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QUANTUM INFORMATION SCIENCE @ UNIPR

MOLECULAR MAGNETISM group

Quantum simulation of magnetic systems

Alessandro Chiesa

Dipartimento di Scienze Matematiche, Fisiche e Informatiche
Università di Parma

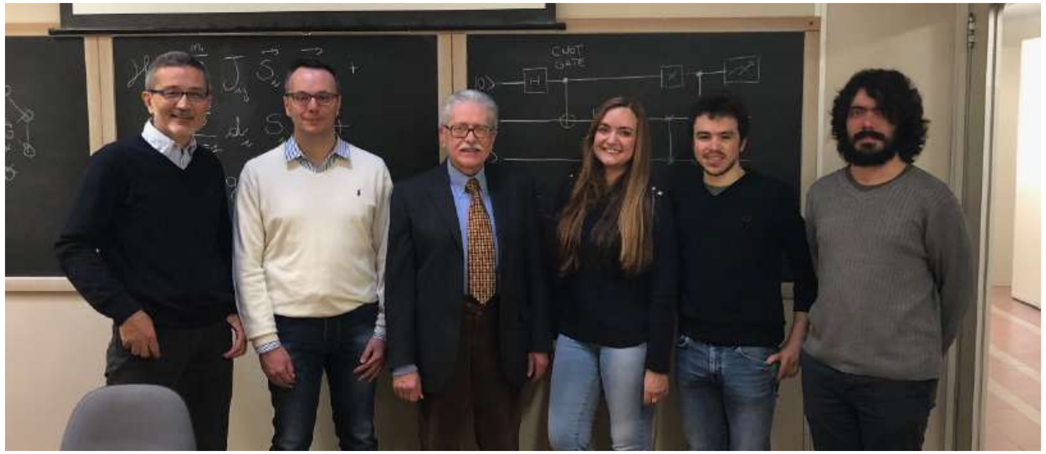
UNIVERSITÀ DI PARMA

MOLECULAR MAGNETISM group

HORIZON 2020

FET - Open

P. Santini, S. Carretta A. Chiesa, E. Macaluso



G. Amoretti, E. Garlatti

QUANTERA

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Progetti di ricerca di Rilevante Interesse Nazionale

