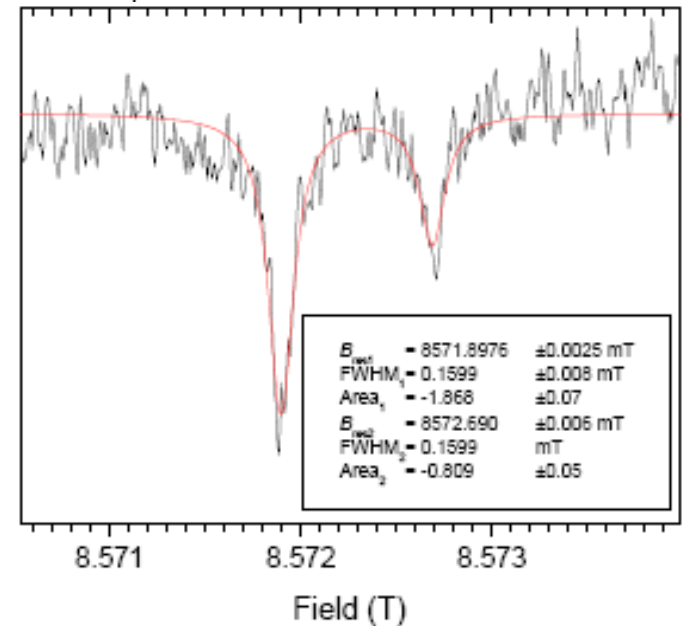
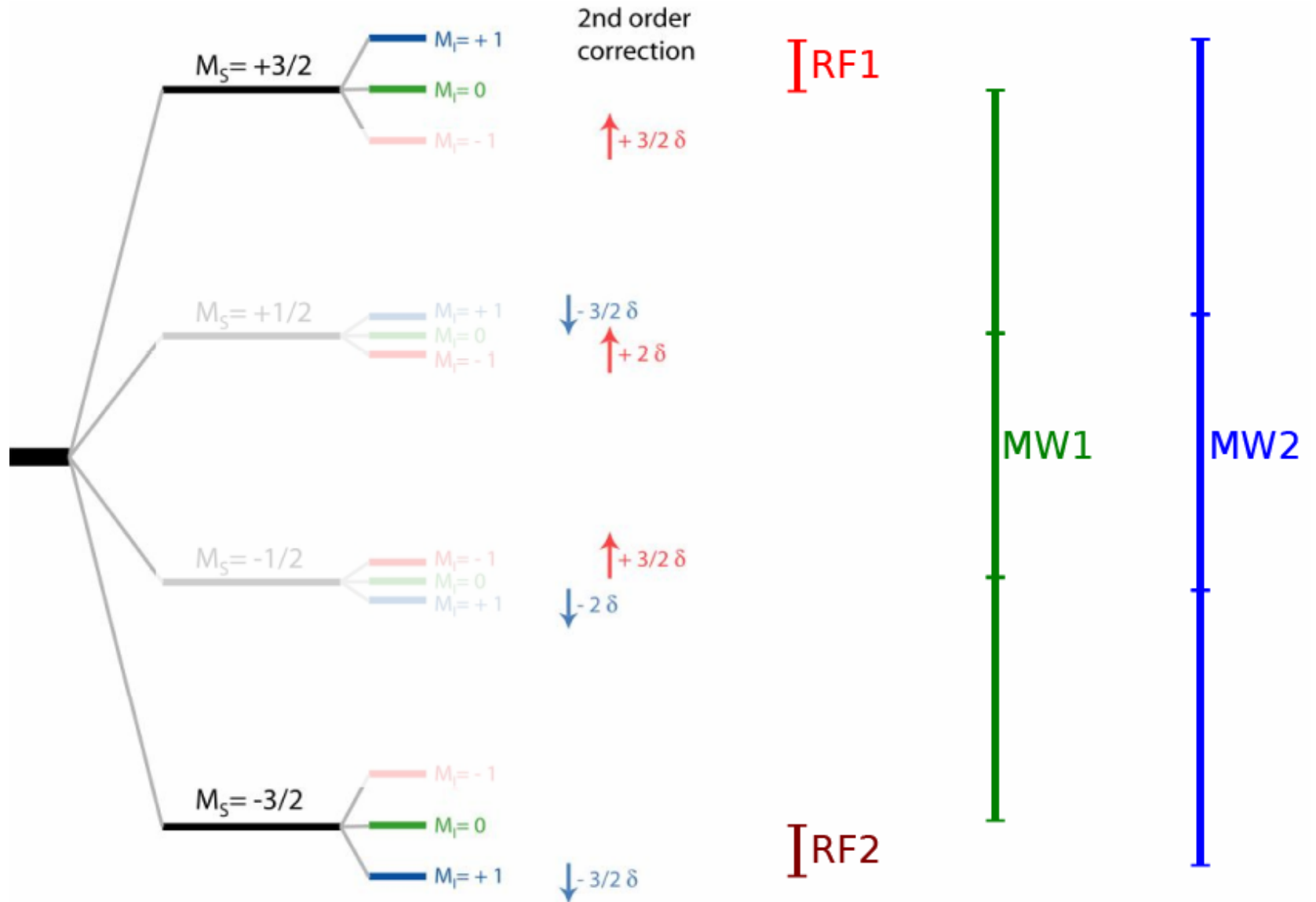


Figure 6.9: CW ESR scan of  $^{15}\text{N}@C_{60}$  at 4.2 K 11.5 hours after DNP polarization. In this time, the polarization has fallen from 4.3 (see Figure 6.6) to 2.3. The red line is the bi-Lorentzian best fit with equal line-widths.

