CHEM40111/CHEM40121

Molecular magnetism

8 Quantum information processing

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Course Overview

1 Fundamentals • Motivation • Origins of magnetism • Bulk magnetism	**5 Single-molecule magnets I** • Single-molecule magnets • Electrostatic model
2 Quantum mechanics of magnetism • Zeeman effect • Statistical mechanics • Magnetisation • Magnetic susceptibility	**6 Single-molecule magnets II** • Measuring magnetic relaxation • Relaxation mechanisms • Latest research
3 Magnetic coupling • Exchange Hamiltonian • Experimental measurements • Vector coupling	**7 Magnetic resonance imaging** • Paramagnetic NMR • Magnetic resonance imaging • Latest research
4 Magnetic anisotropy • Zero-field splitting • Impact on properties • Lanthanides • Spin-orbit coupling	**8 Quantum information processing** • Quantum information • DiVincenzo criteria • Latest research • ***Question time***

Intended learning outcomes

1. Explain the origin of magnetism arising from electrons in atoms and molecules using formal quantum-mechanical terms

2. Compare and contrast the electronic structure of metal ions in molecules and their magnetic properties, for metals across the periodic table

3. Select and apply appropriate models and methods to calculate molecular magnetic properties such as magnetisation, magnetic susceptibility and paramagnetic NMR shift

4. Deconstruct topical examples of molecular magnetism including single-molecule magnetism, molecular quantum information processing and MRI contrast agents