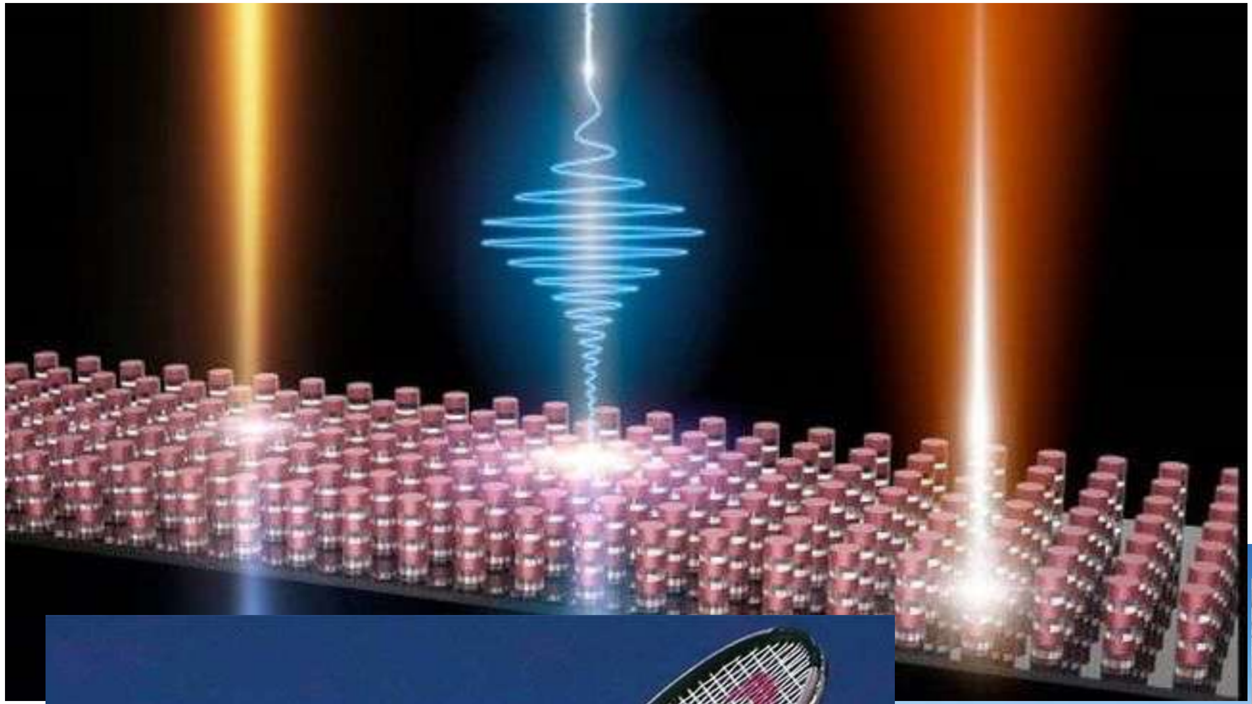
F. Cugini

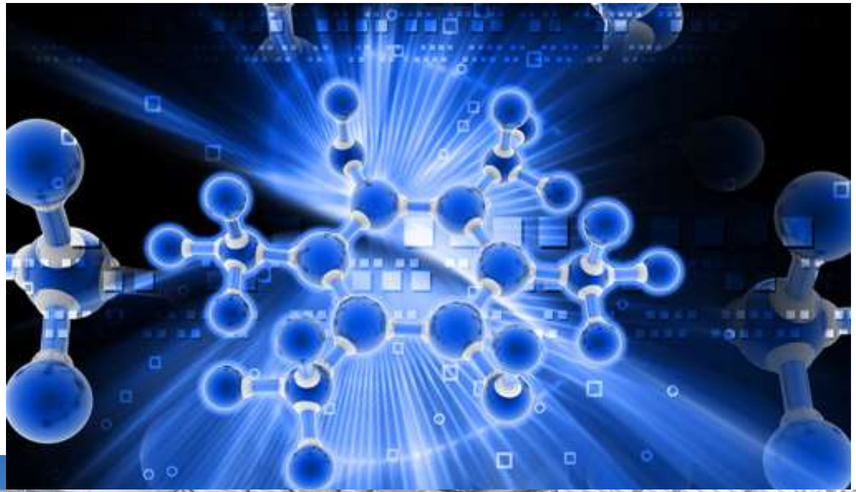
M. Solzi

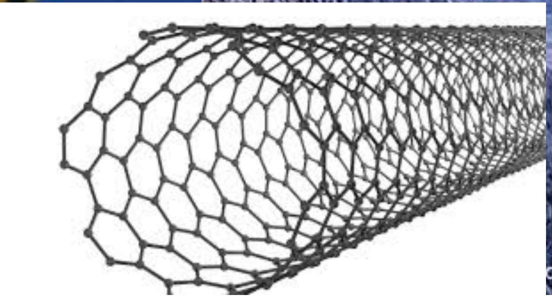
R. Hussain

G. Allodi

R. De Renzi

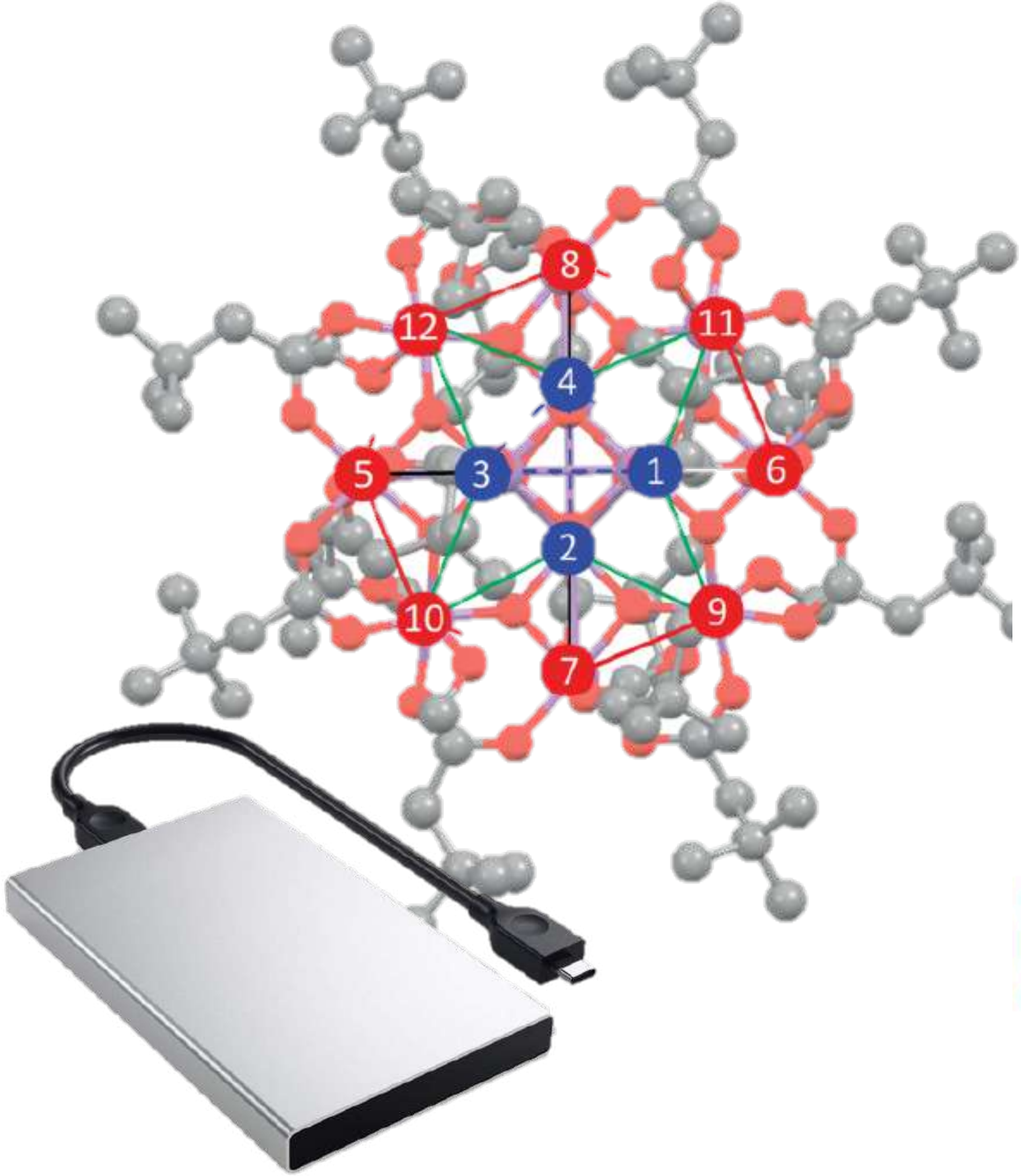




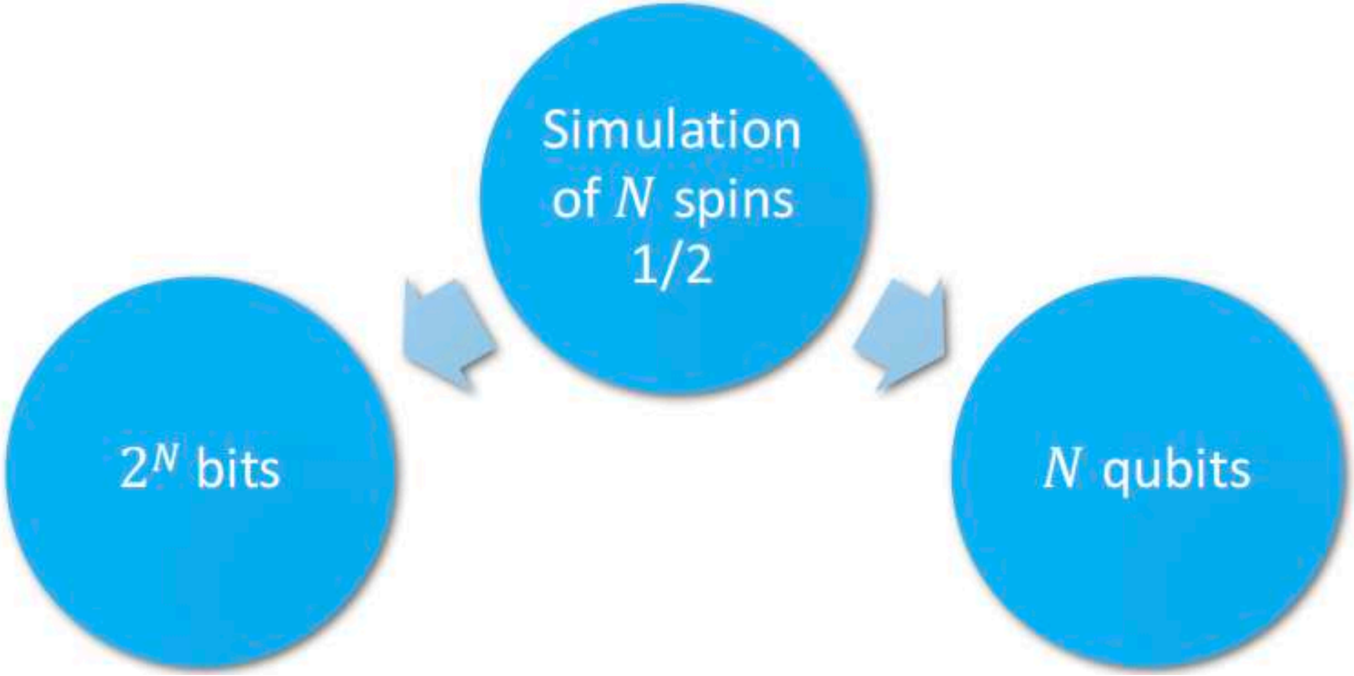


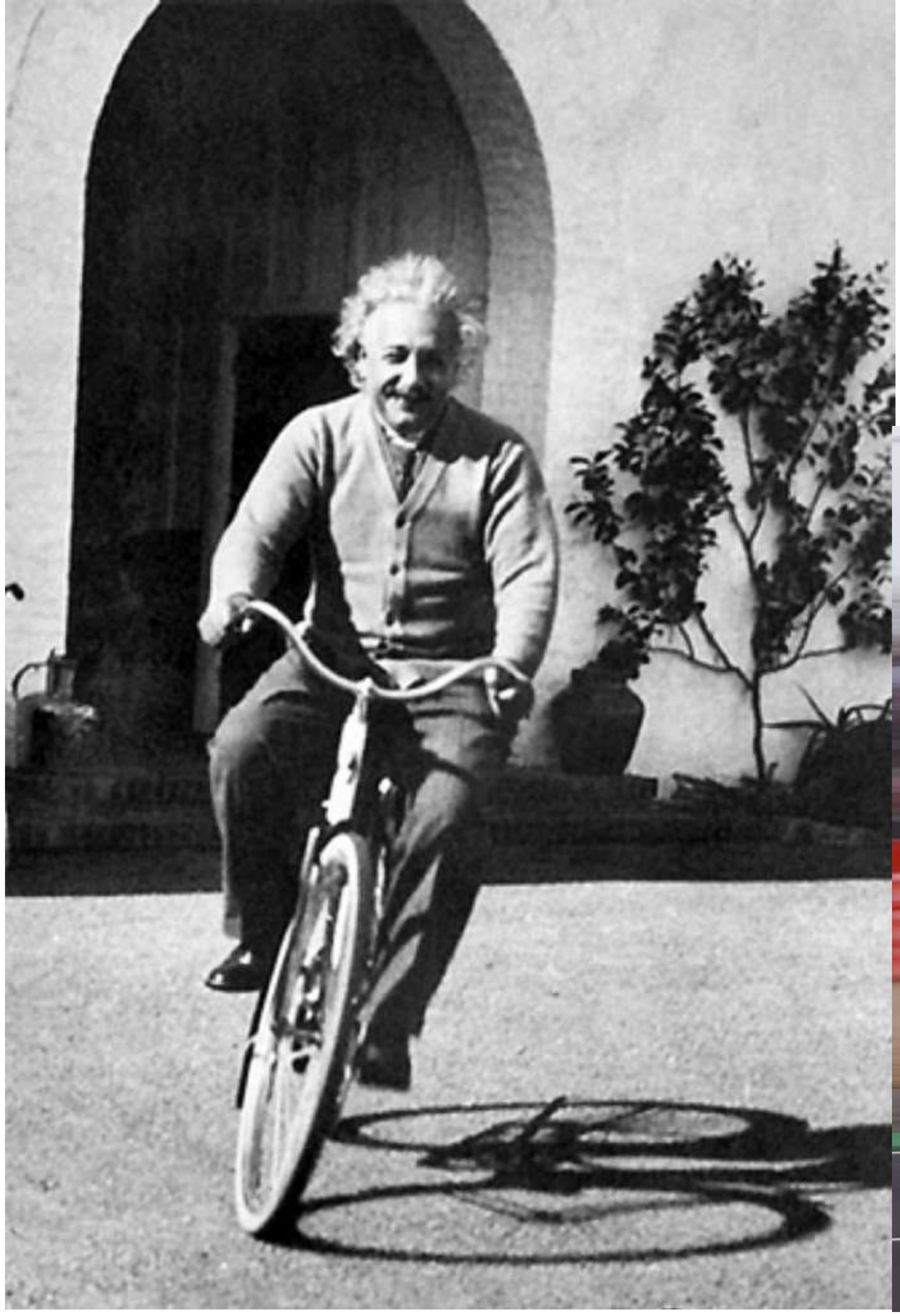
*"Nature isn't classical, dammit, and if you want to make a **simulation of nature**, you'd