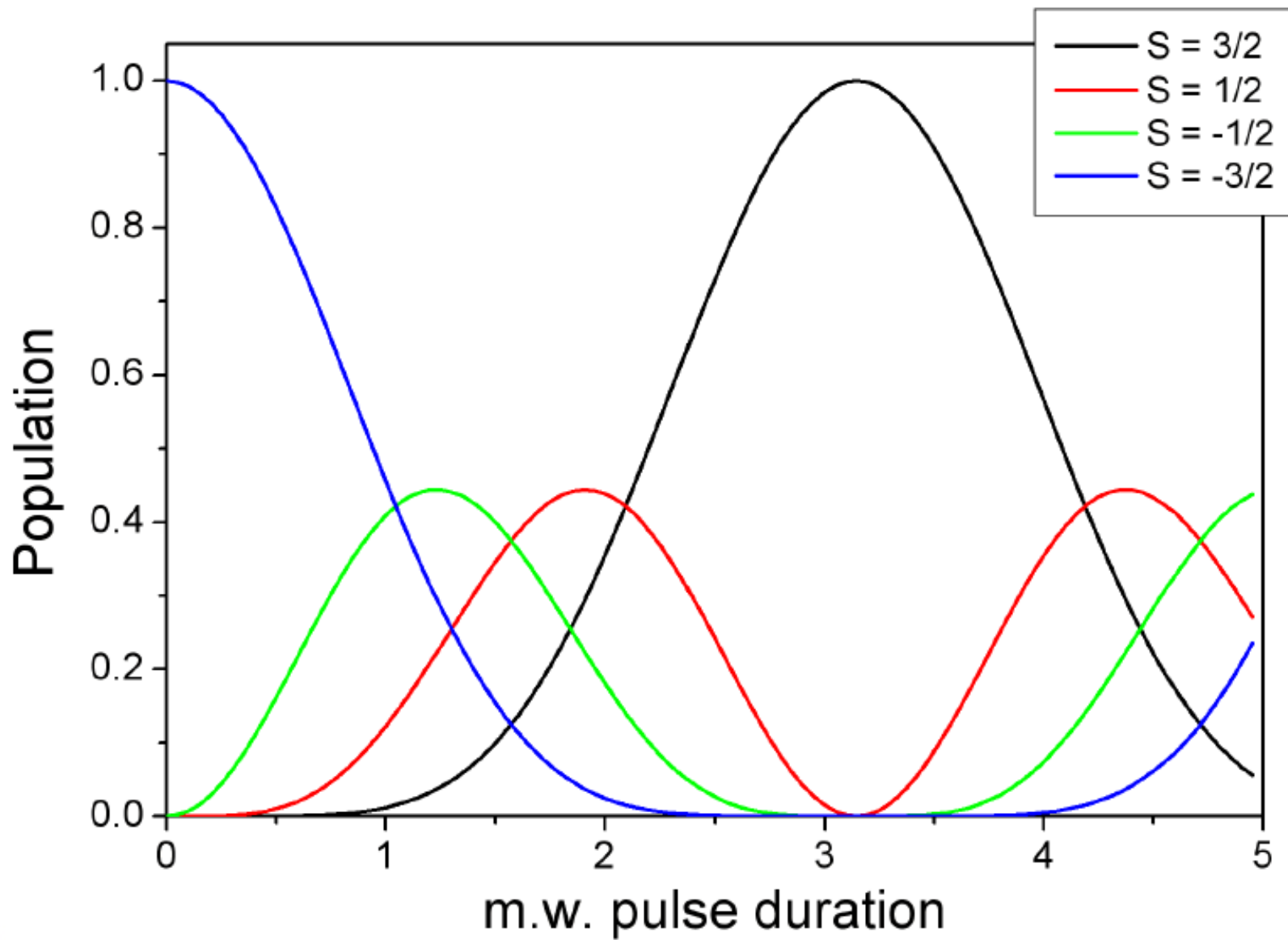
G. Morley *et al.*, *Phys. Rev. Lett.* **98**, 220501 (2007)



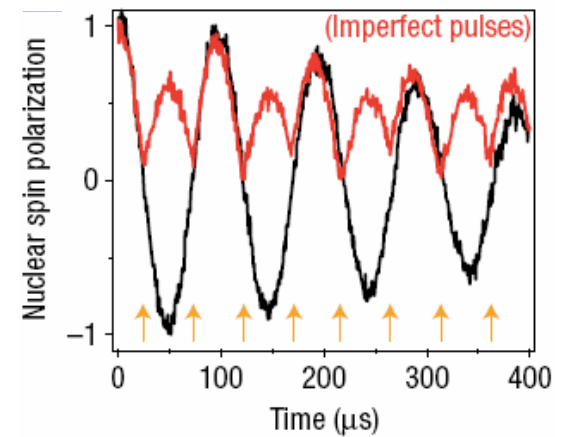
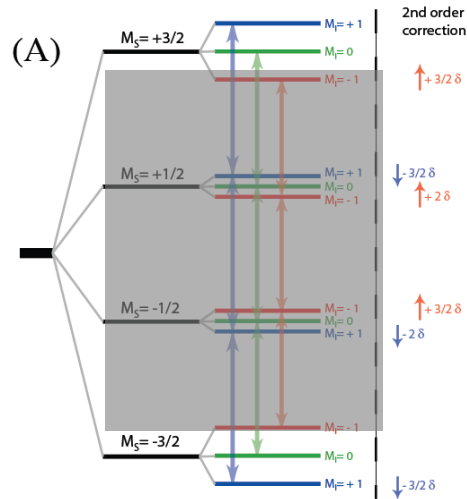
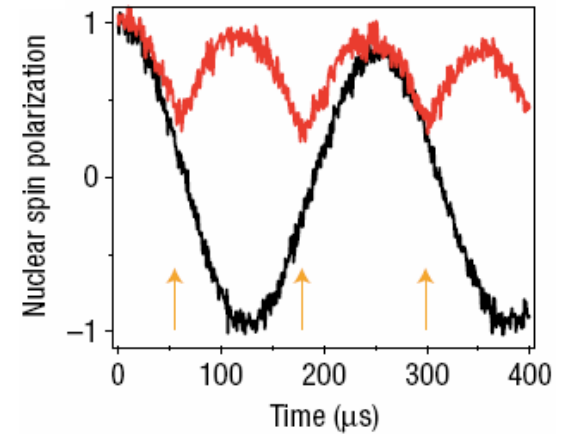
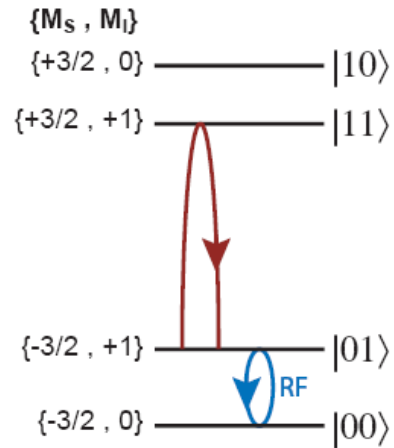
# $^{14}\text{N}@C_{60}$