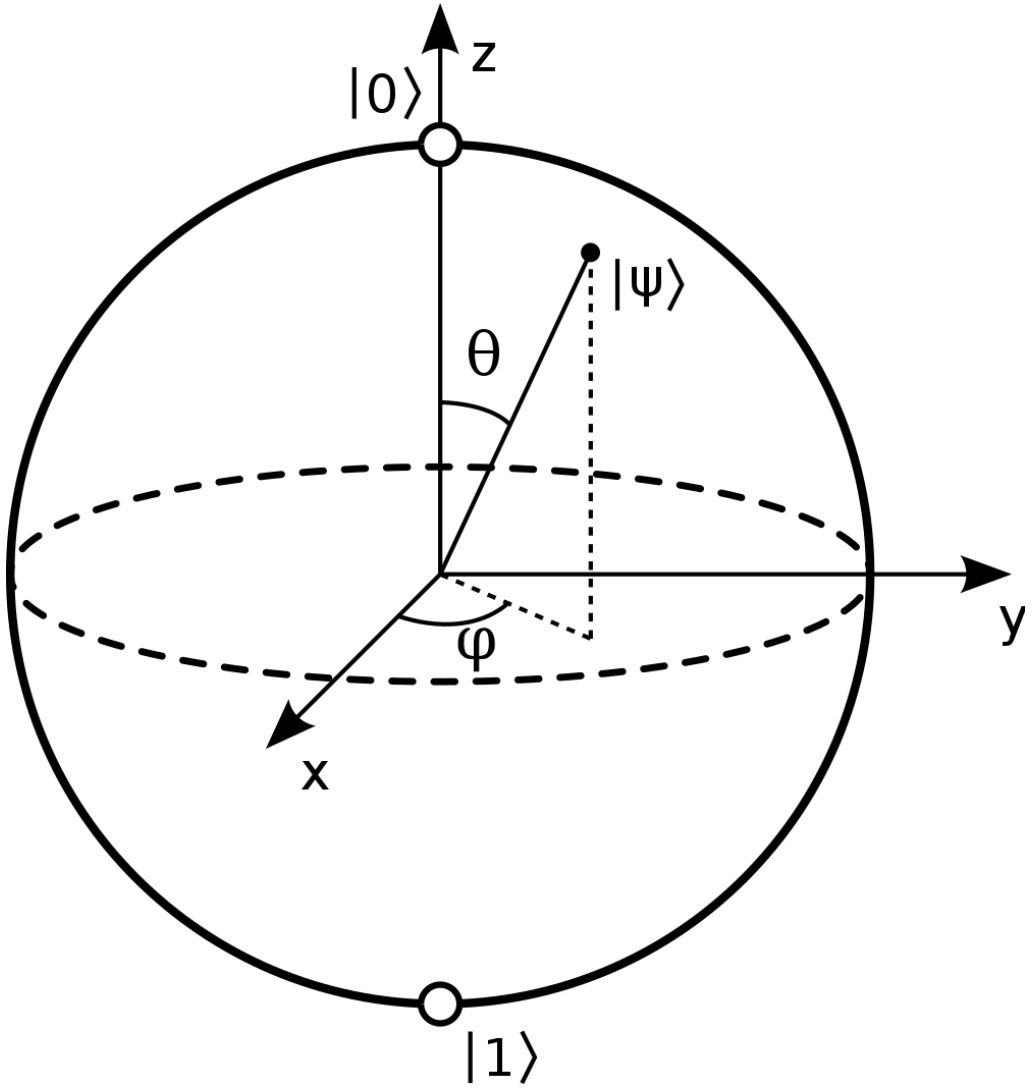
Quantum information

- UP and DOWN states are classical bits

- Quantum bits (qubits) can be anywhere on the Bloch sphere

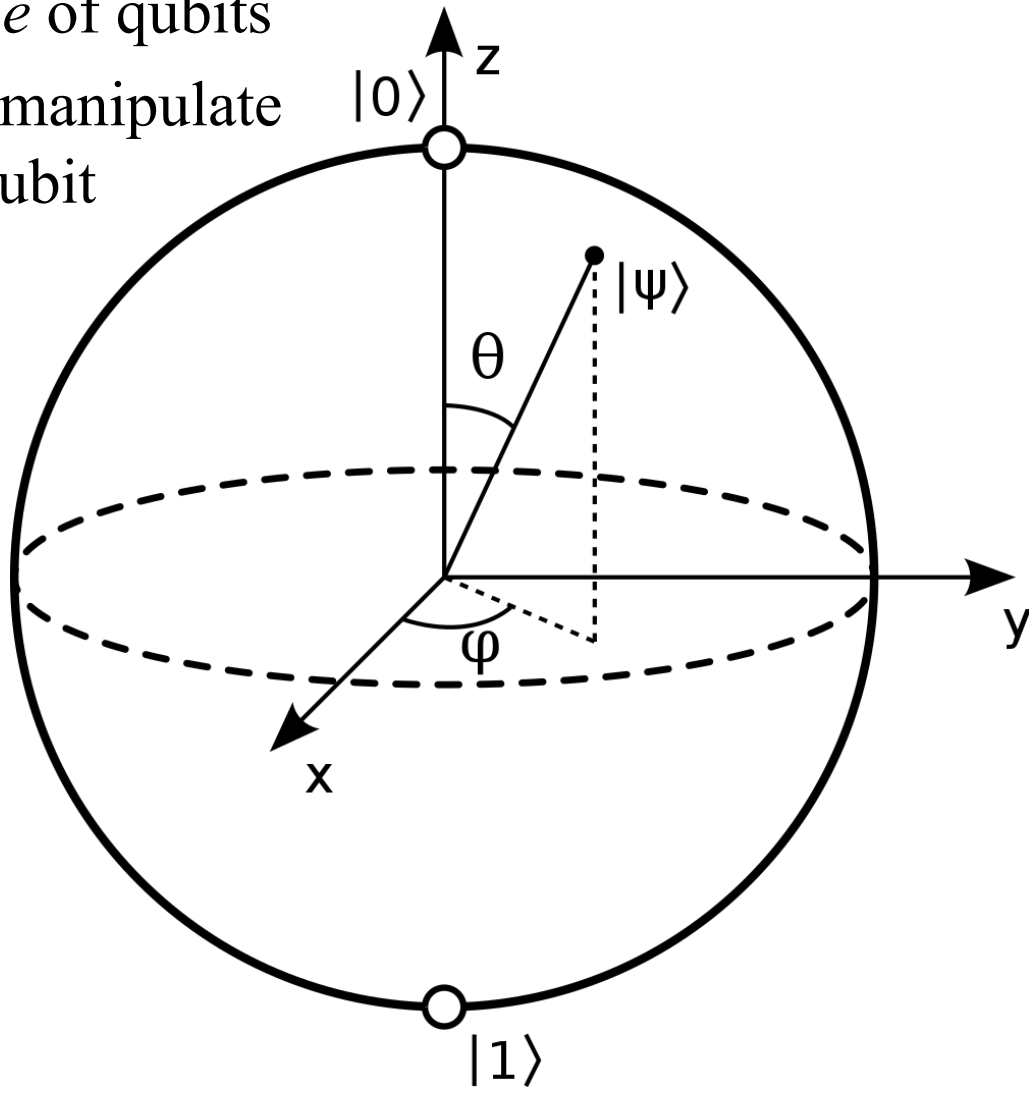
$$|\psi\rangle = \alpha|1\rangle + \beta|0\rangle$$

