Alejandro Gaita-Ariño

ERC Consolidator Grant

DECRESIM

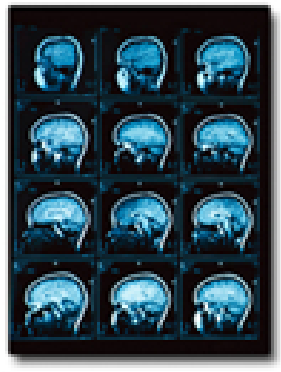
Control Quantum Decoherence using Coordination Chemistry

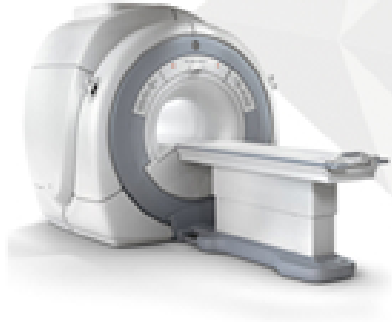
26 / 11 / 2014

Today's electronics run on Quantum Mechanics

$$\hat{H}\Psi = E\Psi$$

"classical" computing





biomedical MRI

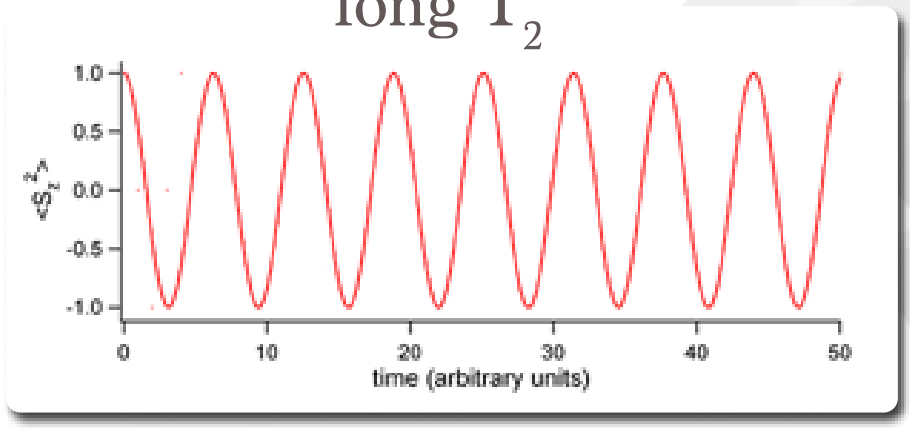
Tomorrow's electronics run on 'cat states'

$\Psi = |\uparrow\rangle + |\downarrow\rangle$

spin-spin relaxation time

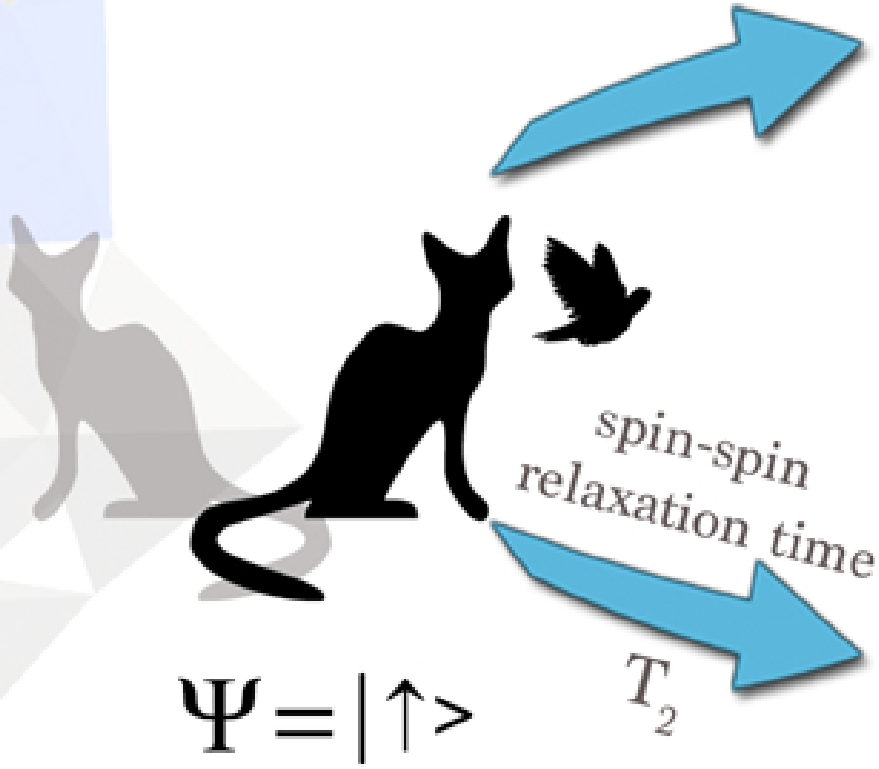
T_2

long T_2

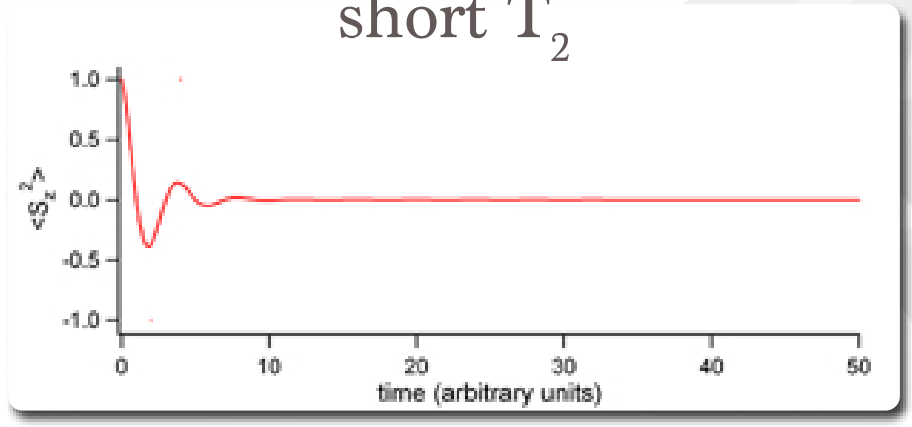


Rabi oscillations

Decoherence kills ‘cat states’