# $N@C_{60}$



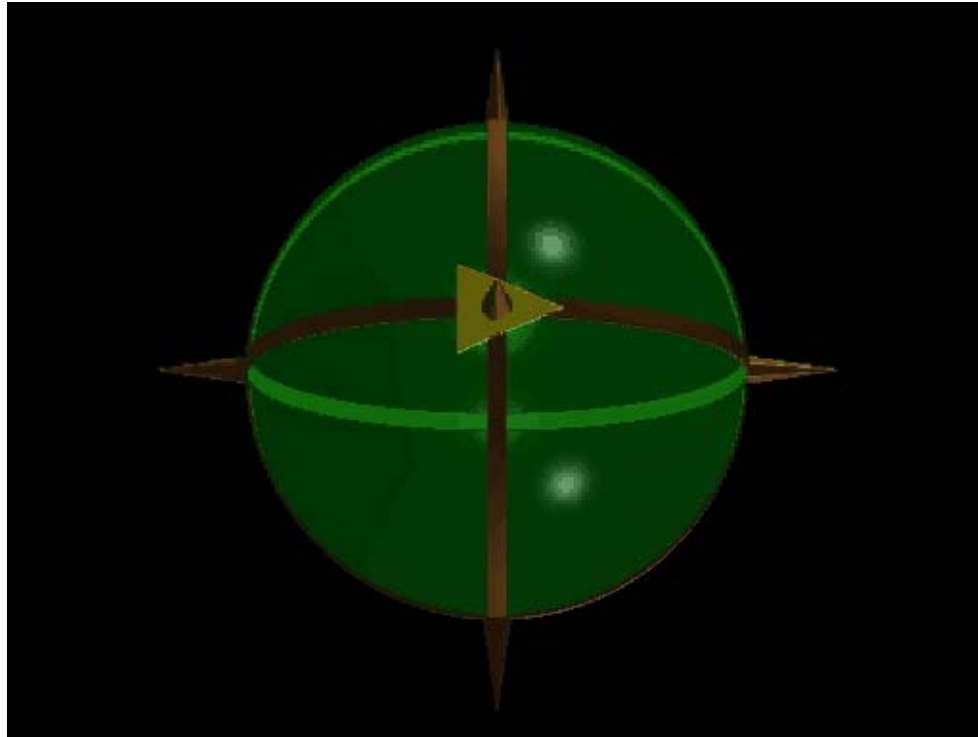
# Bang-bang control



J.J.L. Morton *et al.*, *Nature Physics* **2**, 40-43 (2006)



# *Bang-bang control*

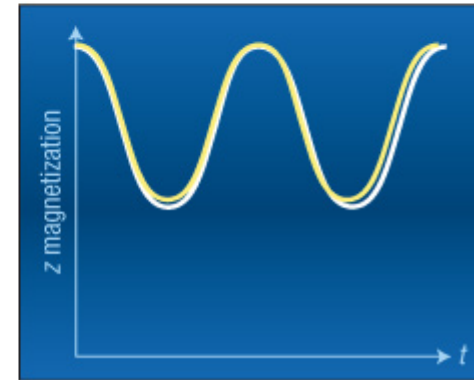
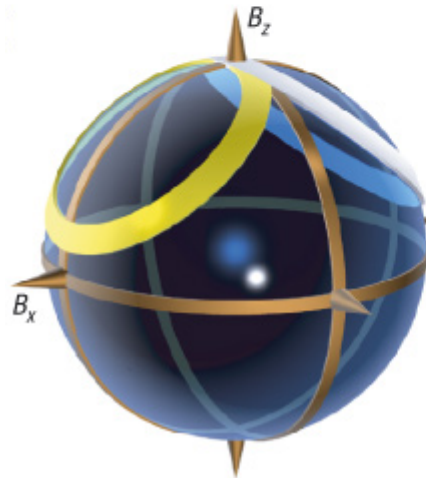
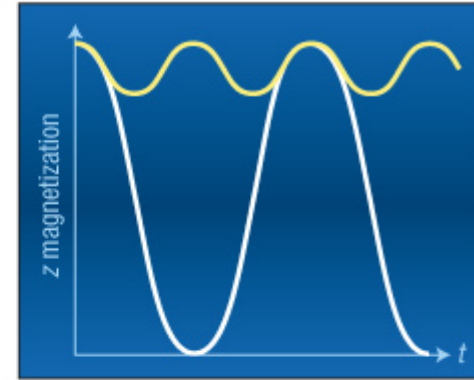
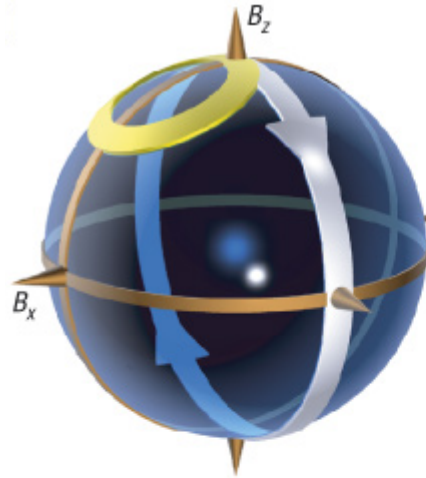
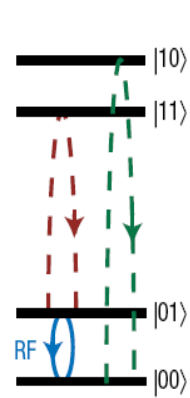
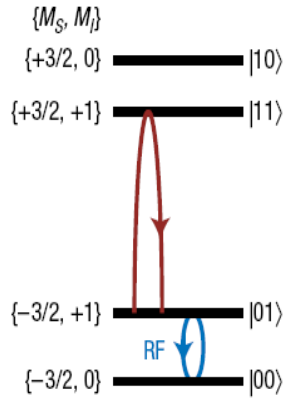


J.J.L. Morton *et al.*, *Nature Physics* **2**, 40-43 (2006)