better make it **quantum mechanical**, and by golly it's a wonderful problem, because it doesn't look so easy"*

1982



The simulation of quantum systems by classical computers is intrinsically inefficient, because the required number of bits and operations grows **exponentially** with the system size.





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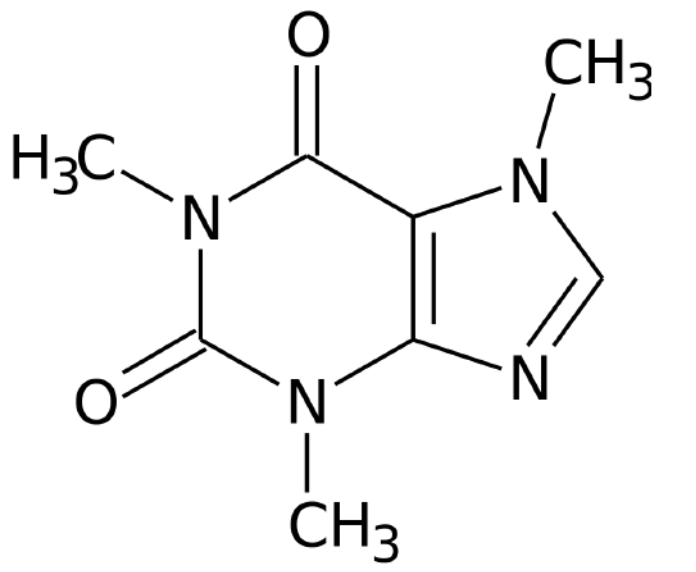