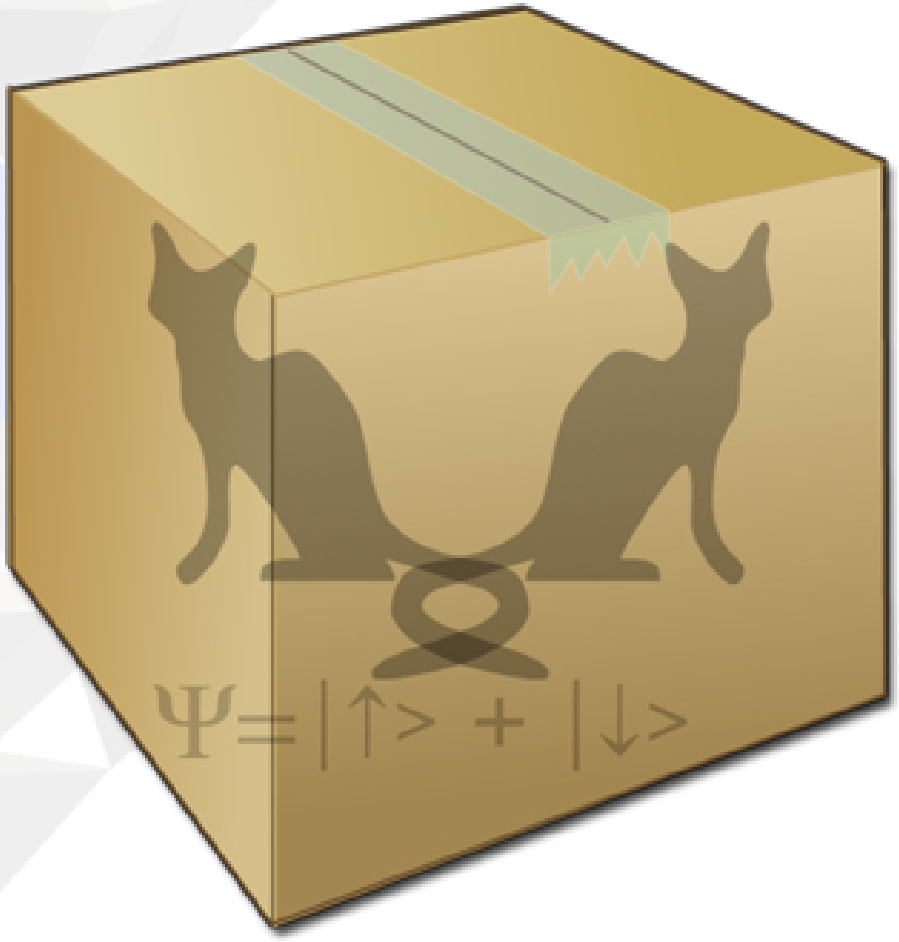


short T_2

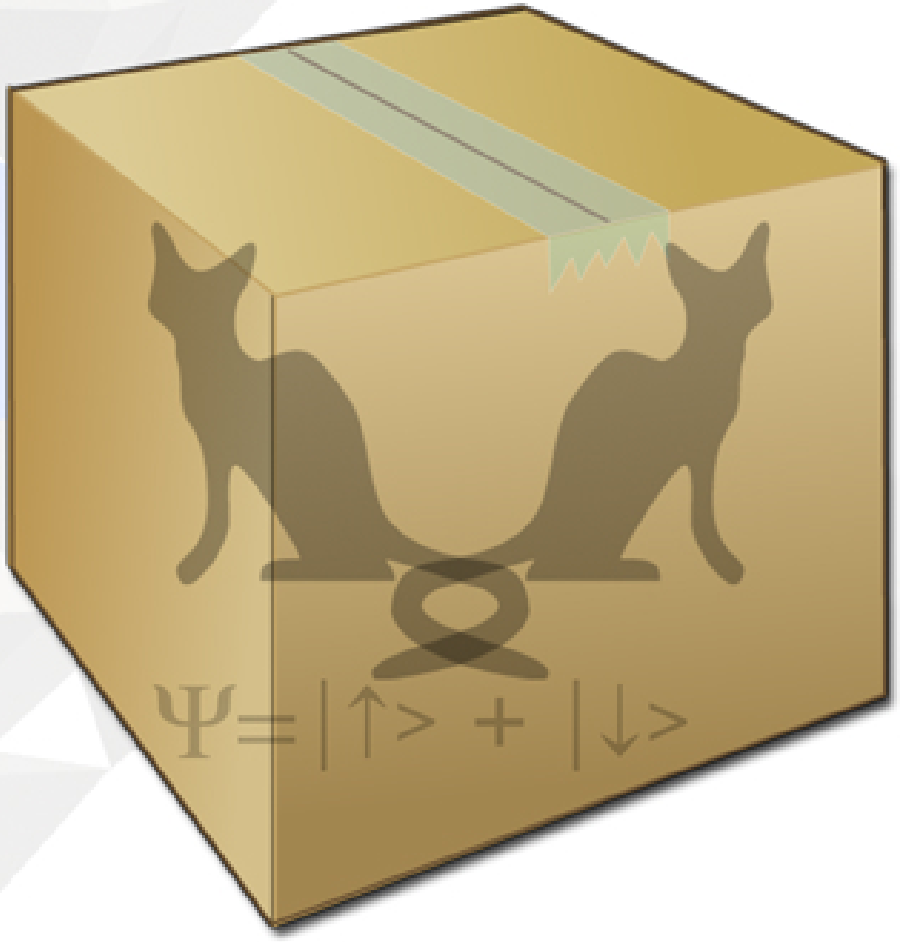


no Rabi oscillations

Chemistry can protect ‘cat states’



Chemistry can protect ‘cat states’



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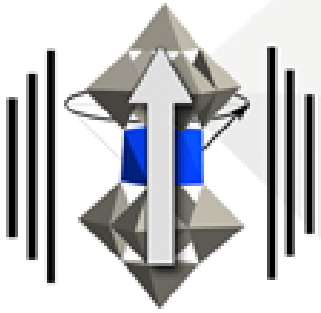
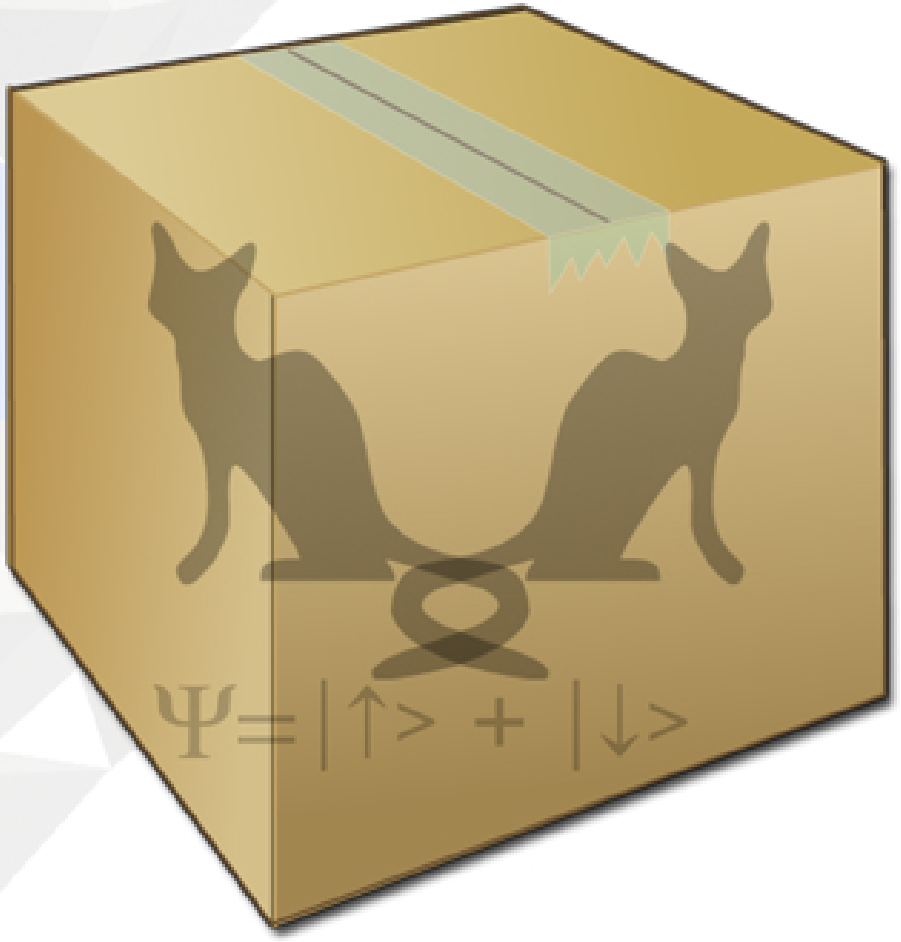


Chemistry can protect ‘cat states’