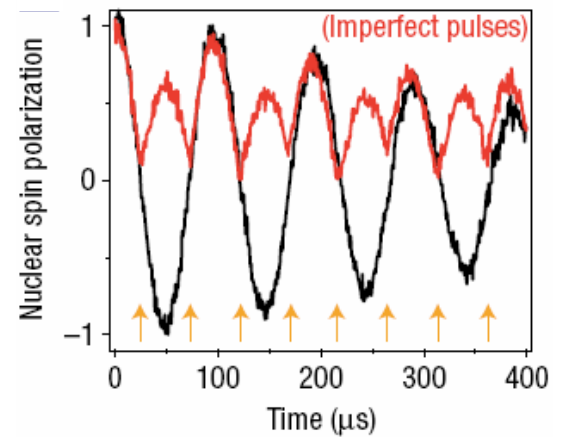
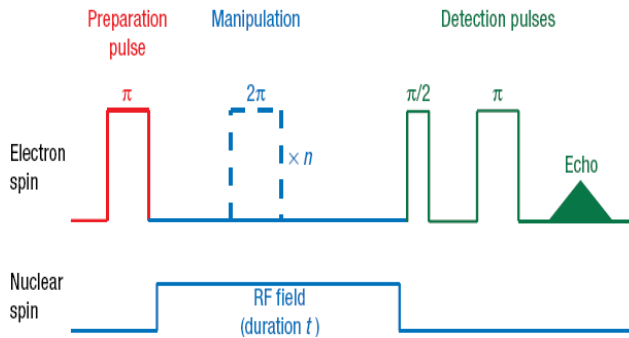
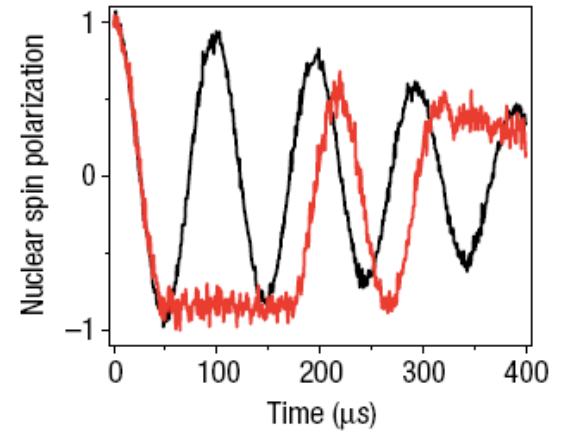
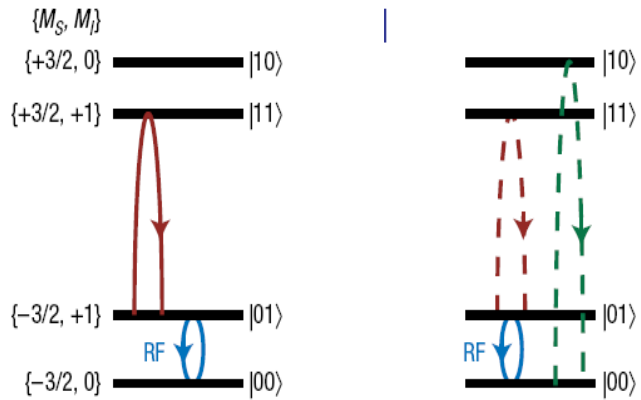
# Bang-bang control



J.J.L. Morton *et al.*, *Nature Physics* **2**, 40-43 (2006)



# Bang-bang control

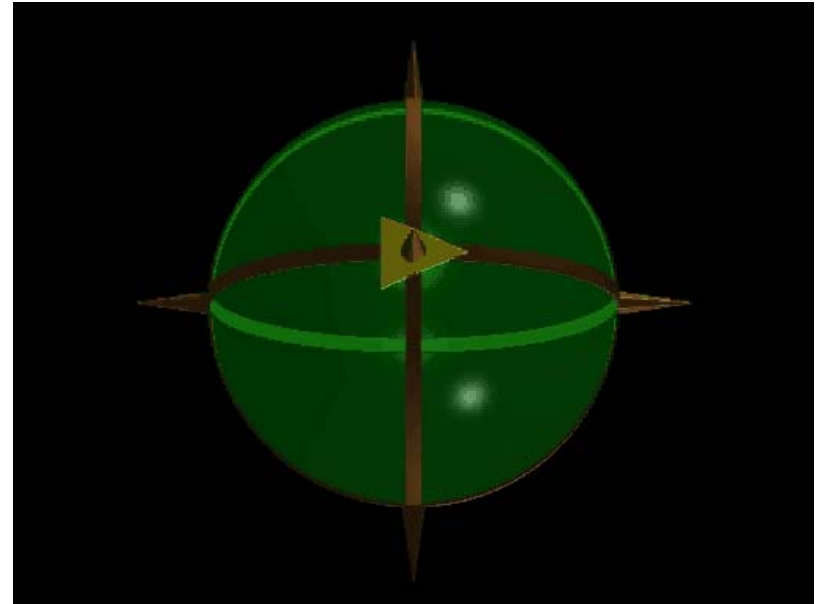


J.J.L. Morton *et al.*, *Nature Physics* **2**, 40-43 (2006)



# *Bang-bang* control

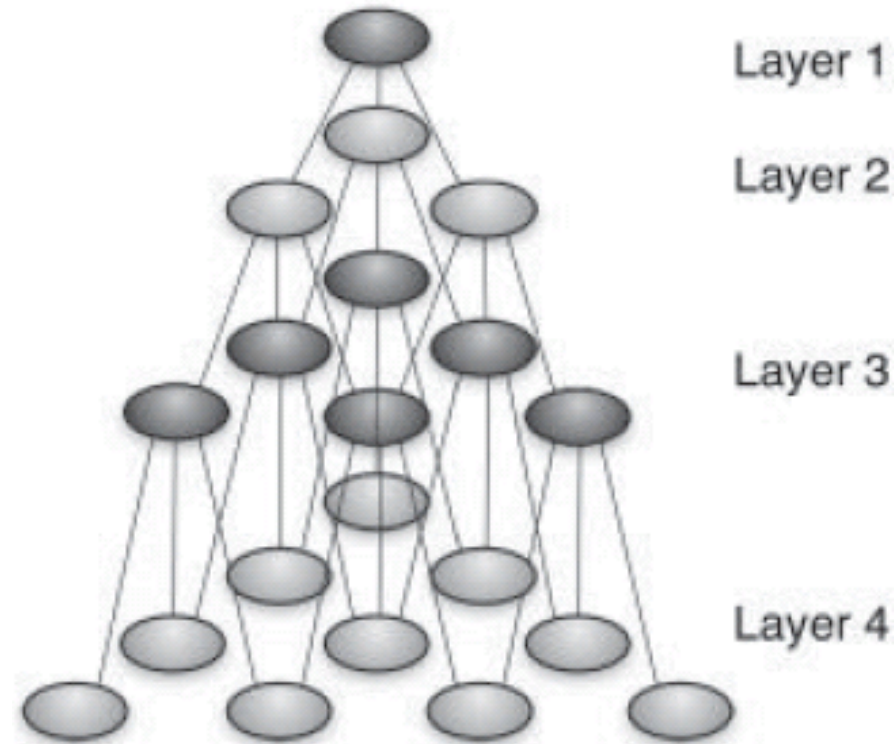
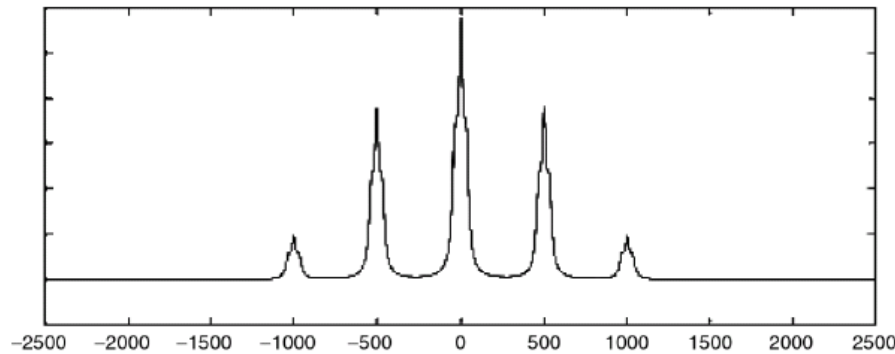
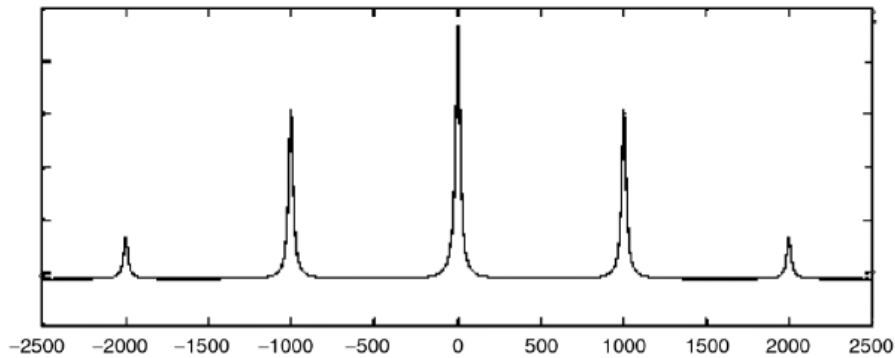
- Unlike quantum Zeno, *bang-bang* control is fully deterministic.
- *Bang-bang* control can be used for control of the nuclear spin qubit with speed determined by the electron spin manipulation.
- The principle of *bang-bang* control can be applied to other systems with three or more levels.