- Allows quantum computers to do things classical computers cannot

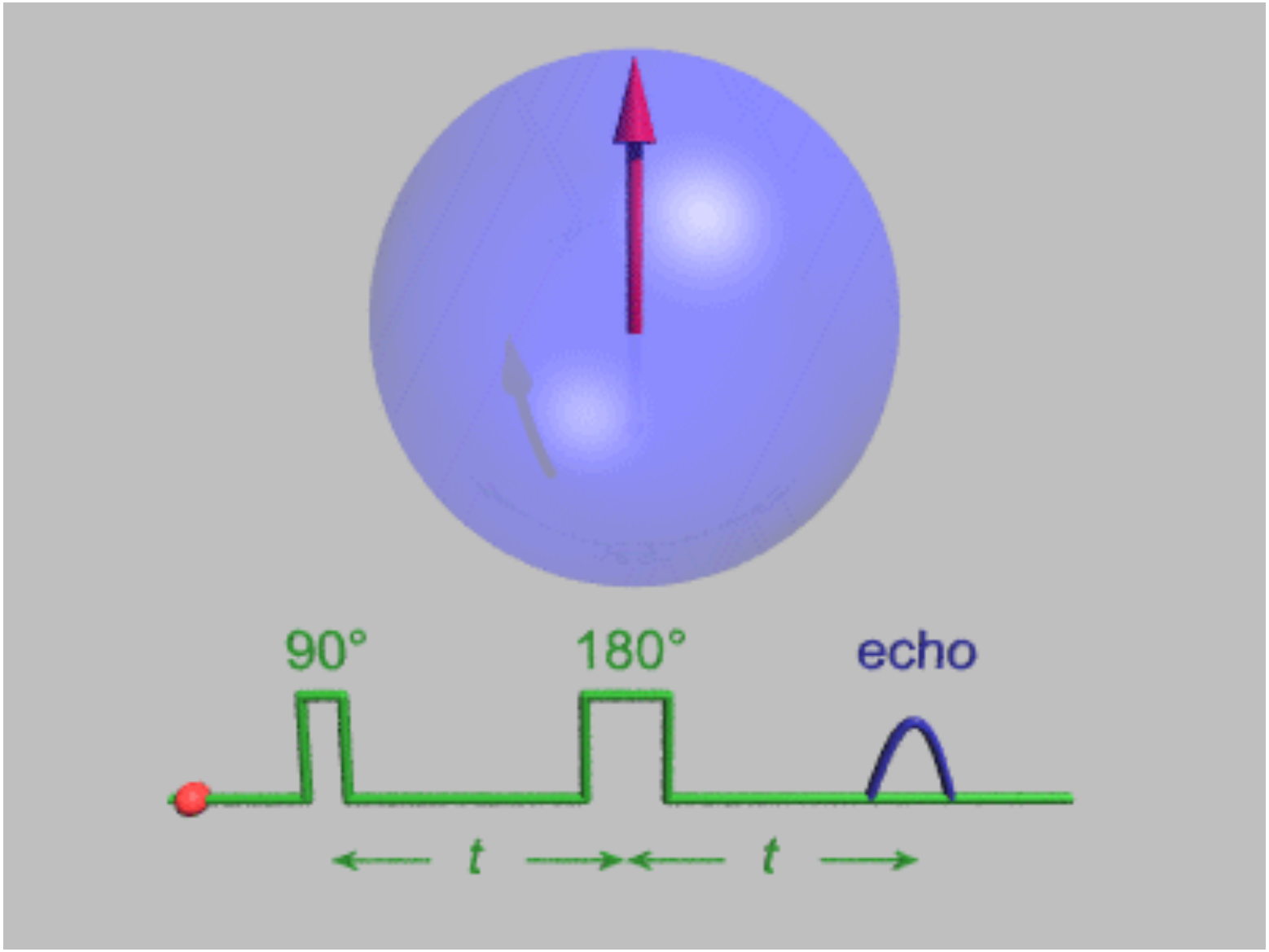


Quantum information

- We talk about *coherence time* of qubits
  - This is how long we can manipulate the state $|\psi\rangle$ before the qubit gets messed up
- We want this to be as long as possible!



Quantum information



Building a quantum computer

- The DiVincenzo criteria:

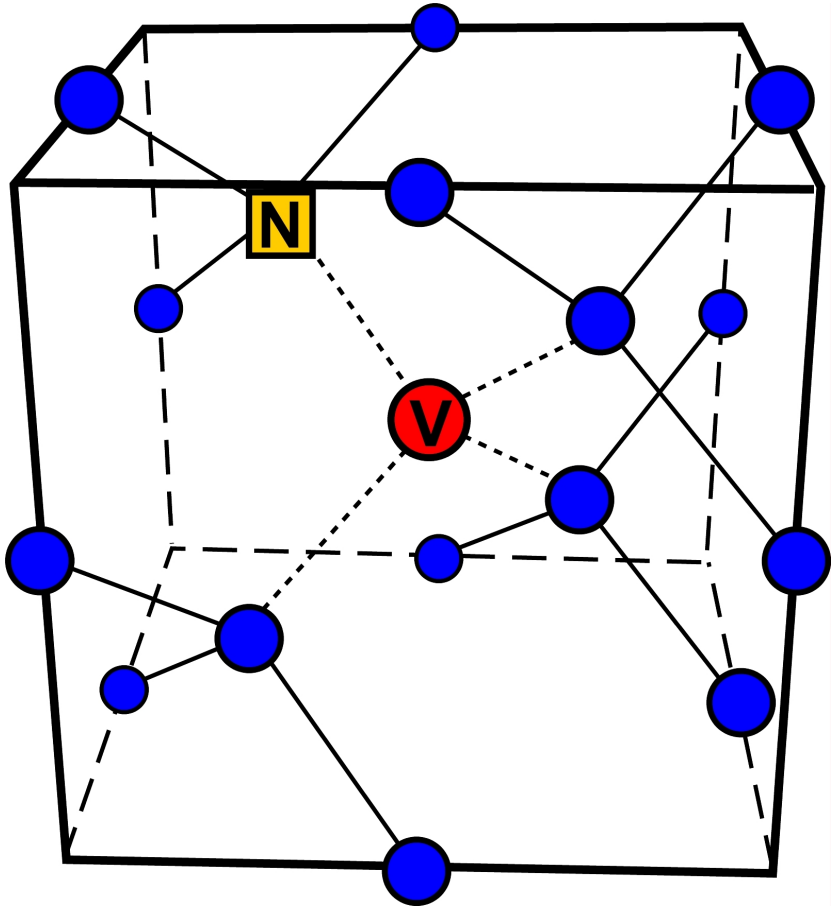
1. Scalable system with well-characterized qubits
2. The ability to initialize the qubits
3. Long coherence times
4. A universal set of quantum gates
5. The ability to readout the qubits

- Many ways to implement qubits:
  - Trapped ions
  - Superconducting circuits (D-Wave, Google, IBM)
  - Defects in diamond
  - Molecular magnets

[1] D. P. DiVincenzo, Fortschritte der Physik, 2000, **48**, 771.

NV centres

- Nitrogen-vacancy (NV) centres are defects in diamond
  - A nitrogen impurity is next to a vacancy, and is charged -1:

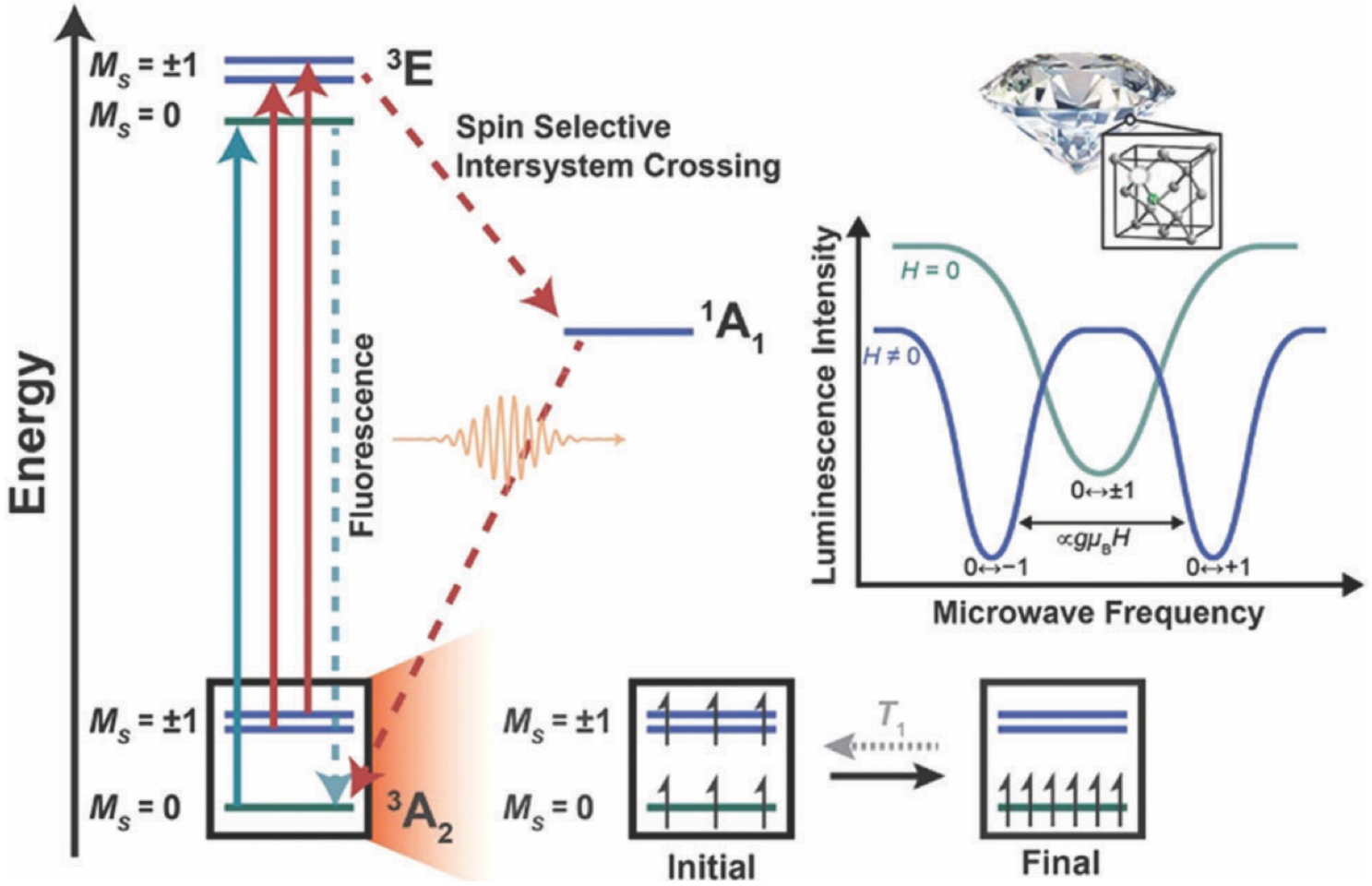


- N atom has three σ-bonds and a lone pair
- Vacancy has three "dangling" σ bonds, each with one electron
- An extra electron resides at the vacancy

- Overall, two electrons pair, and the other two give $S = 1$

NV centres

- The $S = 1$ state has axial ZFS, and there are also excited $S = 1$ and $S = 0$ states:



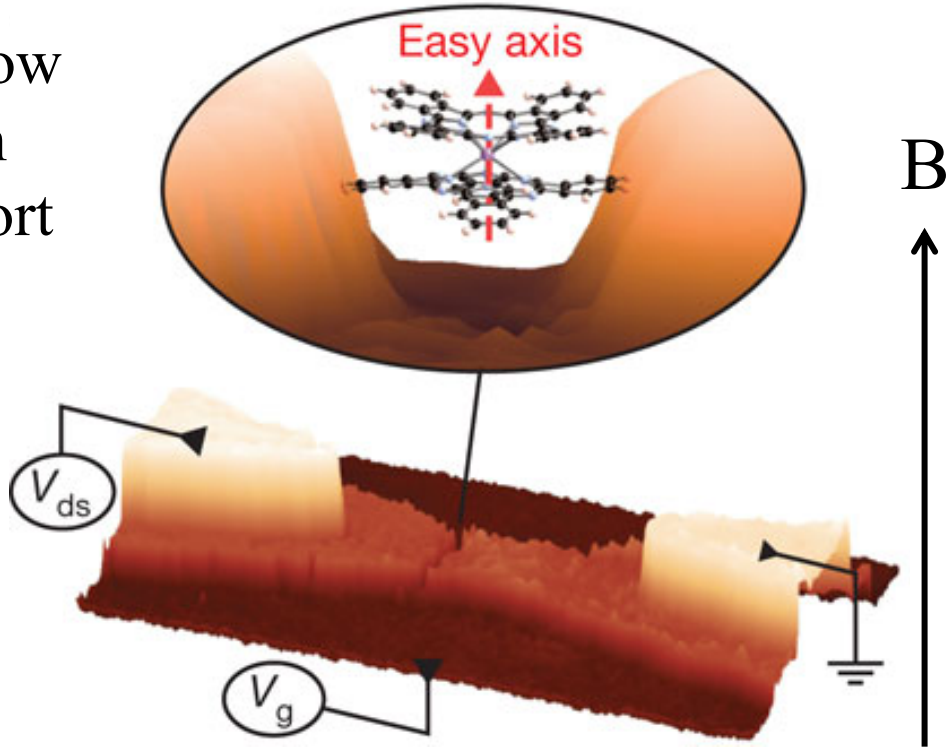
[1] M. S. Fataftah and D. E. Freedman, *Chem. Commun.*, 2018, **54**, 13773.