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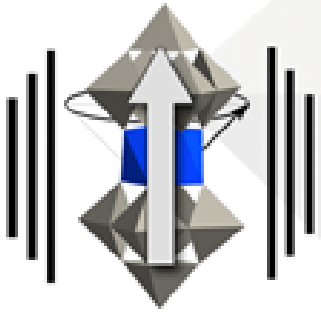
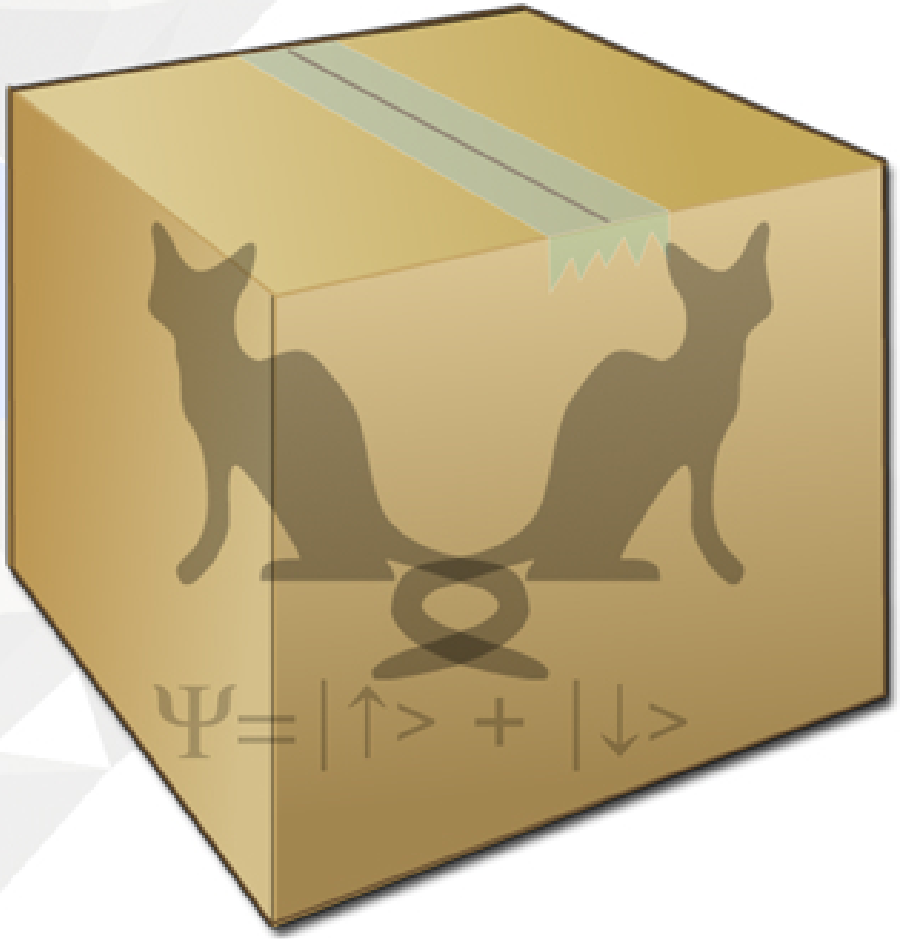
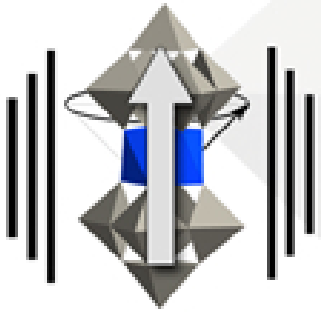


2:

Chemistry can protect ‘cat states’

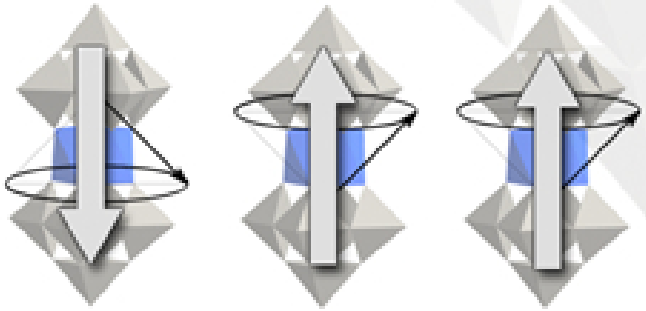


1:



2:

3:



DECRESIM

A chemical approach to molecular spin qubits:
Decoherence and organization of Rare Earth coordination complexes

WP1

Coherence

WP2

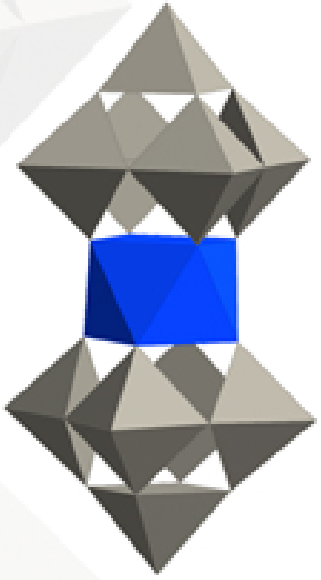
Interaction

WP3

Organization

DECRESIM

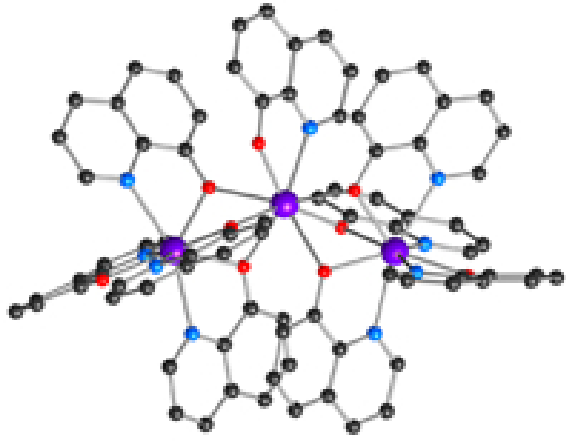
A chemical approach to molecular spin qubits:
Decoherence and organization of Rare Earth coordination complexes