J.J.L. Morton *et al.*, *Nature Physics* **2**, 40-43 (2006)



# Spin amplification for measurement

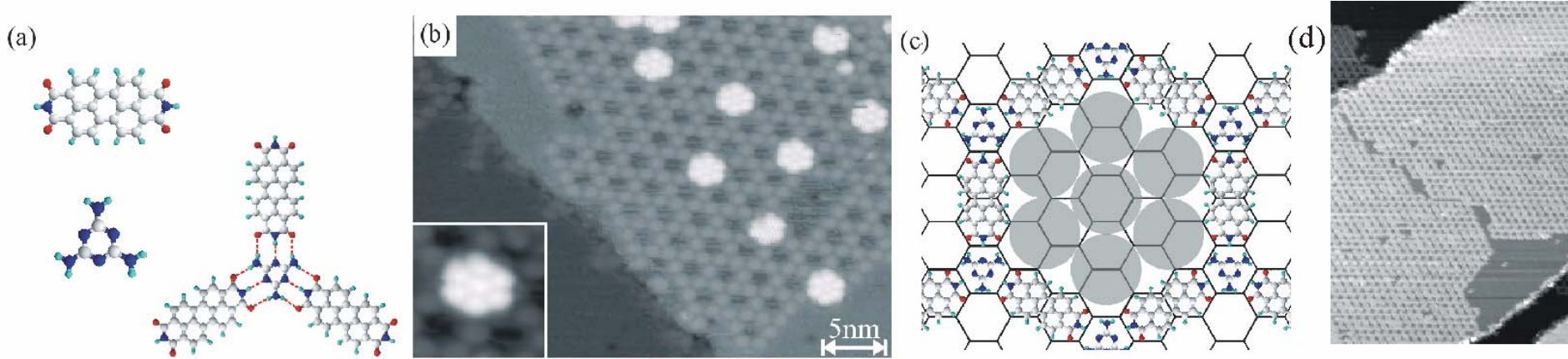


$O(\sqrt[3]{N})$  steps  $\rightarrow$   $N$  correlated spins

Perez-Delgado *et al.*, *Phys. Rev. Lett.* **97**, 100501 (2006)



# 2-D spin arrays



**(a) Component molecules melamine and perylene tetracarboxylic diimide (PTCDI) can be connected by three hydrogen bonds per molecular junction.**

**(b) The molecules are sublimed onto a silicon surface. Melamine forms the vertices and PTCDI forms the edges of a network that assembles spontaneously. The open network provides a template for adsorption of fullerenes.**

**(c) The pores in the network form nanoscale traps which capture fullerene molecules and stabilise heptameric  $C_{60}$  clusters.**

**(d) Networks can extend over several hundreds of nanometres.**

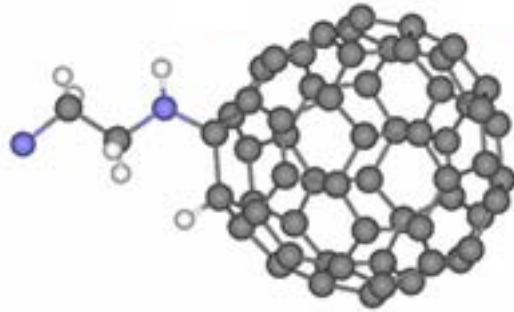


Theobald *et al.*, *Nature* **424**, 1029 (2003)



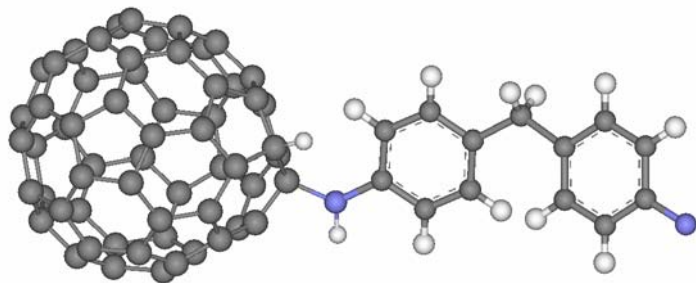
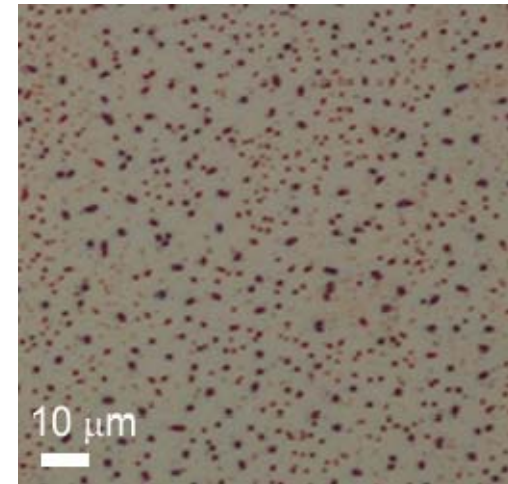
# 3-D spin arrays