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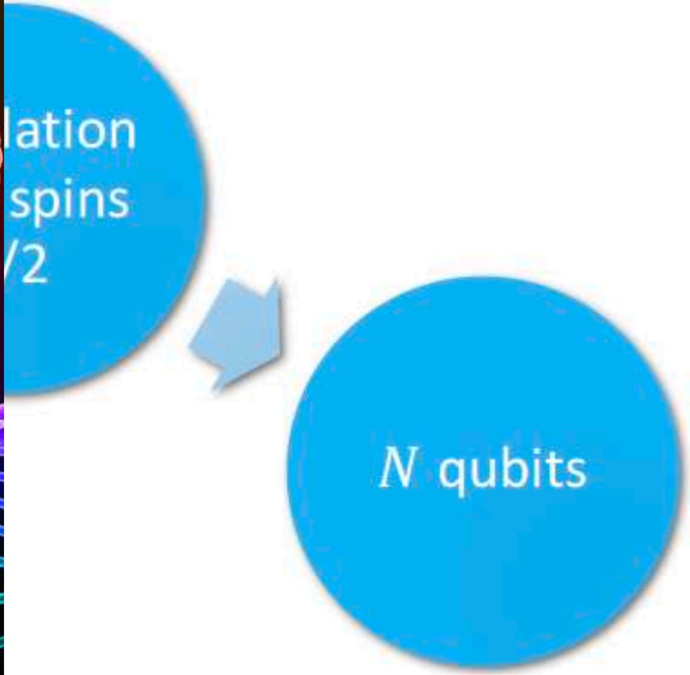
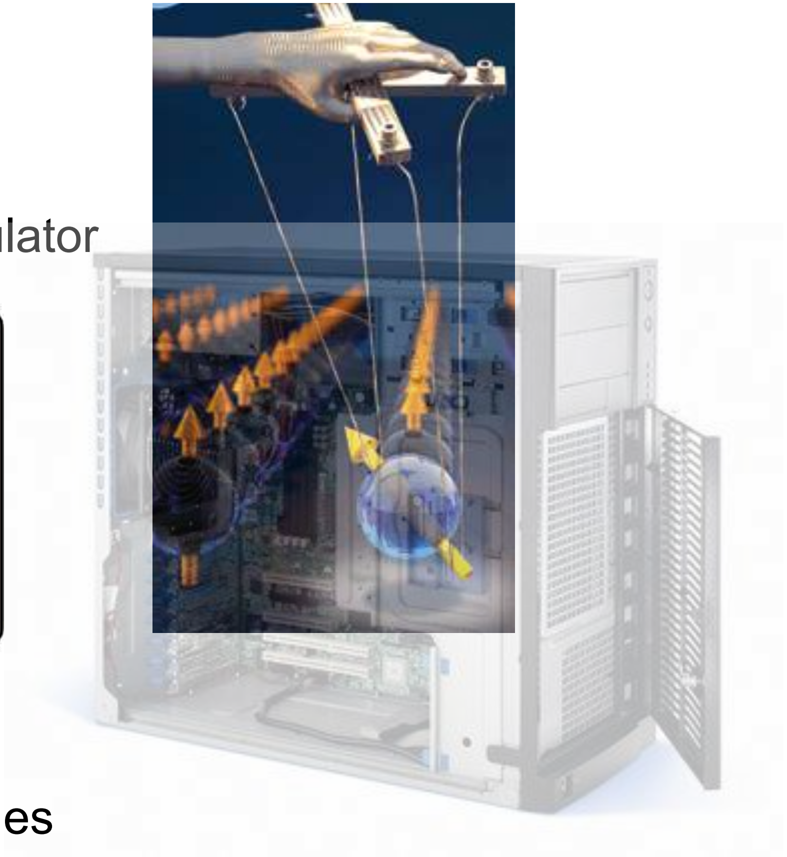


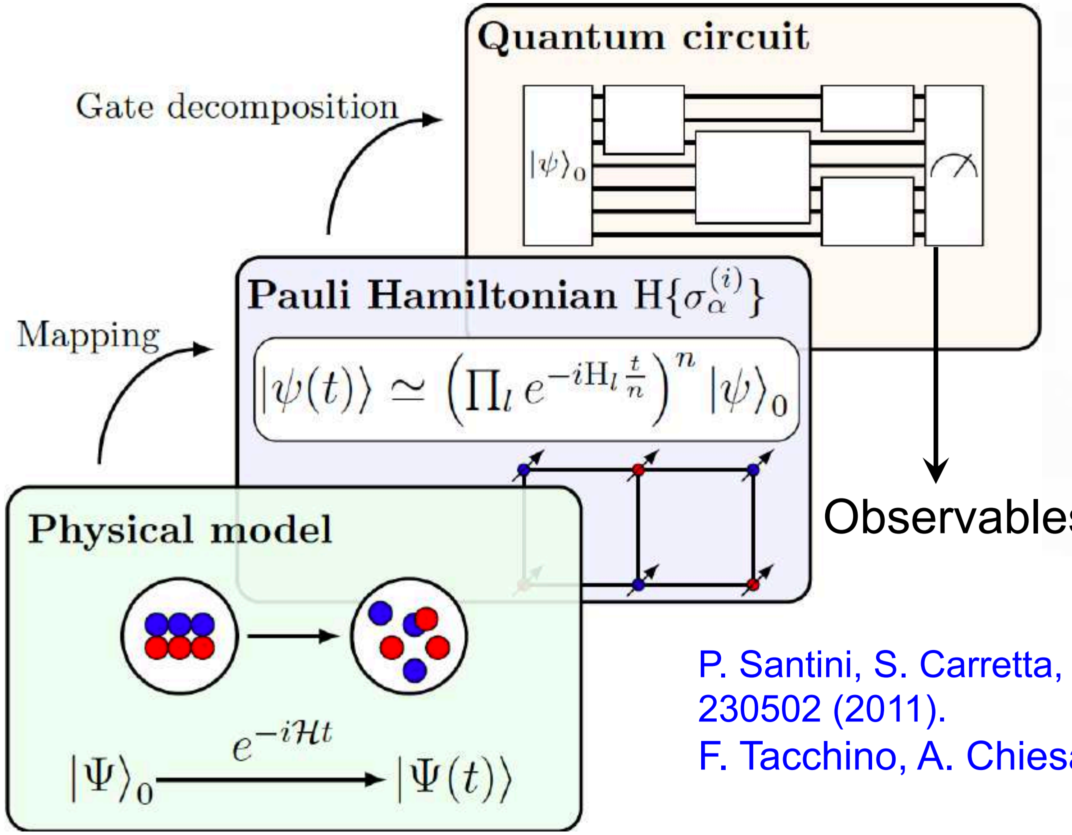
QUANTUM SIMULATORS

encode information in a hardware which operates according to quantum mechanics and whose dynamics can be controlled to mimic the evolution of the target system.