$[Ln(W_5O_{18})_2]^{9-}$
n = 1

WP1

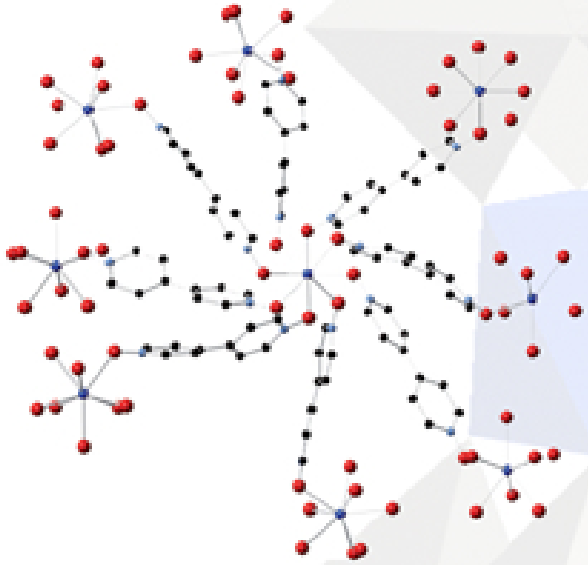
Mononuclear



$Ln_3(OQ)_9$
Q= Quinoline
n = 3

WP2

Polynuclear

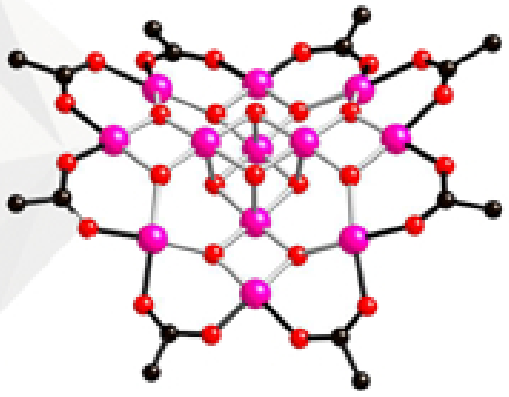


$[Ln(bipyNO)_4]_\infty$
n = ∞

WP3

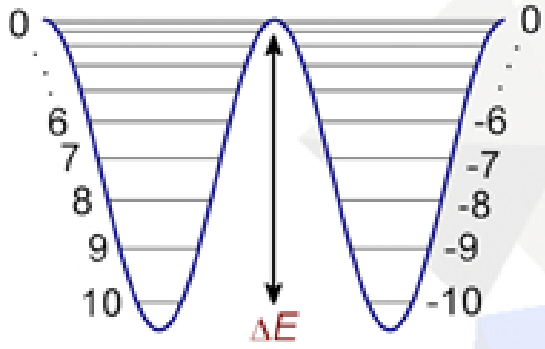
Extended

From SMMs to Spin Qubits

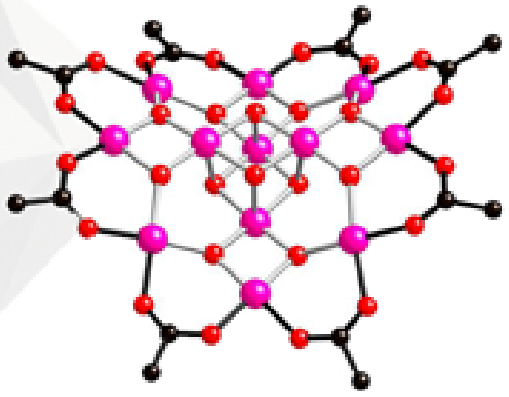


Magnetic Exchange

Zero-Field Splitting

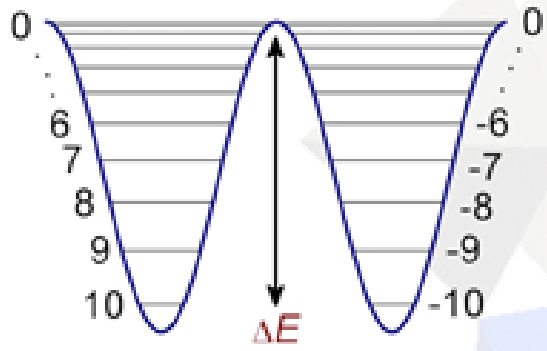


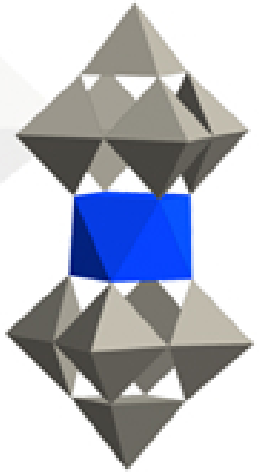
From SMMs to Spin Qubits



Magnetic Exchange

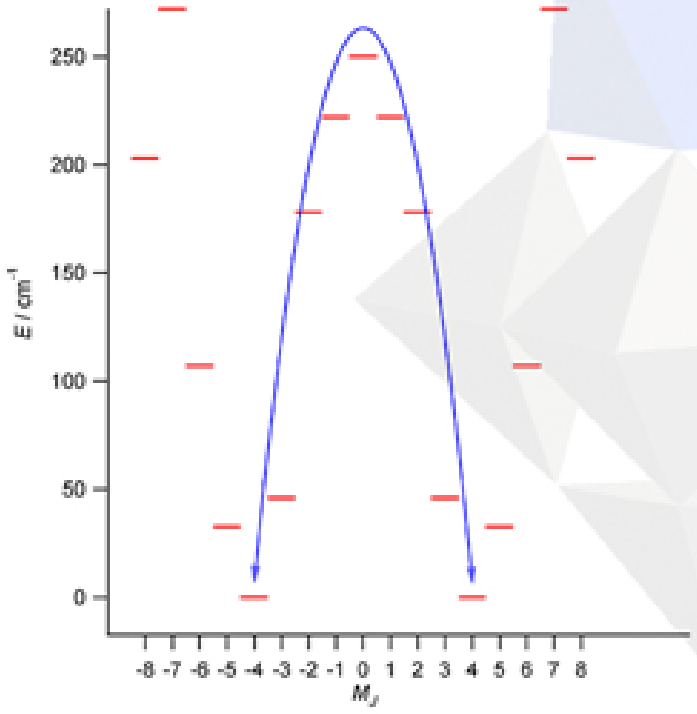
Zero-Field Splitting