## Functionalized fullerenes

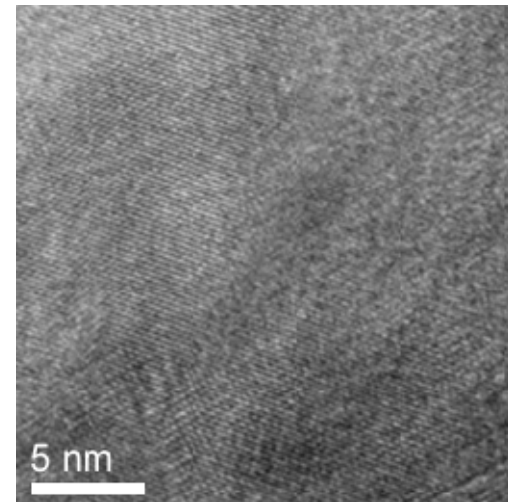
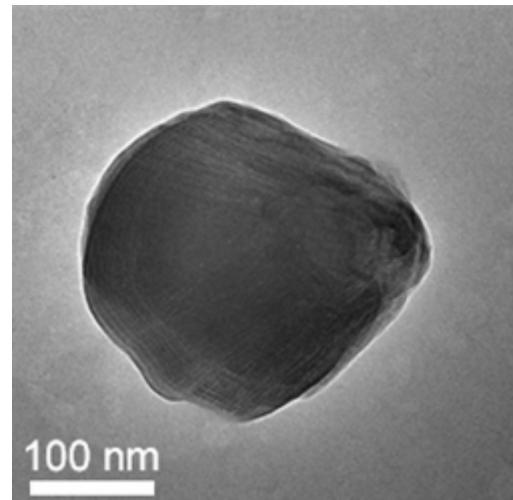


C<sub>60</sub>-ethylenediamine

(a) before  
(b) after  
functionalization



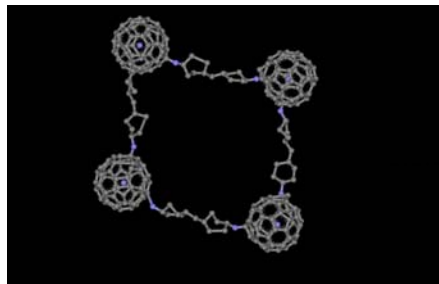
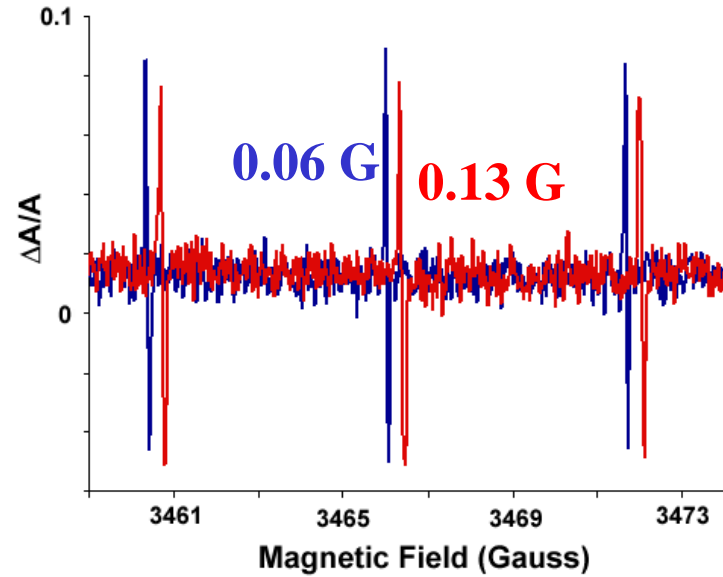
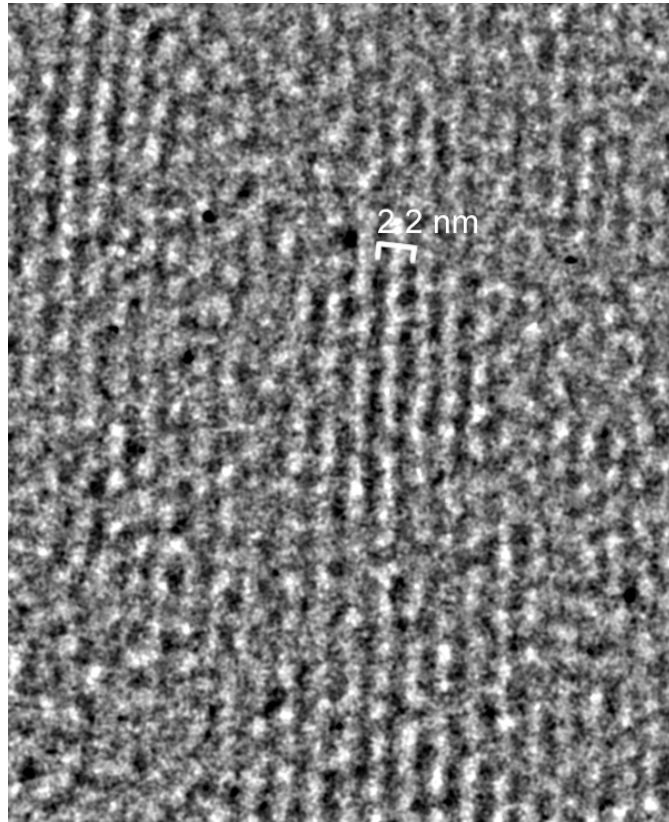
C<sub>60</sub>-4,4'-methylenedianiline



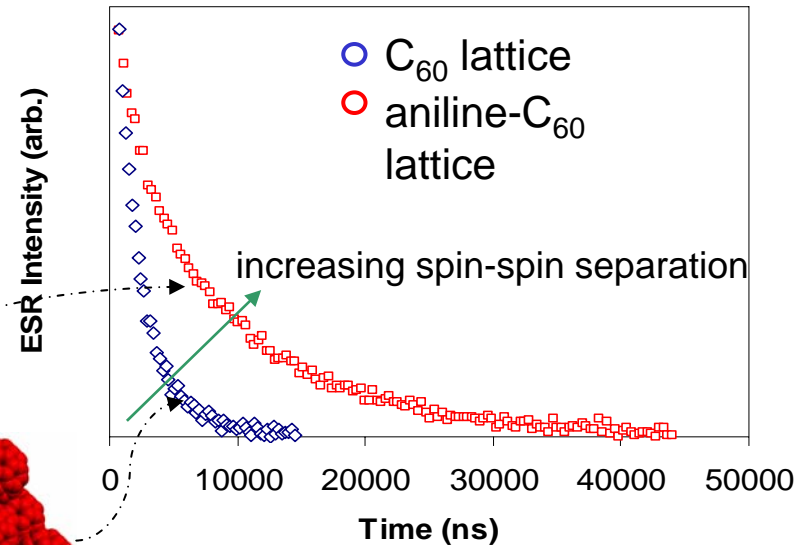
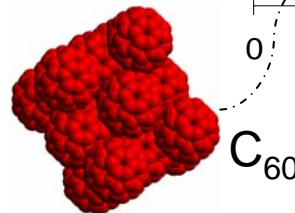
Watt *et al.*, *Chem. Commun.*, 2006, 1944-1946