Controlled evolution

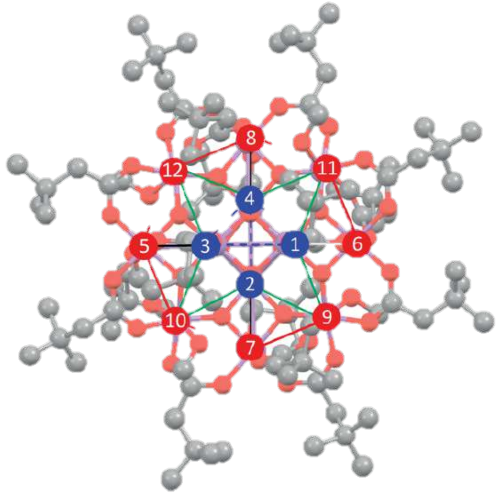


Quantum simulator



Observables

Target system



Evolution according to $\mathcal{H}$

P. Santini, S. Carretta, F. Troiani and G. Amoretti, *Phys. Rev. Lett.* **107**, 230502 (2011).
F. Tacchino, A. Chiesa, S. Carretta, D. Gerace, arXiv:1907.03505.

J. Berezovsky, M. H. Mikkelsen, N. G. Stoltz, L. A. Coldren, D. D. Awschalom, *Science* **320**, 349 (2008).

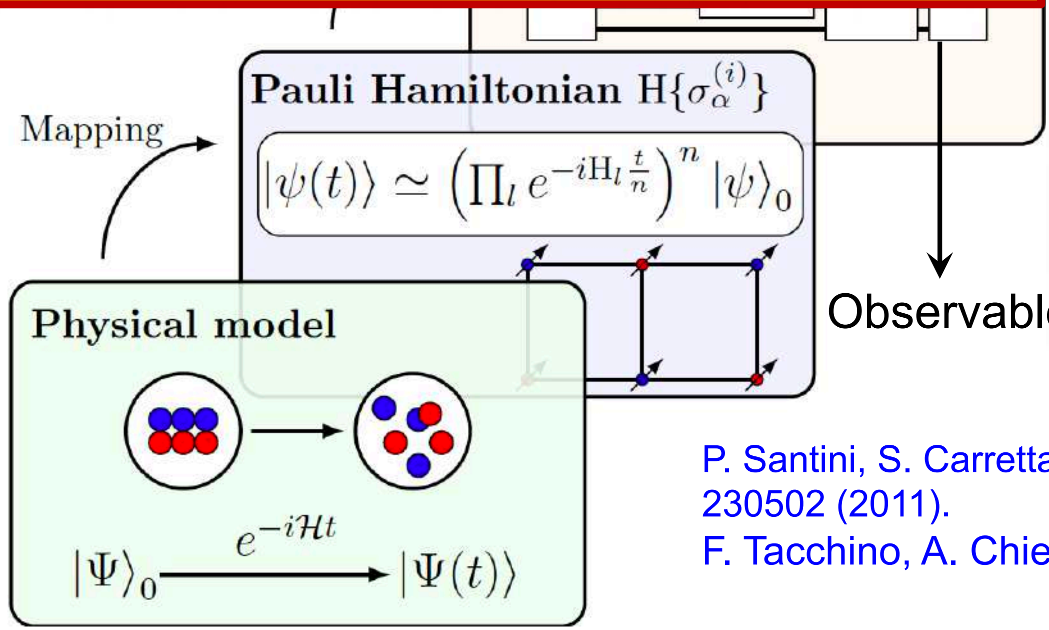
Controlled evolution

QUANTUM SIMULATORS

encode information in a hardware which operates according to quantum mechanics and whose dynamics can be controlled to mimic the evolution of the target system.

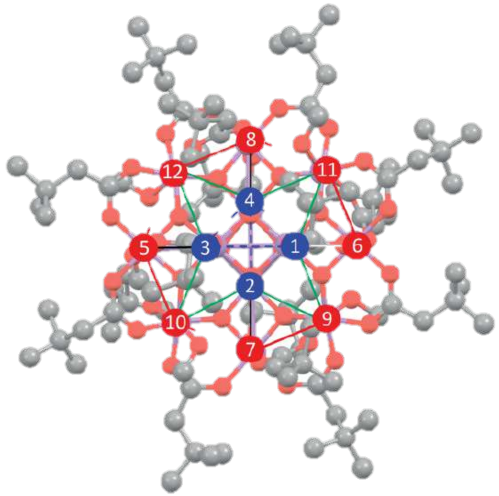
Quantum simulator

A few dozens of controllable qubits could already outperform classical computers



Observables

Target system



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Digital Quantum Simulator

S. Lloyd, *Science* **273**, 1073 (1996)

Digital Quantum Simulator

$$H = \sum_k H_k^{(1)} + \sum_k H_k^{(2)}$$

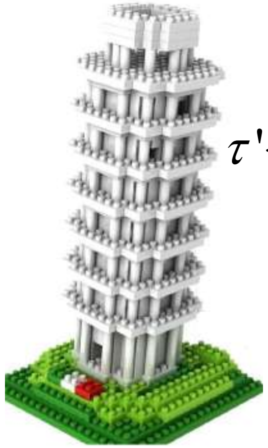
$$U(t,0) = e^{-iHt} \approx \left(\prod_k e^{-iH_k^{(1)}\tau} \prod_k e^{-iH_k^{(2)}\tau} \right)^n \qquad \tau = \frac{t}{n}$$

S. Lloyd, *Science* **273**, 1073 (1996)

Optimizing the digitalization

Target: Pisa tower

Elementary “Trotter” brick in a discretized simulation of the target



$\tau' < \tau \Rightarrow n' > n$

$\rightarrow$

$\tau'' < \tau' \Rightarrow n'' > n'$

$\rightarrow$

$n\tau \gg T_2$

$\rightarrow$

Coarse discretization

Good simulation

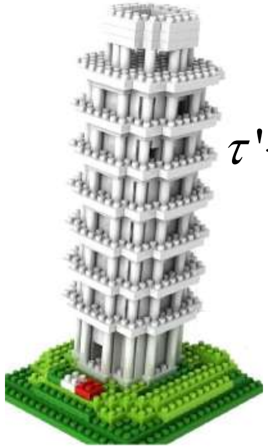
Simulator fails

Optimizing the digitalization

In the **NISQ** (noisy-intermediate scale quantum computing) era
each operation is error-prone

By increasing the circuit depth we increase the error probability.