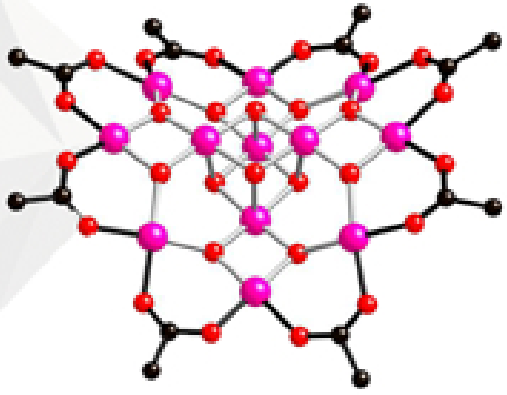


Spin-Orbit Coupling

Crystal Field

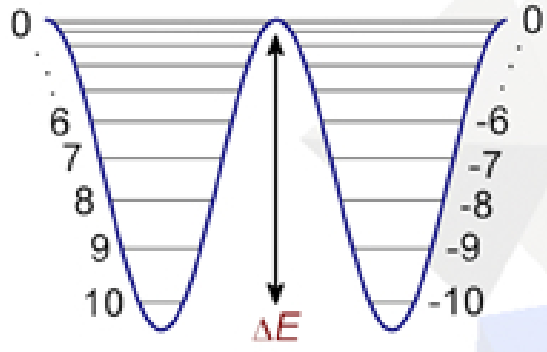


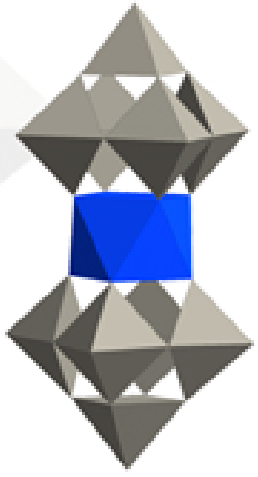
From SMMs to Spin Qubits



Magnetic Exchange

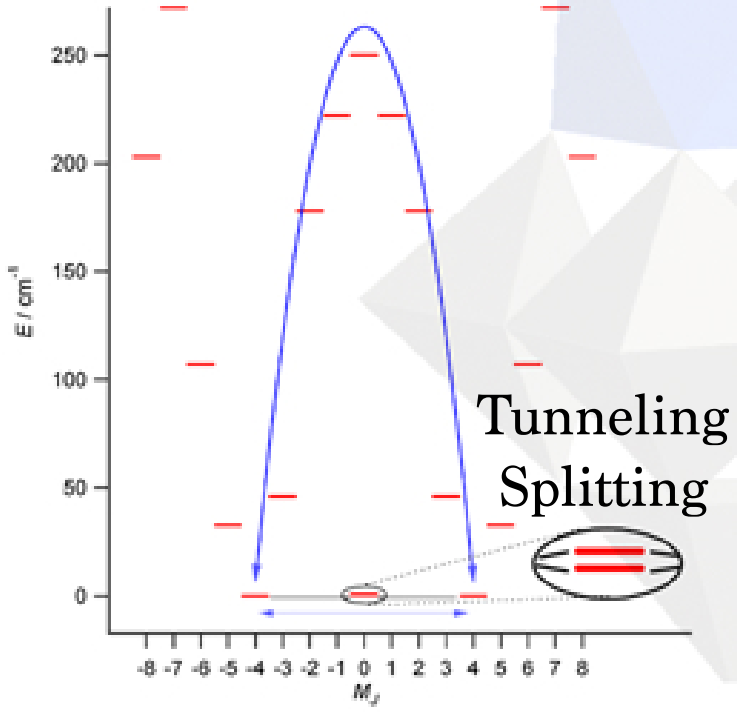
Zero-Field Splitting





Spin-Orbit Coupling

Crystal Field



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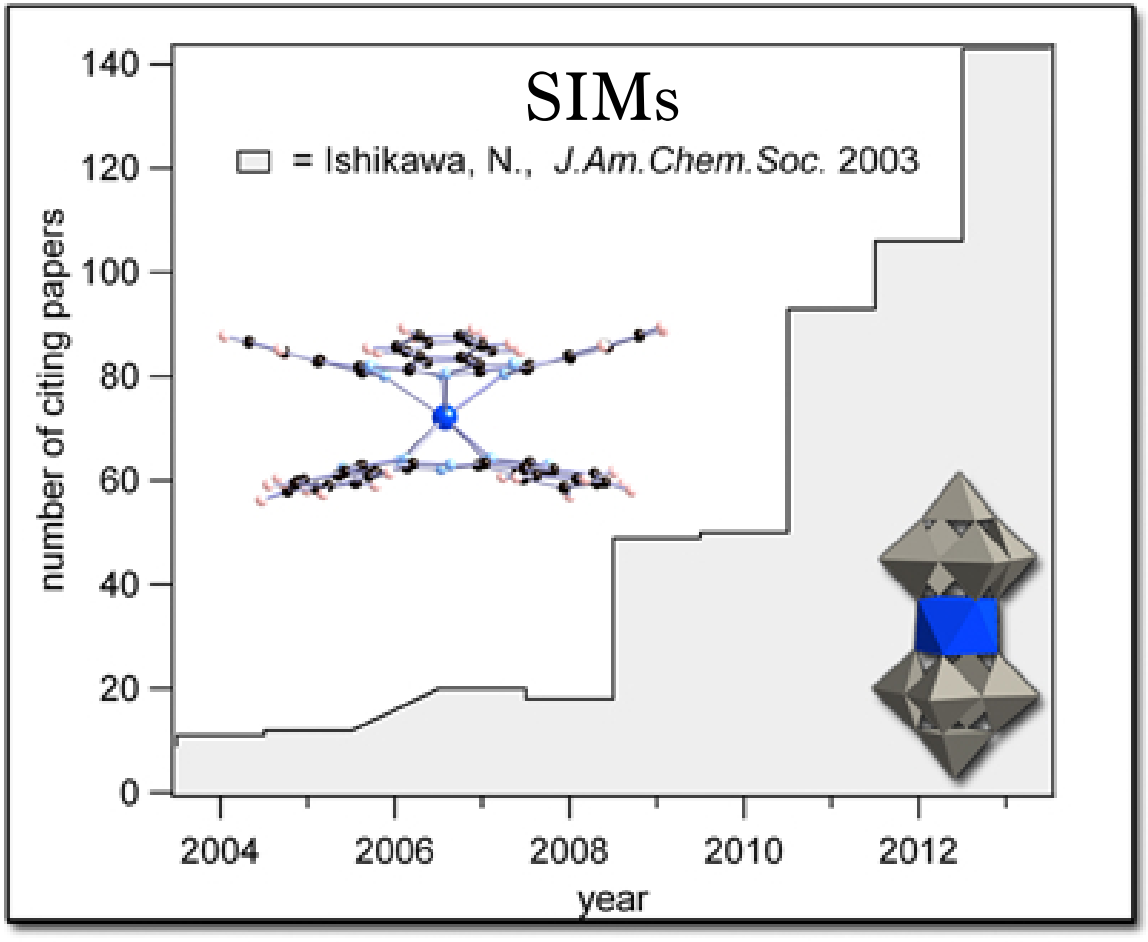
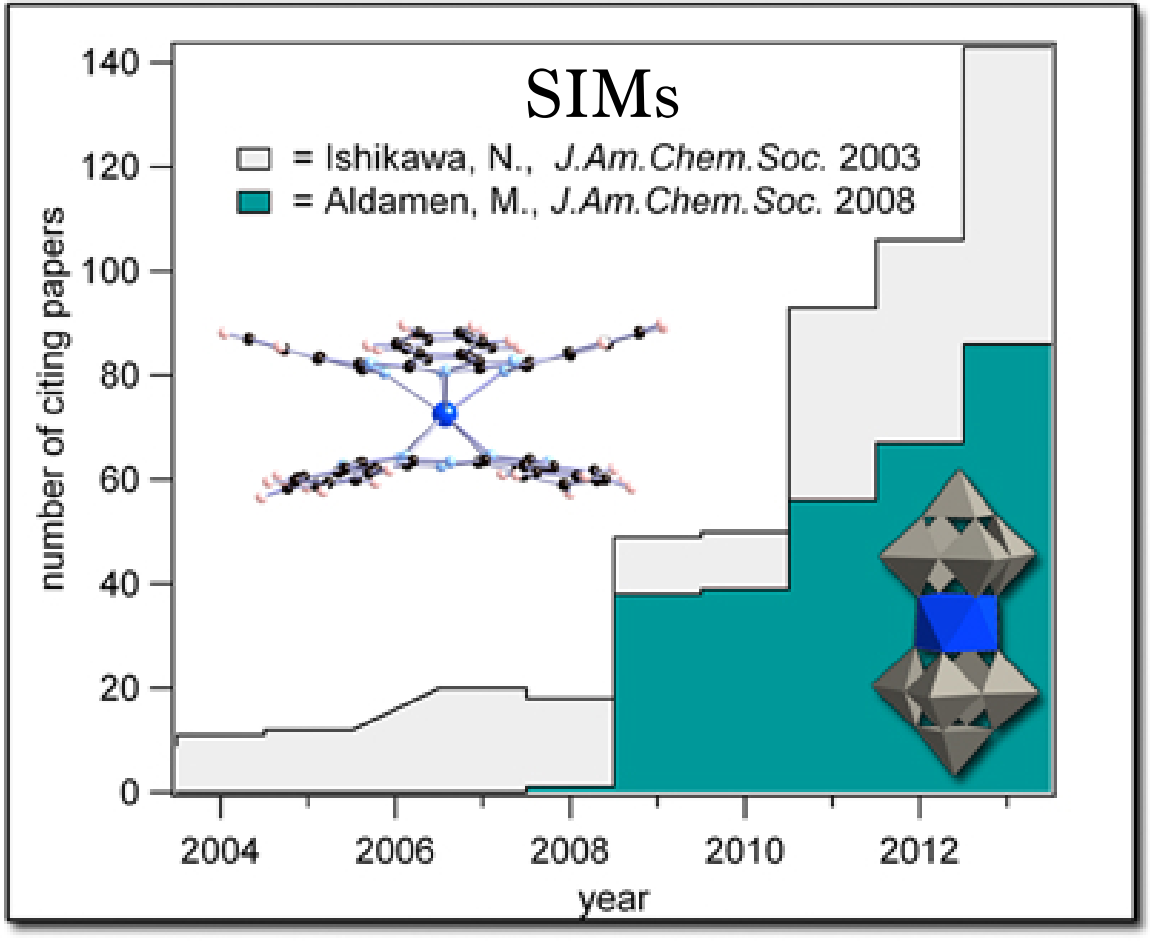


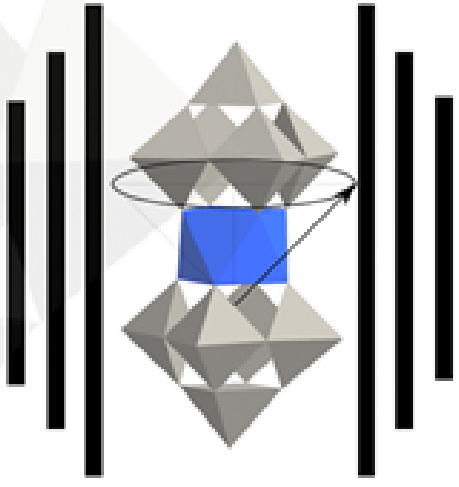
From SMMs to Spin Qubits



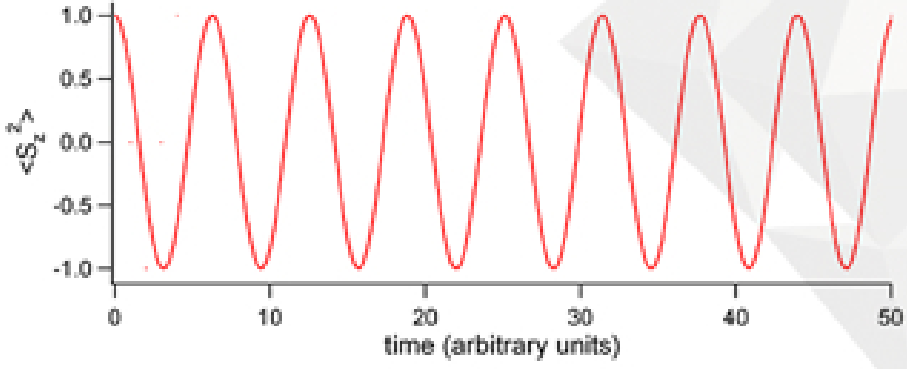
WP1: Decoherence in a mononuclear complex