# 3-D spin arrays

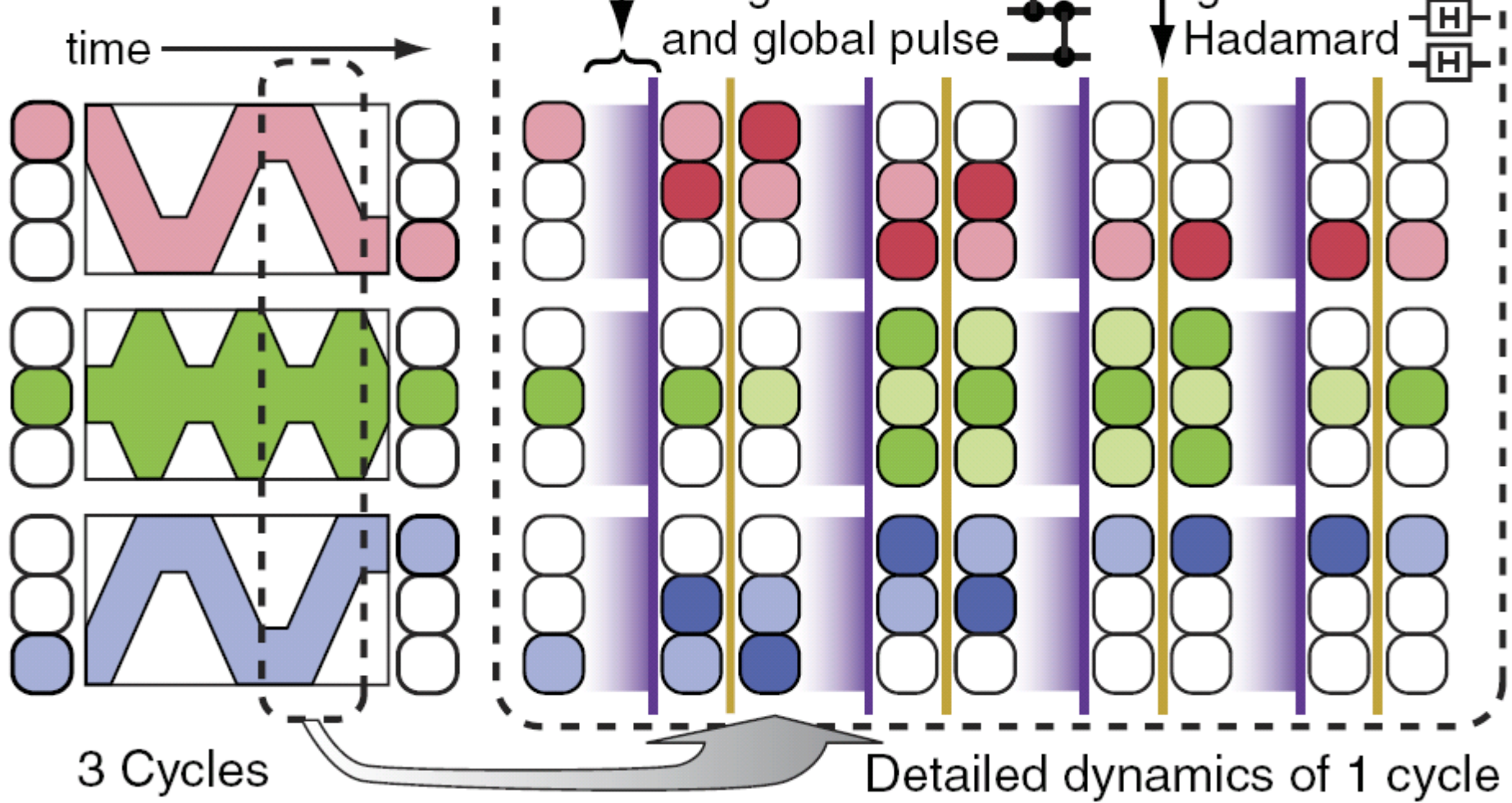


$C_{60}$ -4,4'-methylenedianiline



# Decolocalize-and-revive

(a) Quantum Mirror

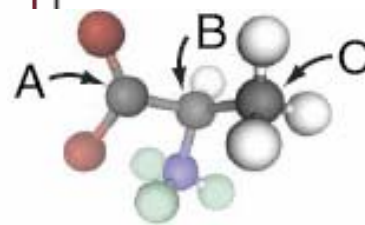
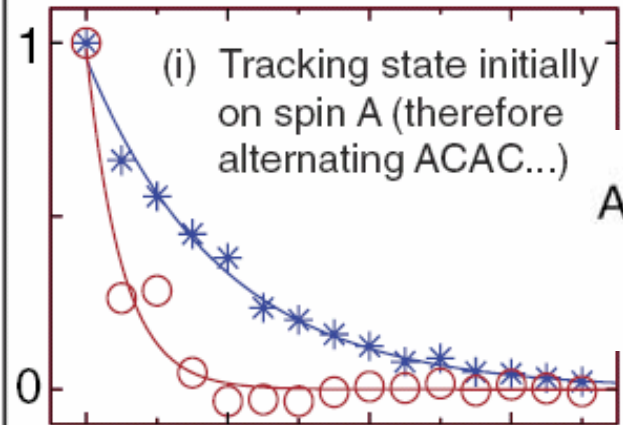
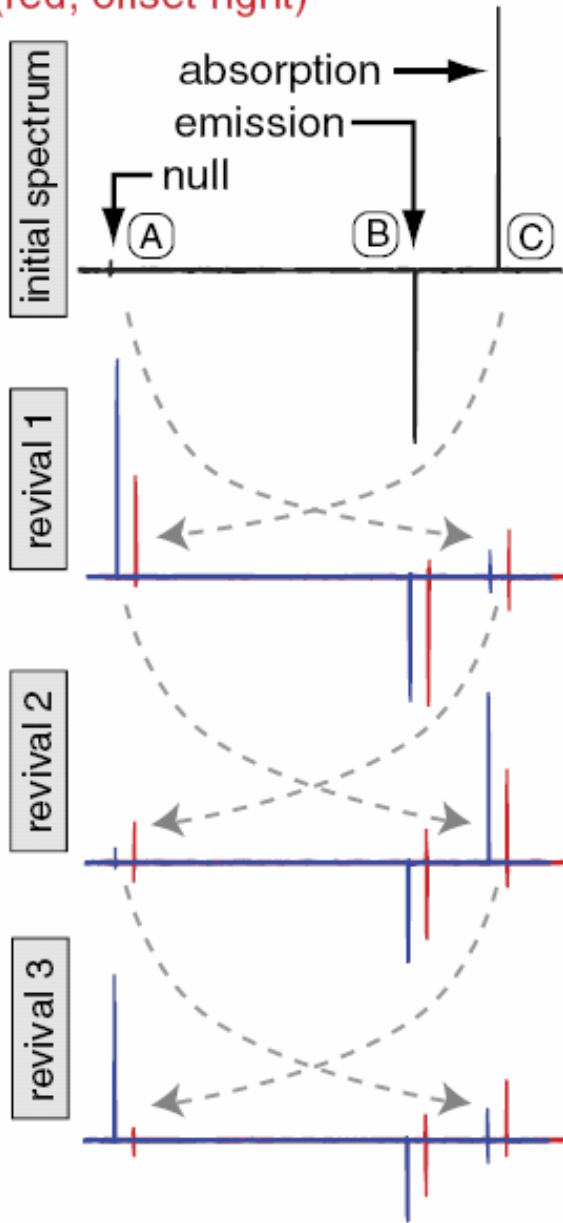