Molecular spin qubits

- A single [Tb(phthalocyanine)$_2$] SMM is placed between gold electrodes and the electron transport is measured (phthalocyanine ligands are good conductors)

- Experiment investigates how electronic and nuclear spin states influence the transport

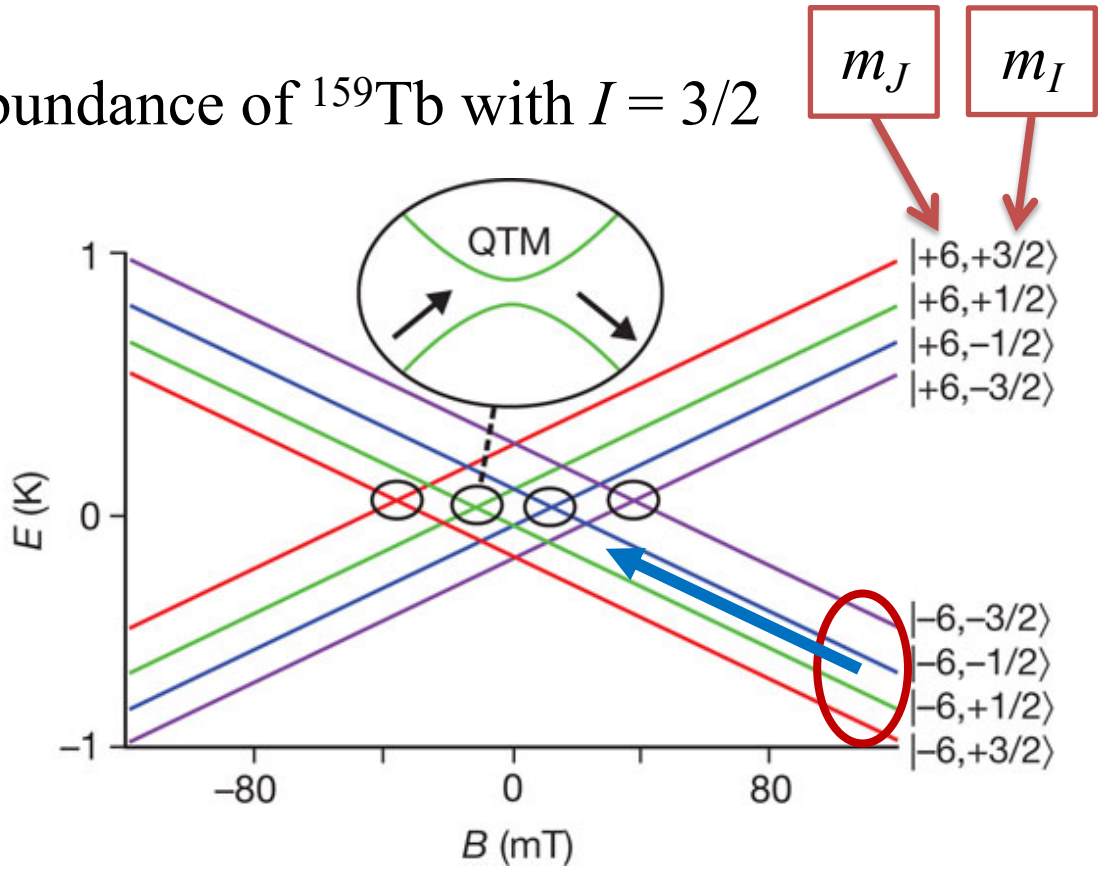
- Variable magnetic field applied



[1] Vincent *et. al.*, *Nature*, 2012, **488**, 357; [2] Thiele *et. al.*, *Science*, 2014, **344**, 1135

Molecular spin qubits

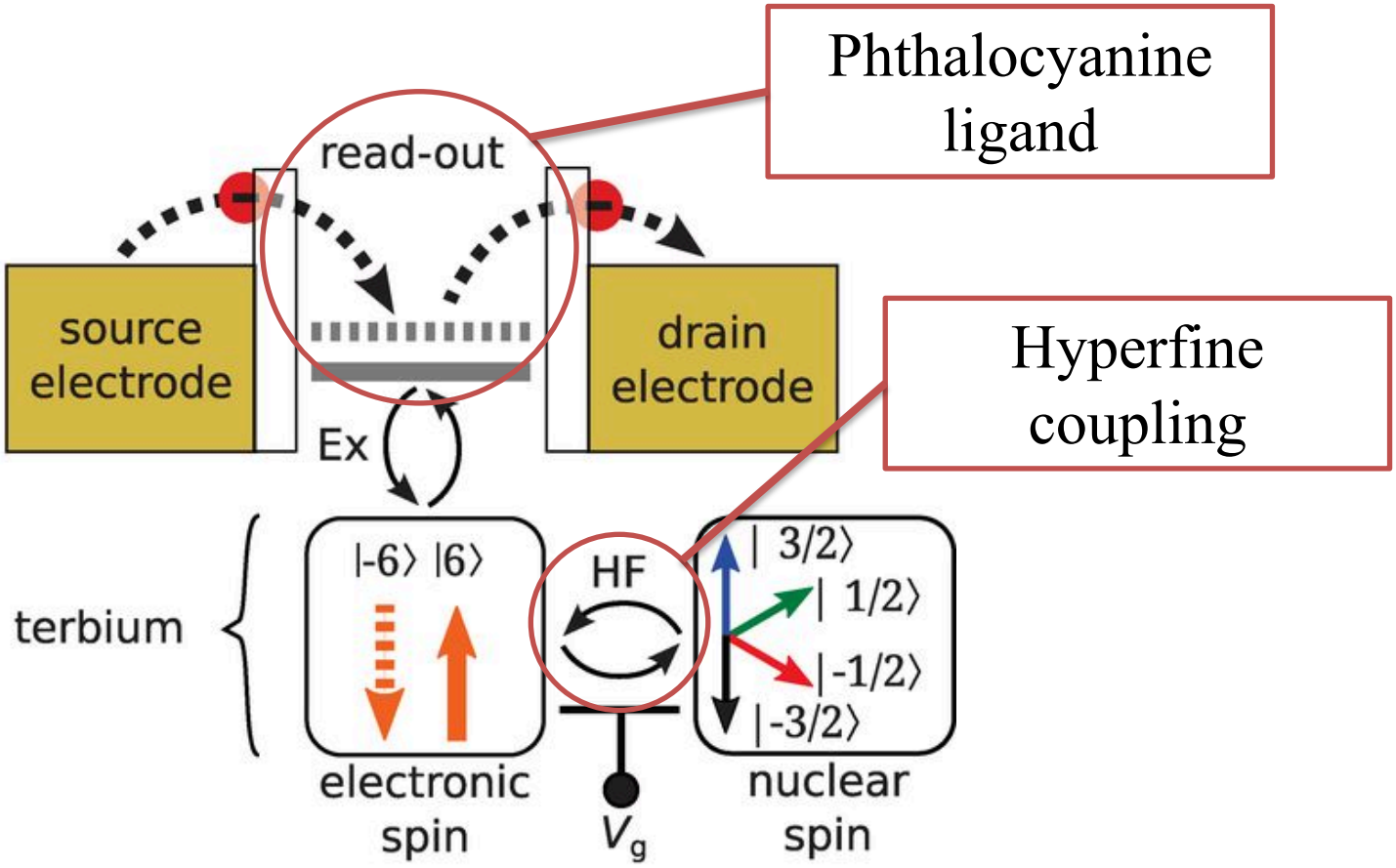
- The molecule is kept at ~ 0.08 K and so only ground electronic states are relevant, which are $m_J = \pm 6$
- Tb has 100% isotopic abundance of ^{159}Tb with $I = 3/2$
- When molecule is magnetised, one of four states are occupied
- Avoided crossings near B = 0 allows magnetic relaxation