Theory

Experiment

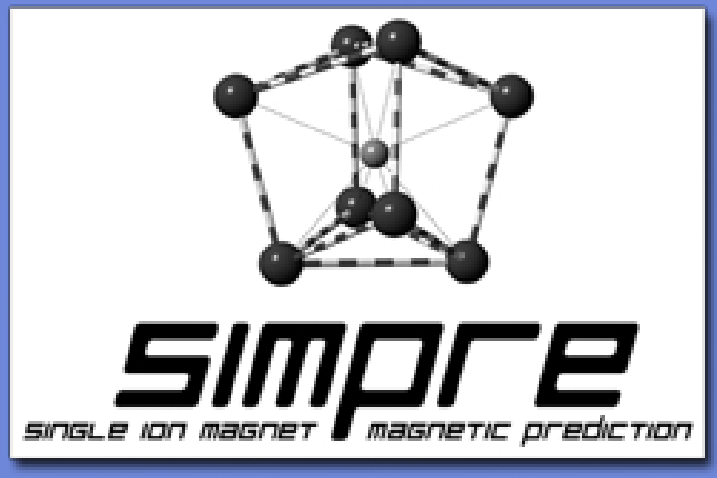


Time



Rabi Oscillations

From coordination environment to Crystal Field Hamiltonian



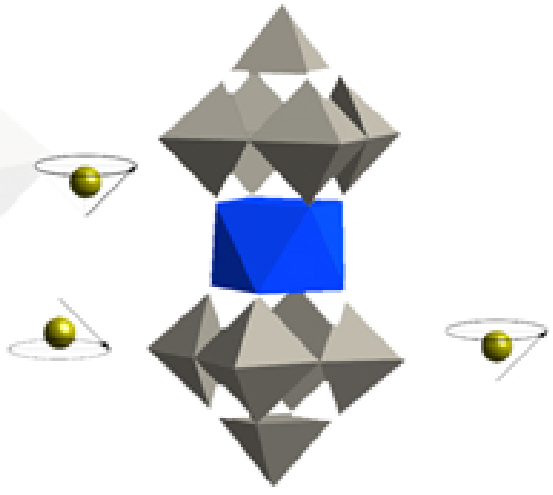
Upcoming Features in 2.0

Parameterization of common ligands

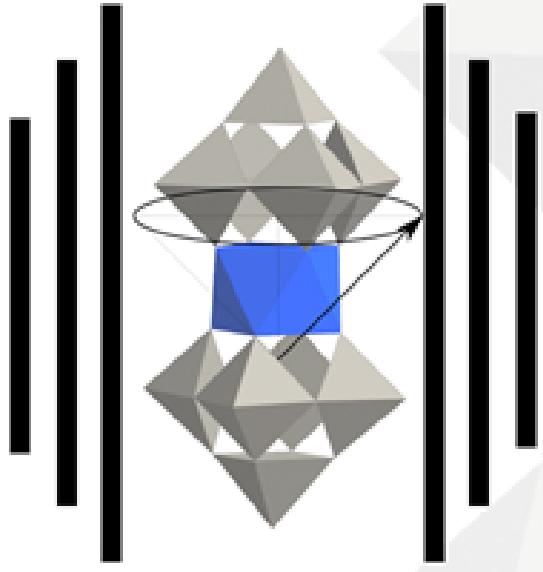
Consideration of spin-orbit coupling

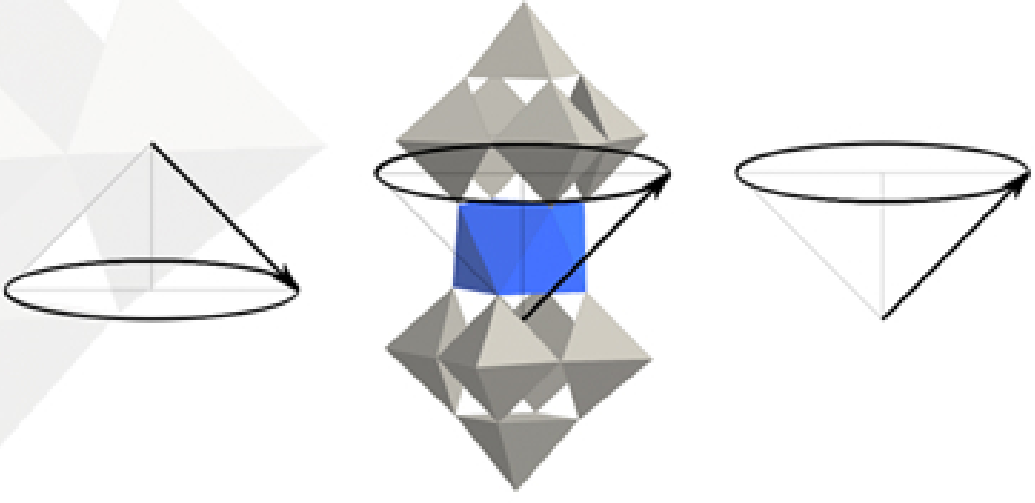
J. Am. Chem. Soc., **2012**, 134, 14982.
Inorg. Chem., **2012**, 51, 1256.
Dalton Trans., **2012**, 41, 13705.
Chem. Sci., **2013**, 4, 938.
J. Comp. Chem., **2013**, 34, 1961.
J. Comp. Chem., **2014**, 35, 1930.
Chem. Eur. J., **2014**, 20, 10695.
Inorg. Chem., **2014**, 53, 9976.
Inorg. Chem., **2014**, 53, 11323.
and 9 more works in preparation.

Coupling to the environment



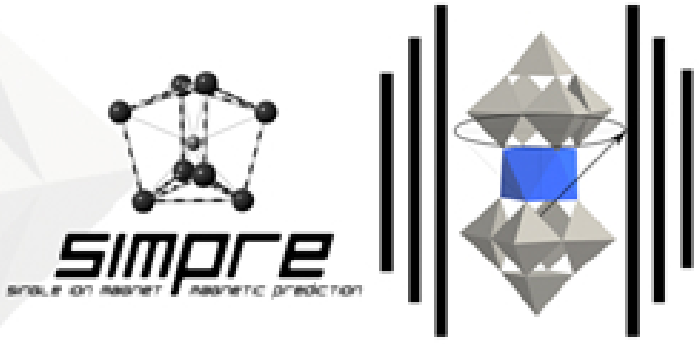
$[Ln(W_5O_{18})_2]^{9-}$

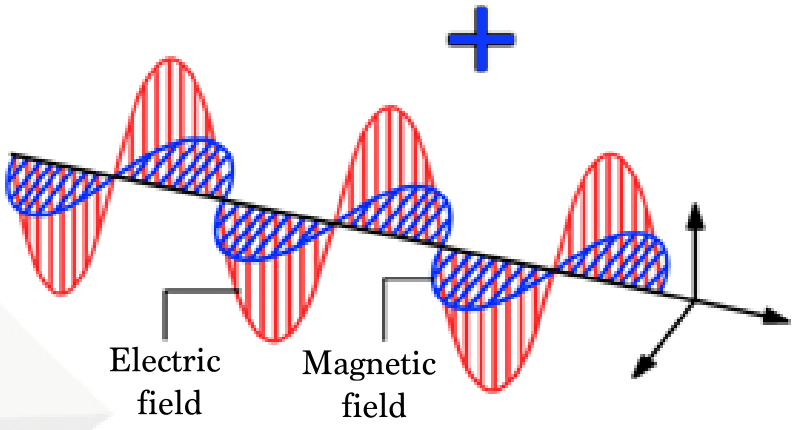




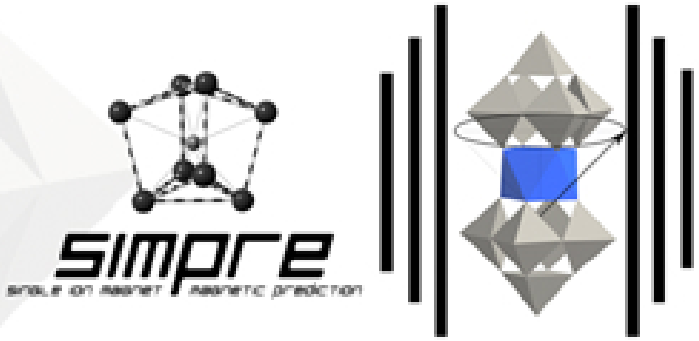
Phys. Rev. Lett, **2011**, 107, 105504
Phys. Rev. B **2012**, 86, 024432
Int. J. Quant. Chem. **2012**, 112, 2957
arXiv:1405.2217, submitted to Phys. Rev. B
arXiv:1408.5321, submitted to Int. J. Num. Met. Eng.