*J. Fitzsimons et al., Phys. Rev. Lett. 99, 030501 (2007)*

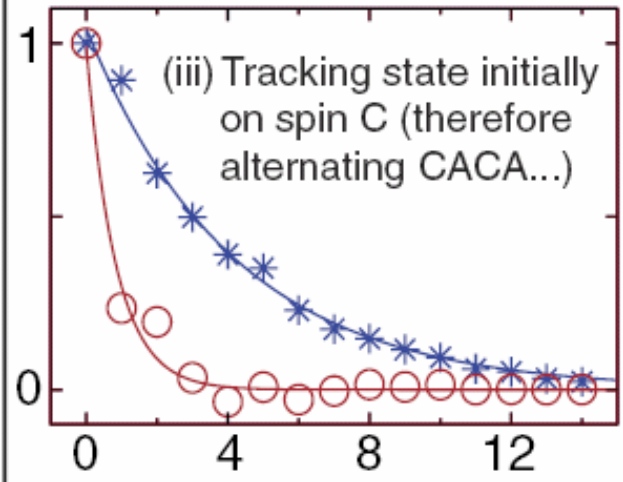
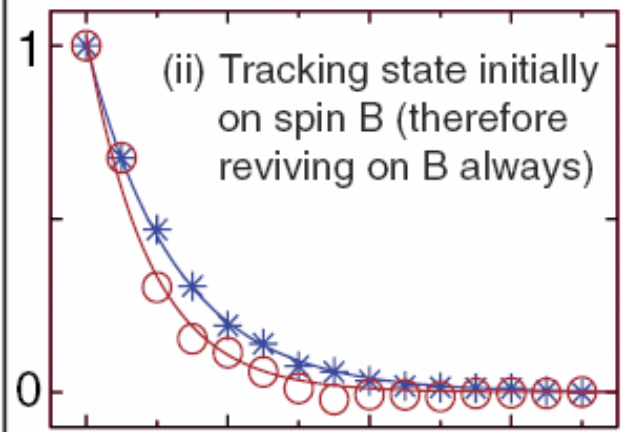




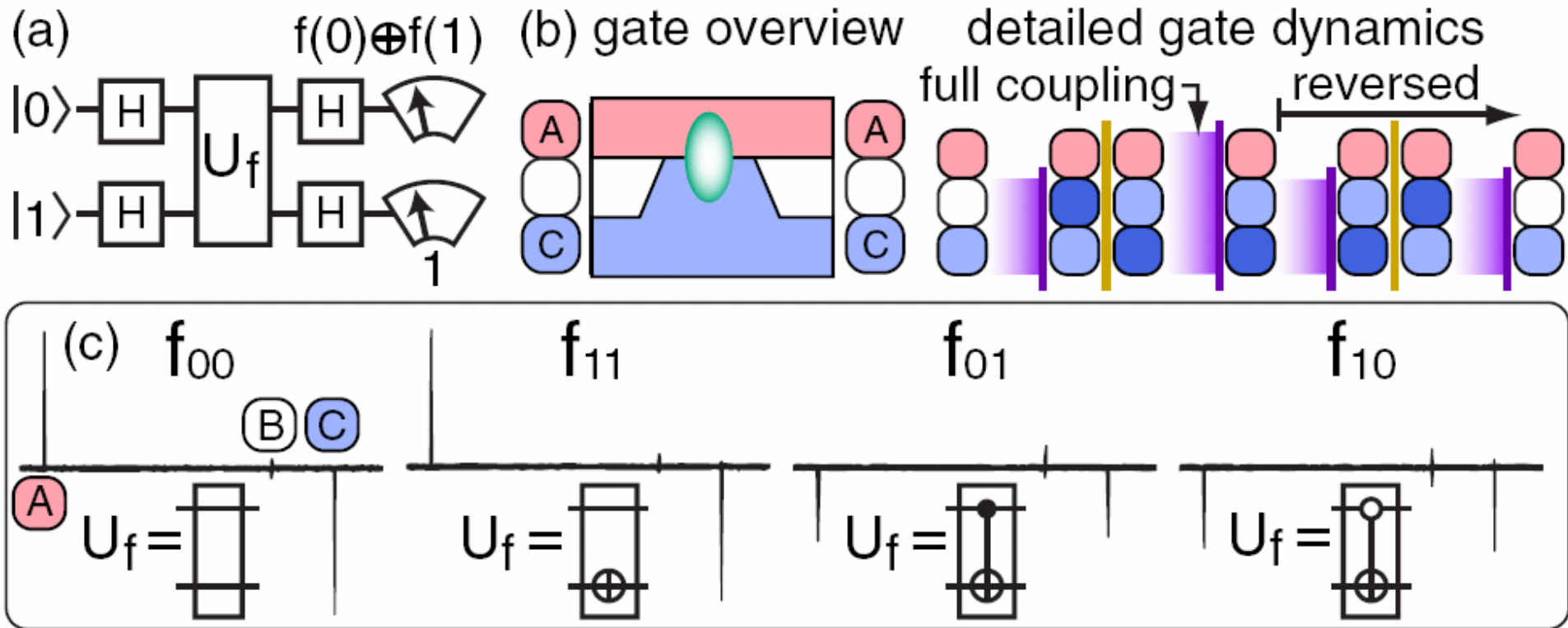
Quantum mirror (blue) versus SWAP network (red, offset right)



<sup>13</sup>C-labeled aniline in D<sub>2</sub>O



# Deutsch's algorithm



J. Fitzsimons *et al.*, *Phys. Rev. Lett.* **99**, 030501 (2007)



# Can you build a quantum computer with carbon?