Trade-off **Targeted error mitigation strategies**



$\tau' < \tau \Rightarrow n' > n$ $\rightarrow$

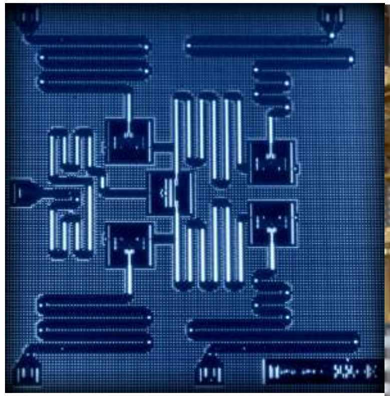
$\tau'' < \tau' \Rightarrow n'' > n'$ $\rightarrow$

$n\tau \gg T_2$ $\rightarrow$

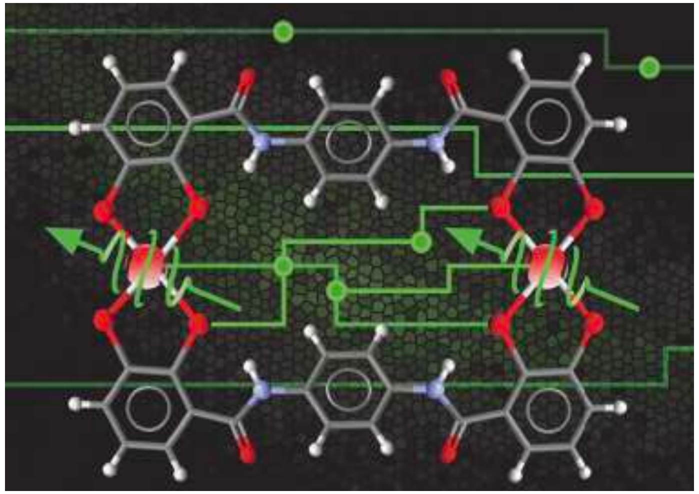
Coarse discretization Good simulation Simulator fails

Physical implementation: a few examples

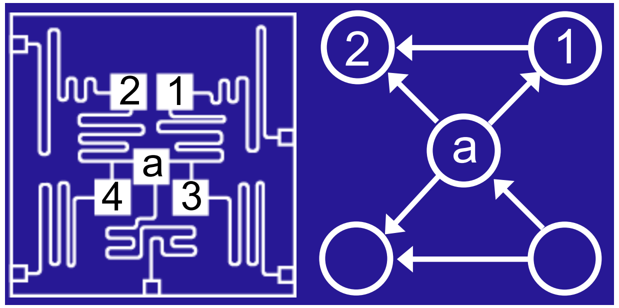
- State-of-the-art **leading** technologies: superconducting (transmon) qubits
  - Existing chips with 5-53 qubits enable to implement non trivial quantum algorithms.
  - Other leading technology: trapped ions



- **Prospective** technologies: Molecular Nanomagnets
  - Other promising platforms: photons, quantum dots...