[1] Vincent *et. al.*, *Nature*, 2012, **488**, 357; [2] Thiele *et. al.*, *Science*, 2014, **344**, 1135

Molecular spin qubits

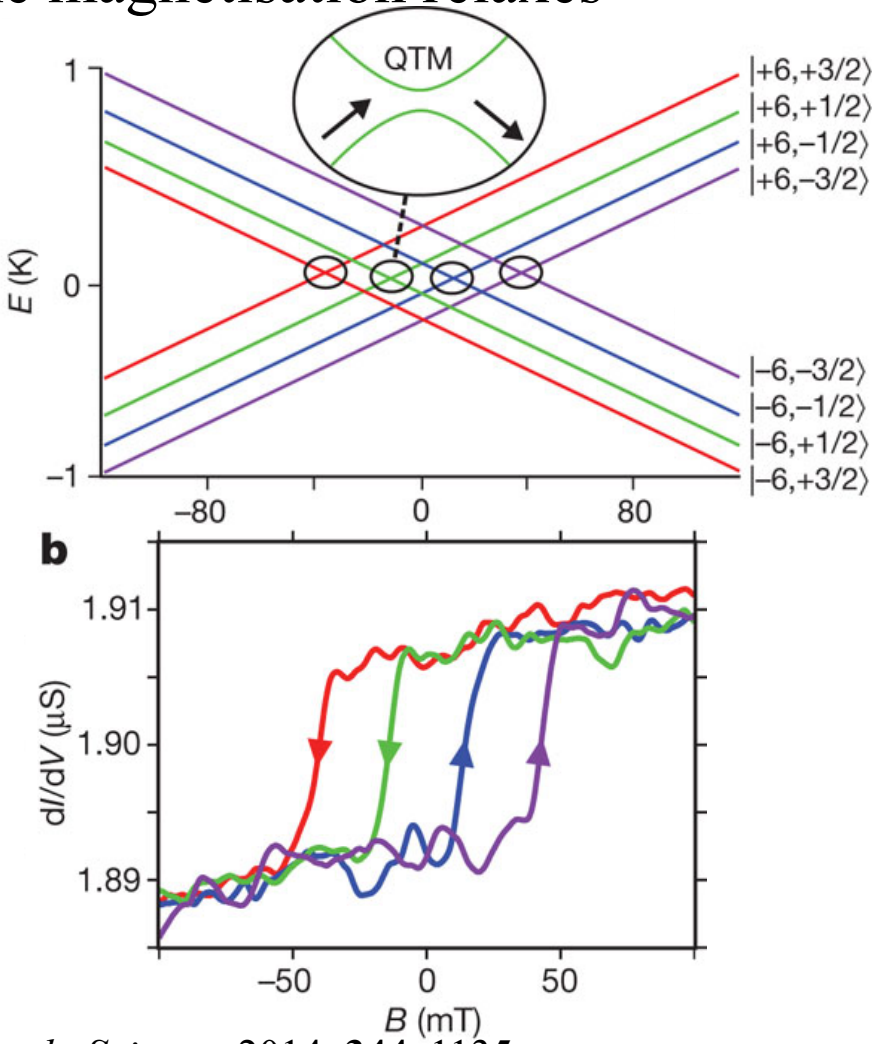
- The electron transport (i.e. conductivity) of the molecule is measured



[1] Vincent *et. al.*, *Nature*, 2012, **488**, 357; [2] Thiele *et. al.*, *Science*, 2014, **344**, 1135