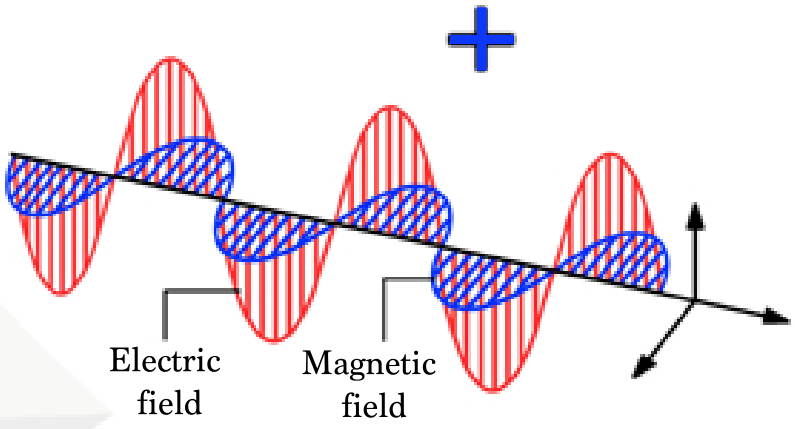
Dynamical properties - Time Evolution

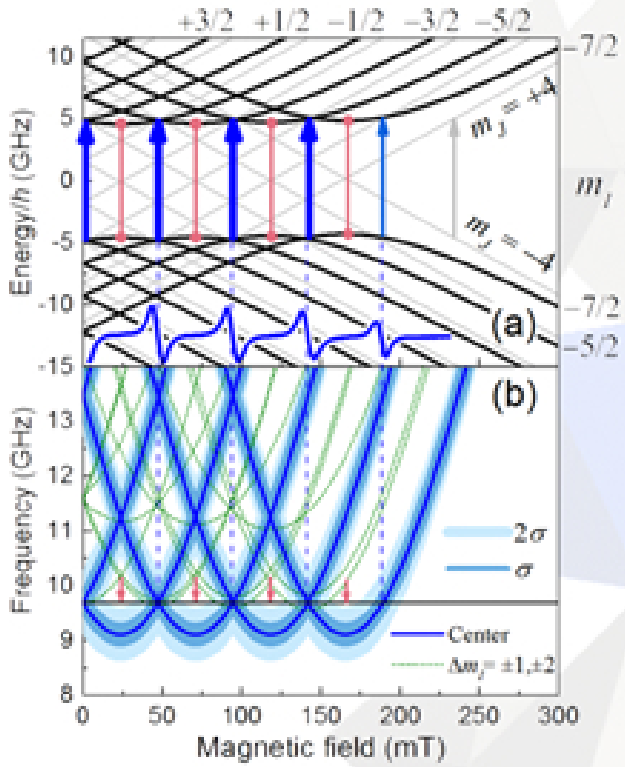




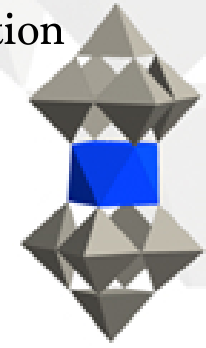
Dynamical properties - Time Evolution



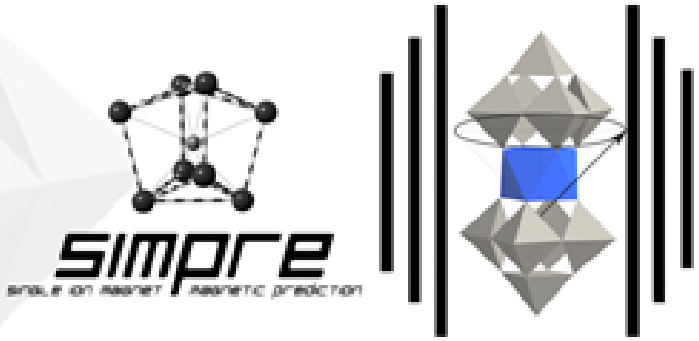


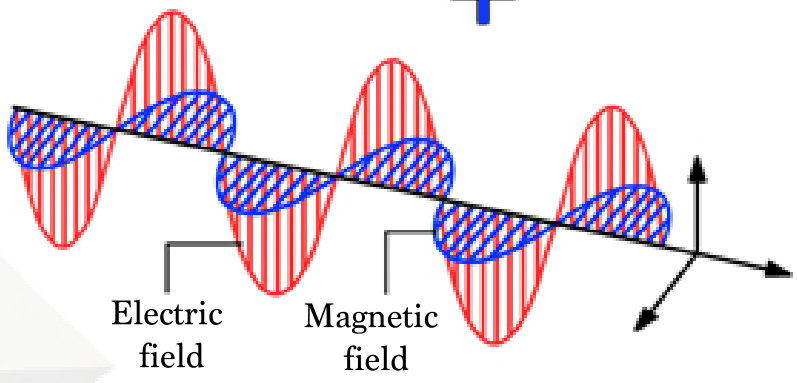


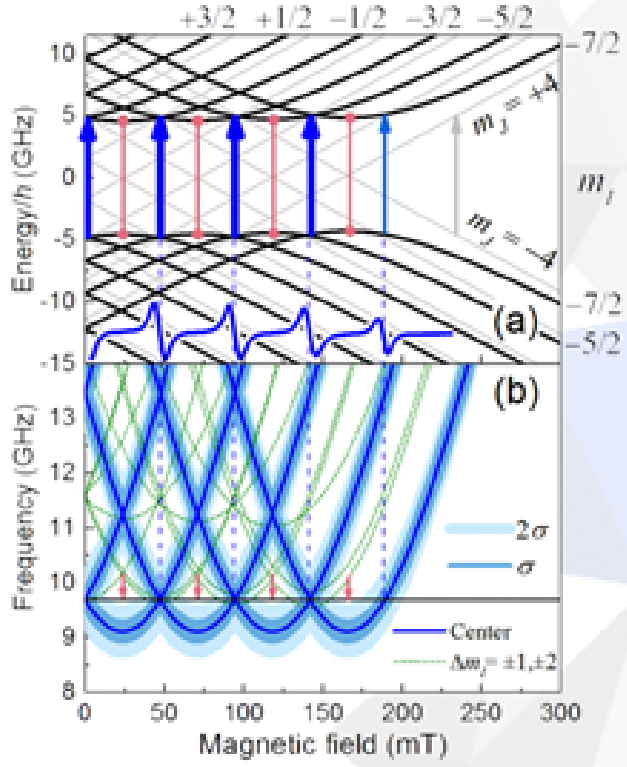
Clock transitions,
Long T_2 with no dilution
$[Ho(W_5O_{18})_2]^{9-}$



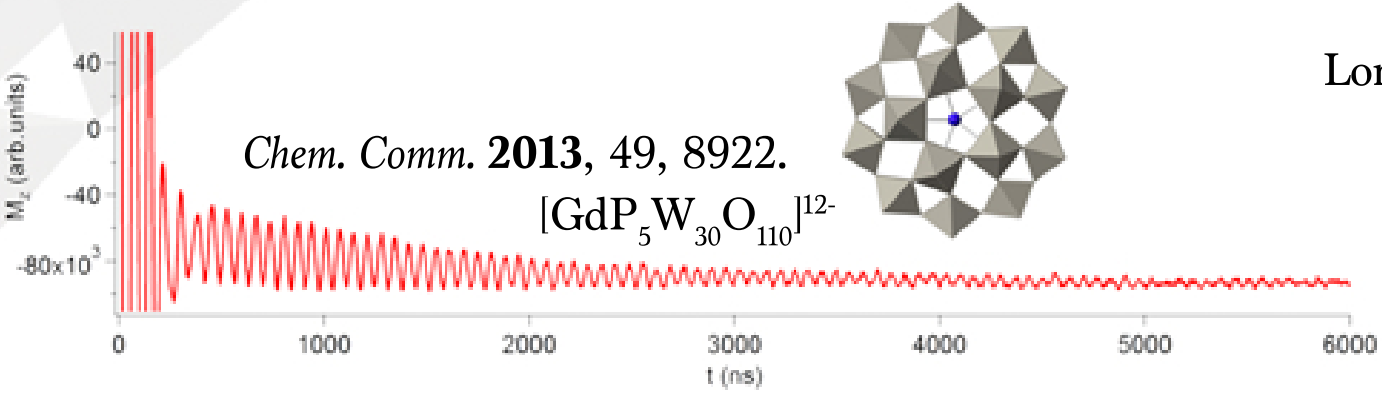
Dynamical properties - Time Evolution



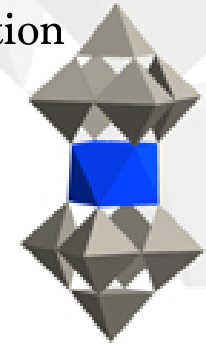




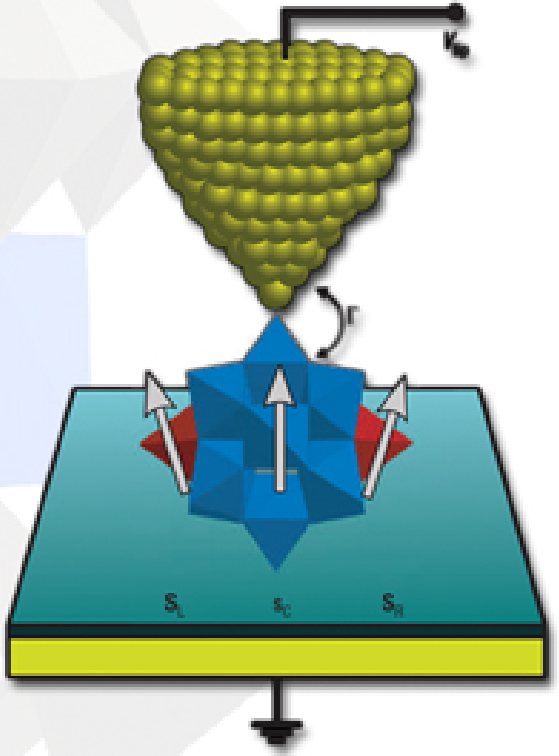
Clock transitions,
Long T_2 with no dilution
$[Ho(W_5O_{18})_2]^{9-}$