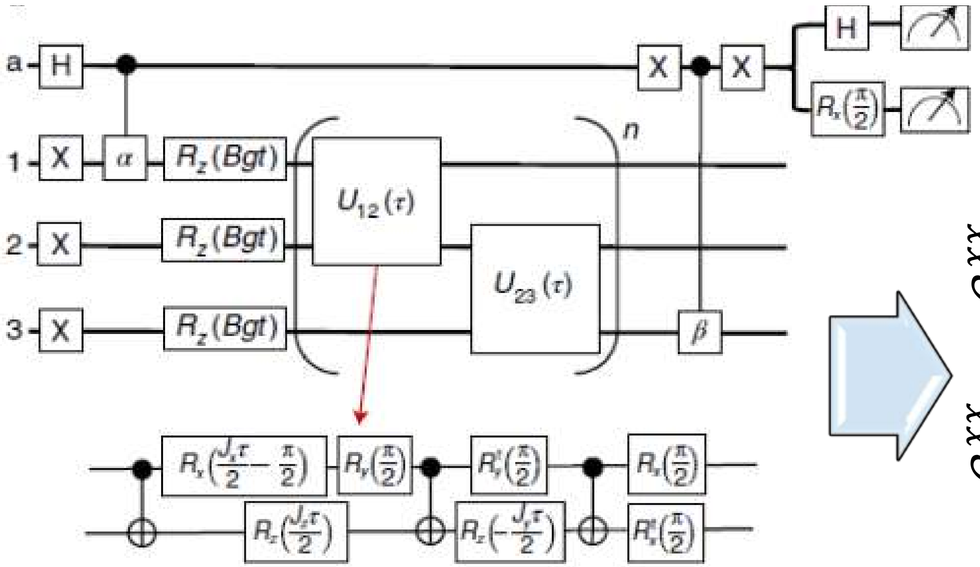


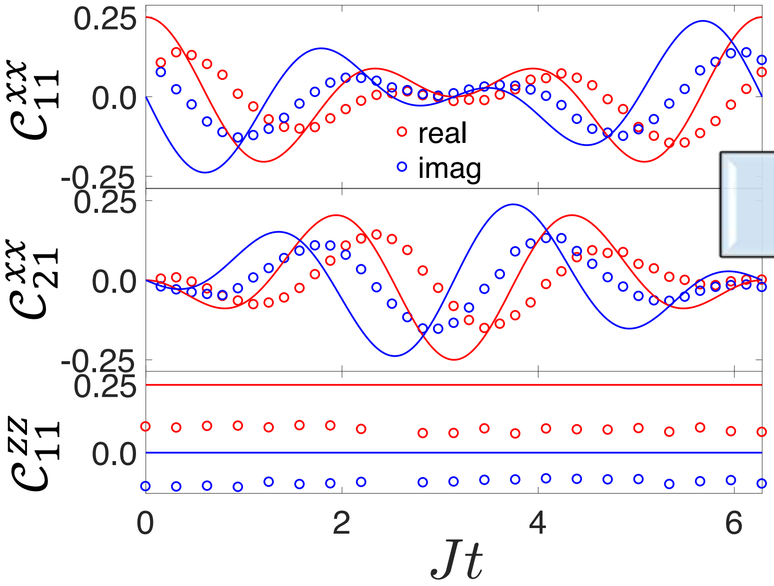
Superconducting qubits

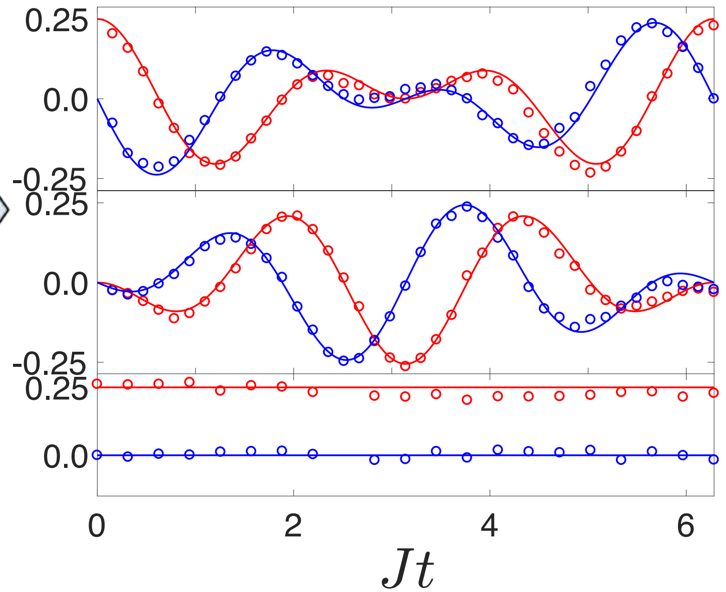


The quantum dynamics of spin chains can be simulated by concatenating elementary gates.

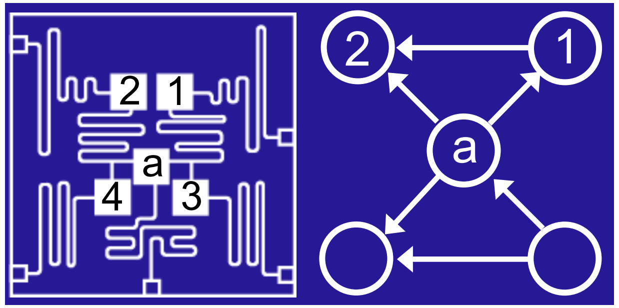
Noisy results are corrected by exploiting symmetries of the extracted observables, thus recovering the correct dynamics.







Superconducting qubits



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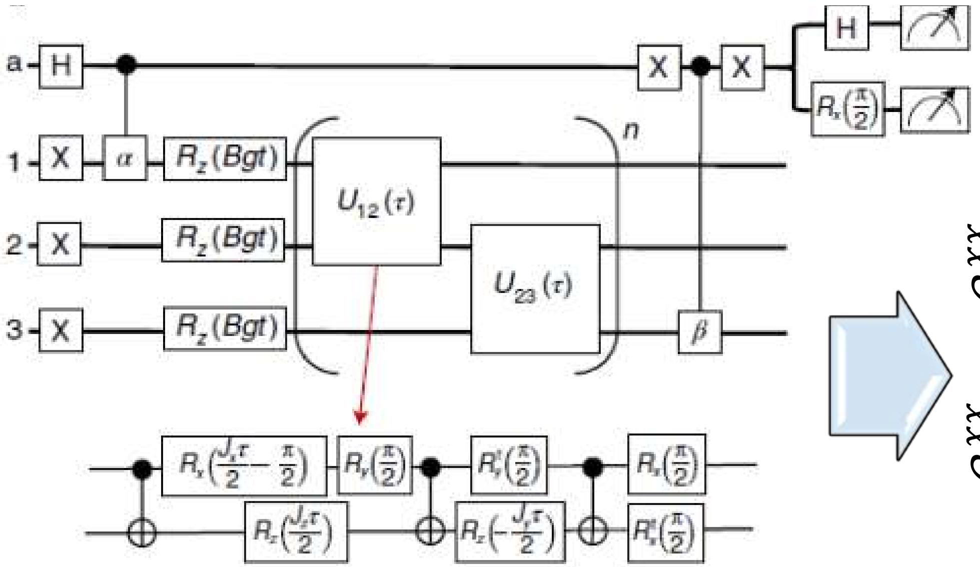
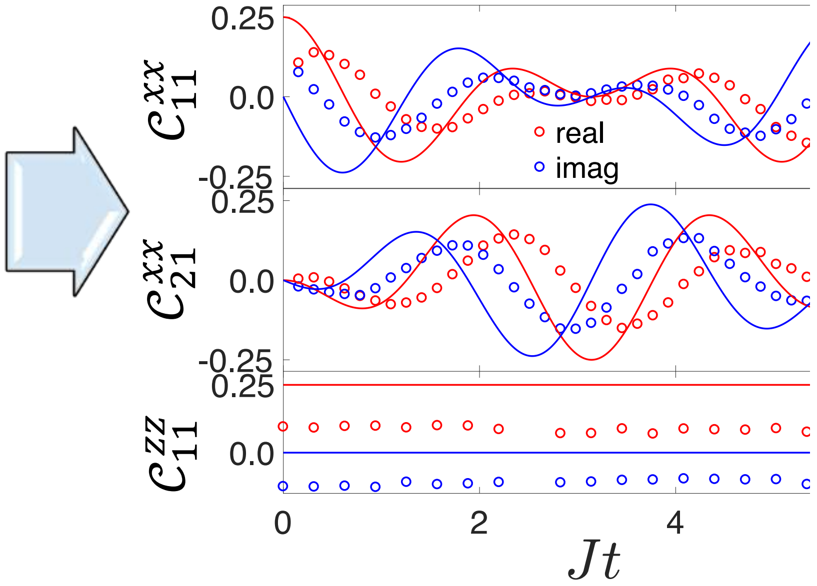
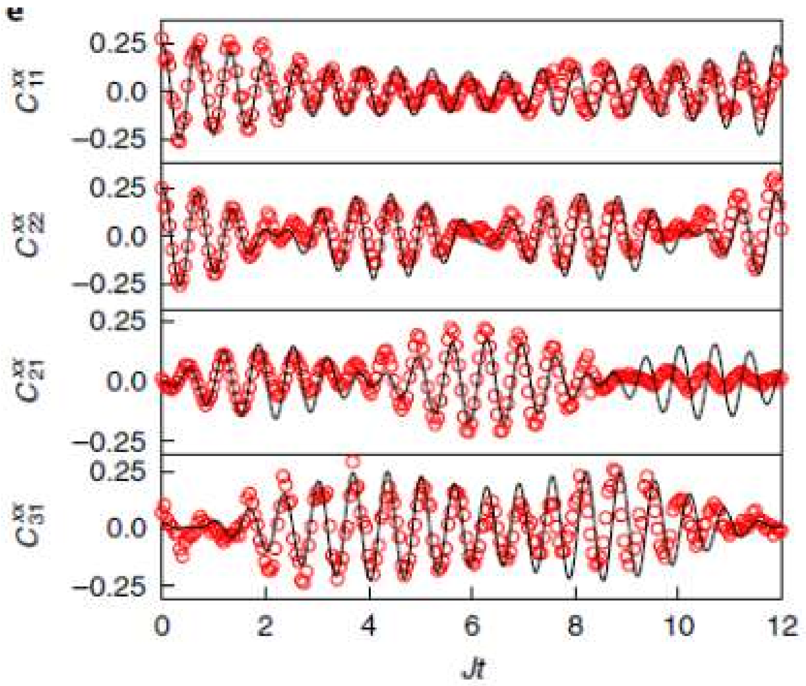
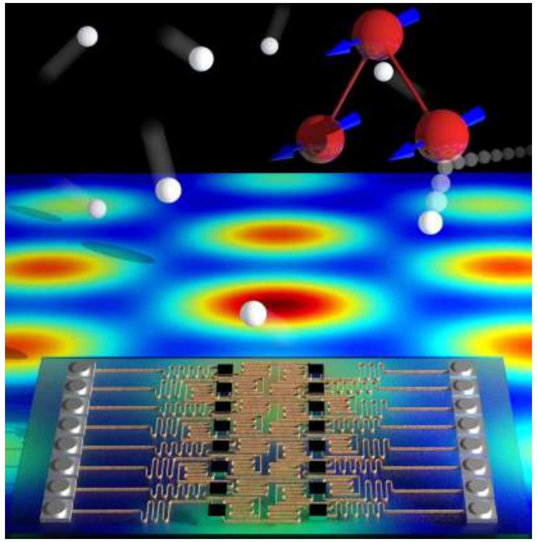