Molecular spin qubits

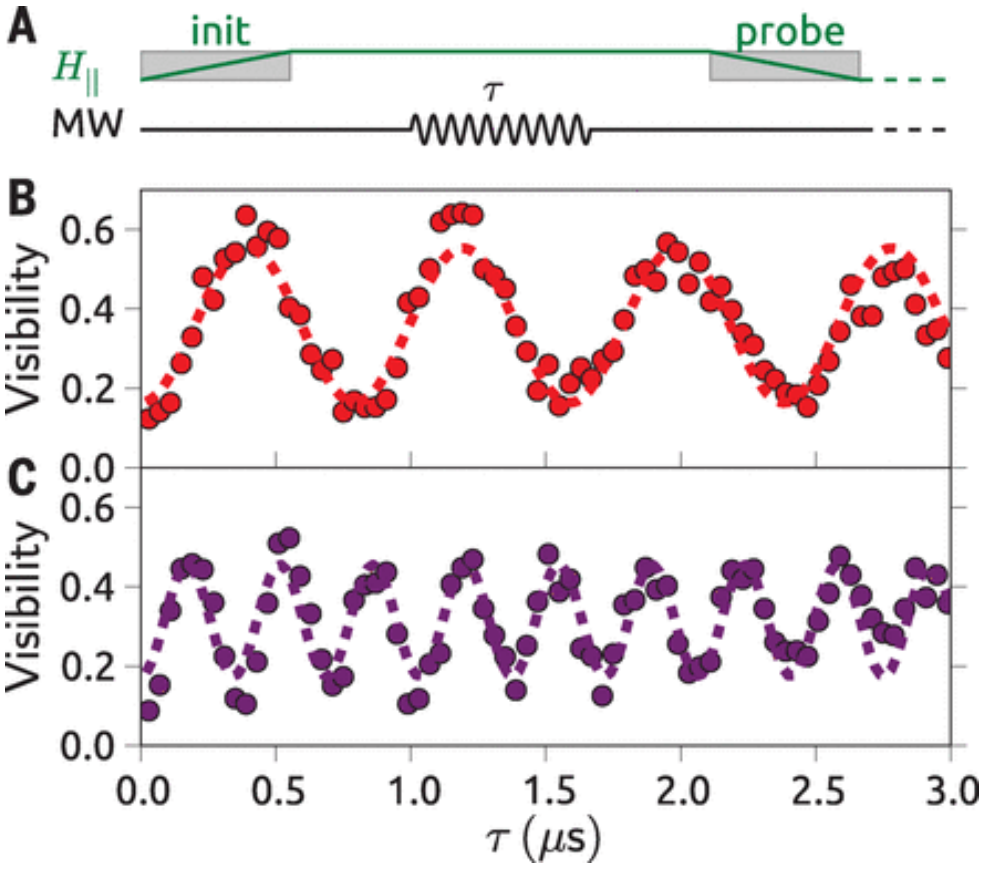
- The conductivity jumps when the magnetisation relaxes
- This directly measures the relaxation of a single molecule (multiple scans needed to see the different steps)
- Nuclear spin states live long enough to control coherently...



[1] Vincent *et. al.*, *Nature*, 2012, **488**, 357; [2] Thiele *et. al.*, *Science*, 2014, **344**, 1135

Molecular spin qubits

- Nuclear spin is initialised in the $m_I = +3/2$ state with magnetic field
- Microwave pulse induces oscillations between $m_I = +3/2$ and $m_I = +1/2$
- Sweep magnetic field back to read-out m_I state



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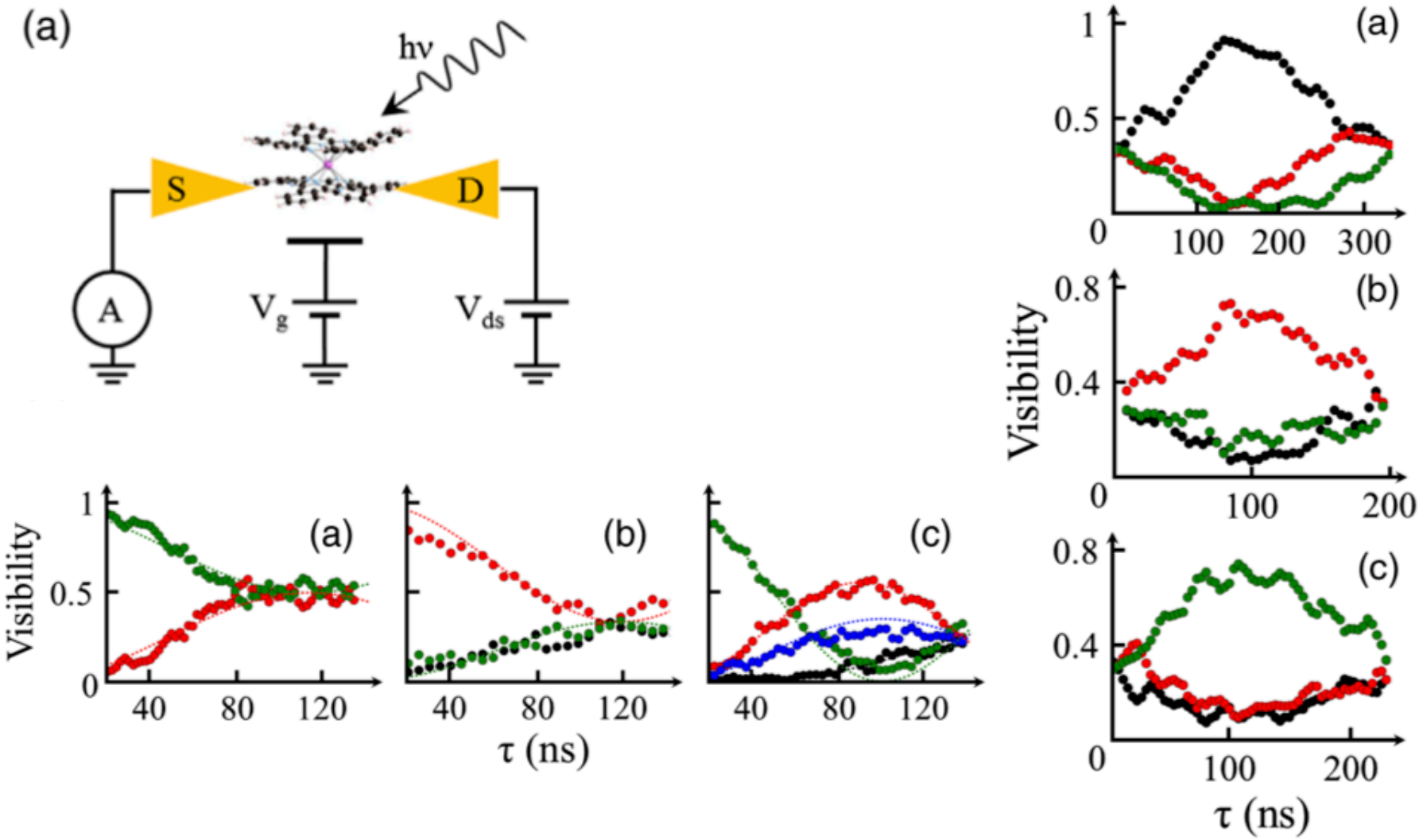
Grover's algorithm in a molecule



[1] C. Godfrin *et al.*, *Phys. Rev. Lett.*, 2017, **119**, 187702.