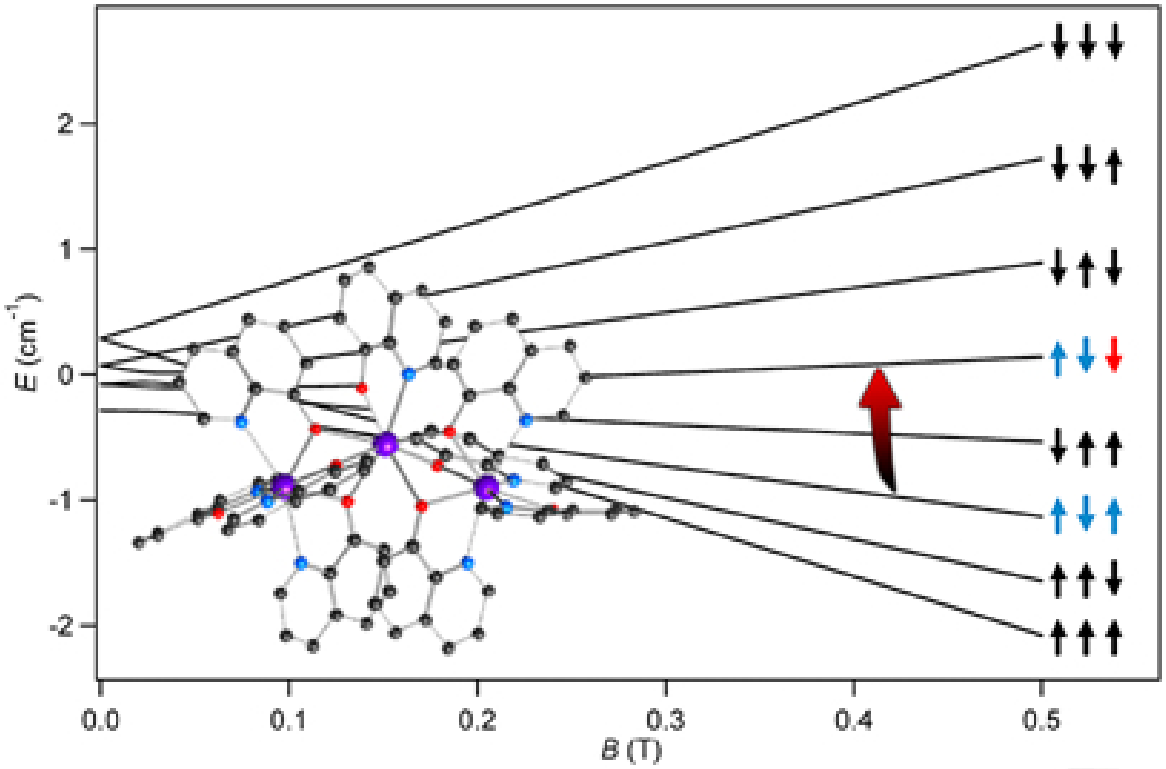
Chem. Comm. **2013**, 49, 8922.
$[GdP_5W_{30}O_{110}]^{12-}$



WP2+3: Quantum Gates, Quantum Algorithms



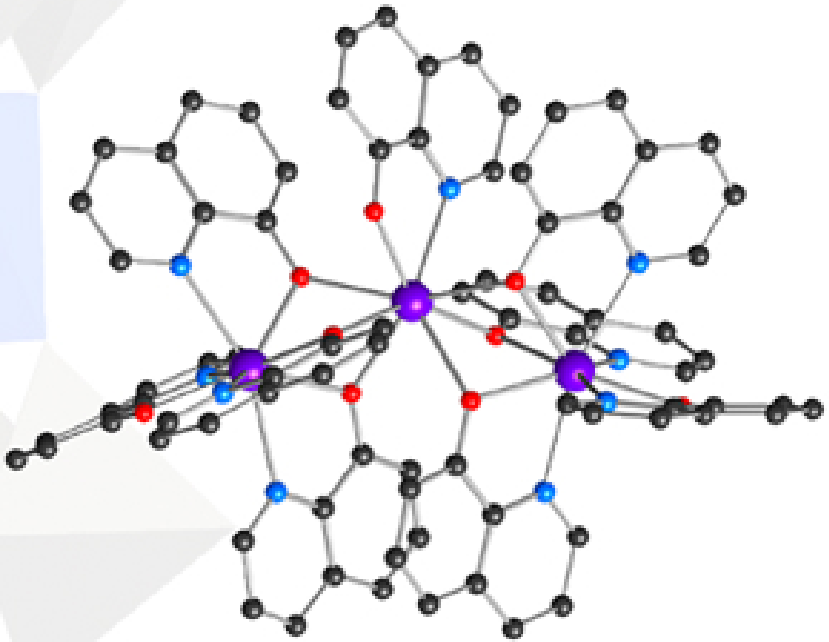
$[PMo_{12}O_{40}(VO)_2]^{q-}$



Nature Nanotech., **2007**, *2*, 312.

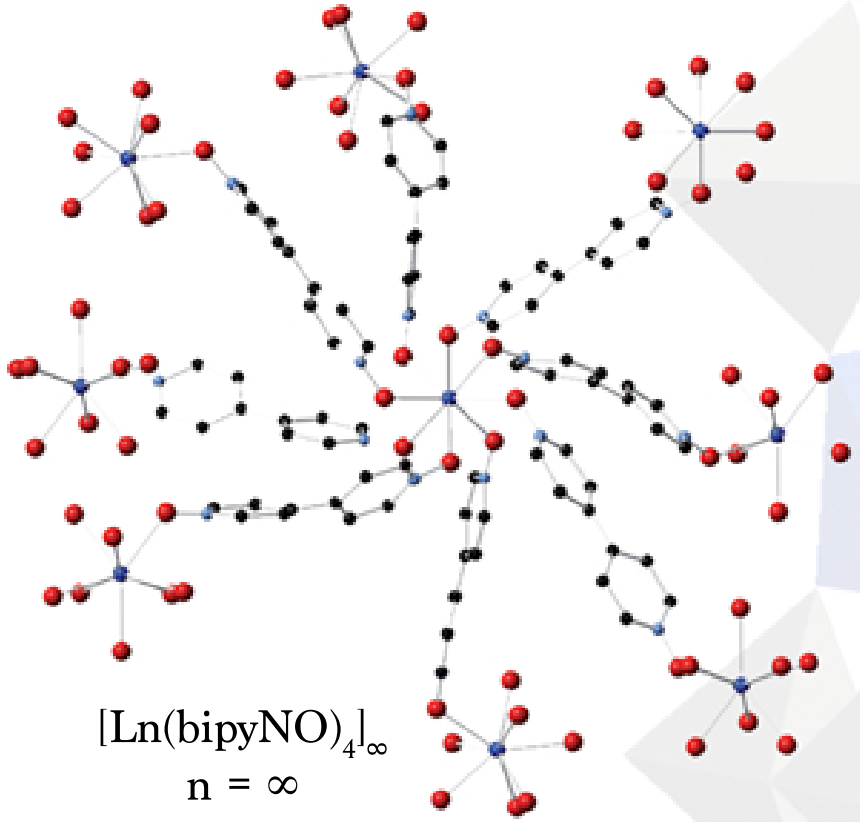
WP2+3: Interaction and Organization

Polynuclear Complexes
Quantum algorithm



$Ln_3(OQ)_9$
Q= Quinoline
n = 3

Phys. Rev. A, submitted



$[Ln(bipyNO)_4]_\infty$
n = ∞

Extended Systems
Quantum automata

Chem. Eur. J., **2014**, *20*, 10695

DECRESIM

Control Quantum Decoherence using Coordination Chemistry