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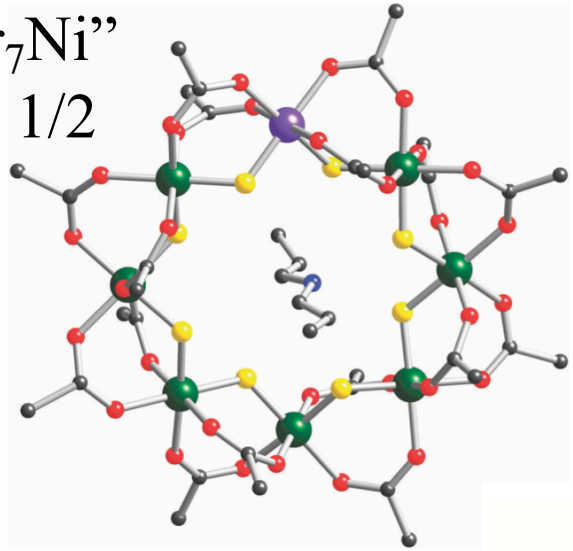
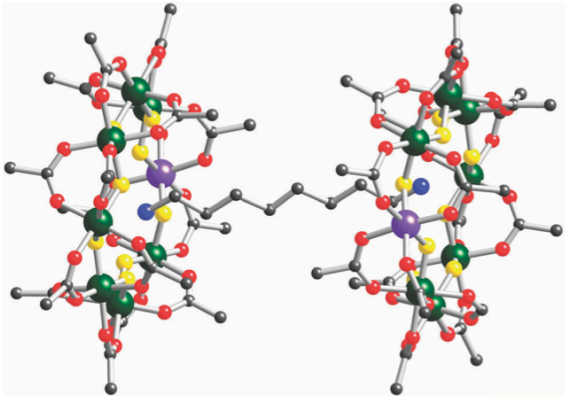
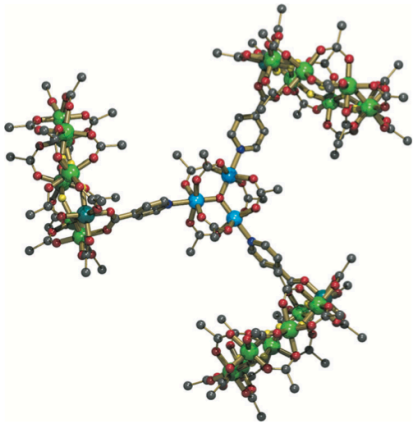
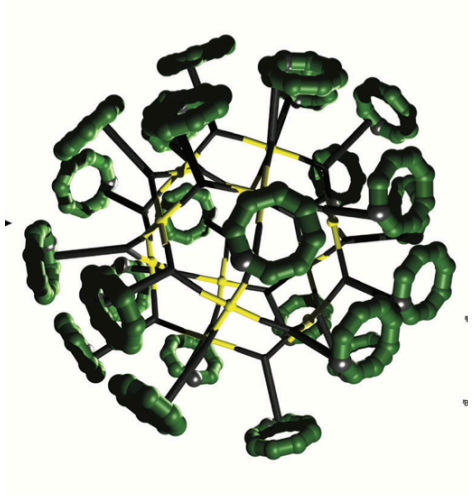
Qubits

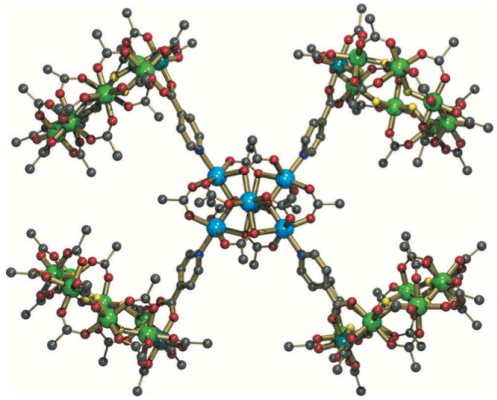
"Cr_7Ni"
S = 1/2

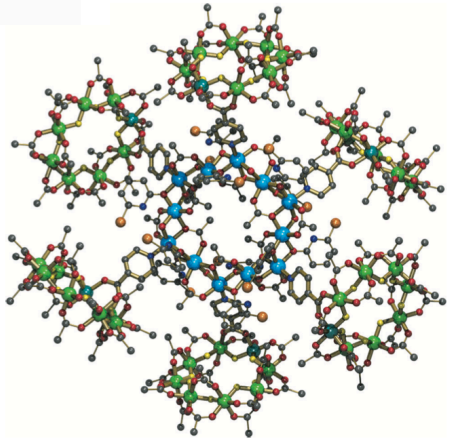












Richard Winpenny
Eric McInnes

[1] E. J. L. McInnes *et al.*, *Angew. Chem. Int. Ed.*, 2015, **54**, 14244; [2] C. J. Wedge et al., *Phys. Rev. B*, 2012, **108**, 107204; [3] J. Ferrando-Soria *et al.*, *Nature Commun.*, 2016, **7**, 11377.