Extracting experimental observables



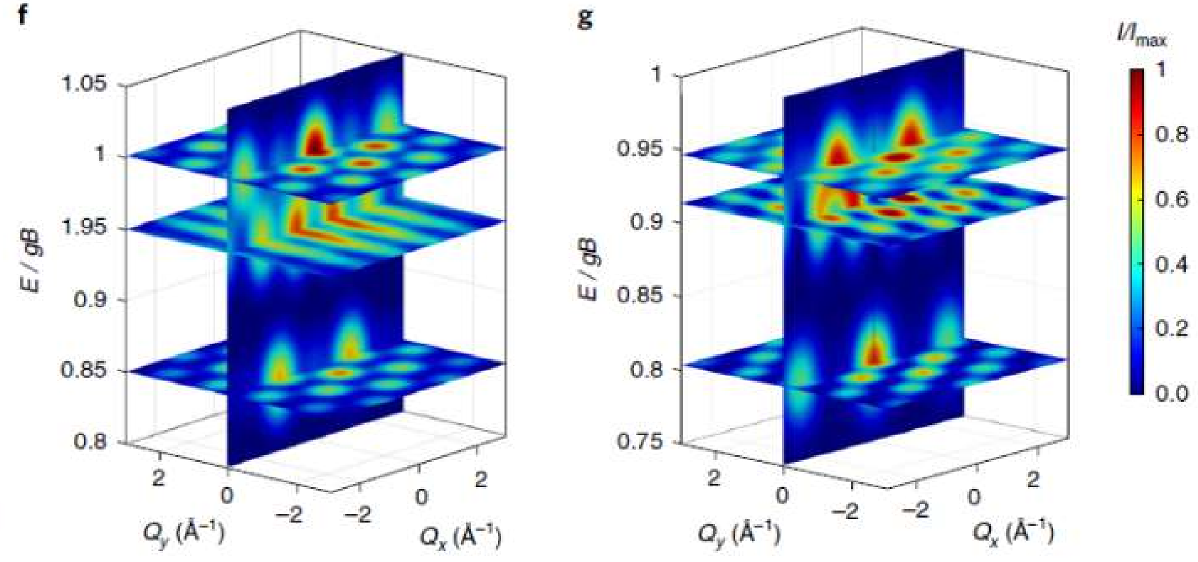
nature physics

LETTERS

https://doi.org/10.1038/s41567-019-0437-4

Quantum hardware simulating four-dimensional inelastic neutron scattering

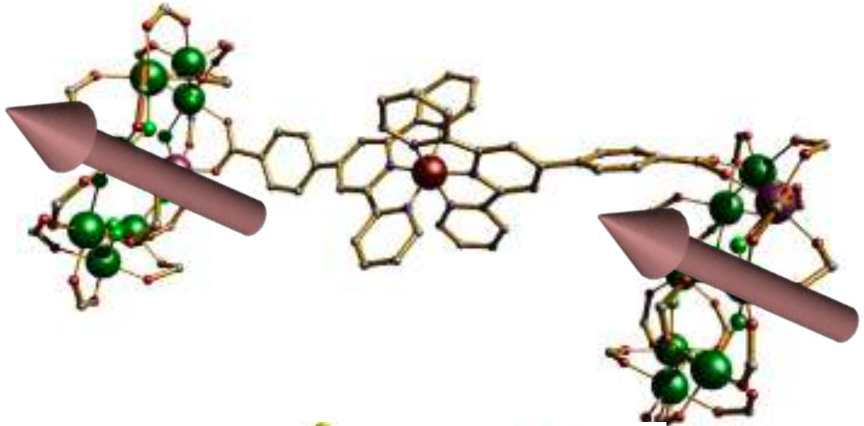
A. Chiesa[1,5], F. Tacchino[2,5], M. Grossi[2,3], P. Santini[1], I. Tavernelli[4], D. Gerace[2] and S. Carretta[1*]



Quantum simulations of the spin dynamics of prototypical spin systems are used to calculate the 4D inelastic neutron cross-section

In the near future, quantum computers will be used to interpret experiments which cannot be modeled by classical machines

Molecular Nanomagnets

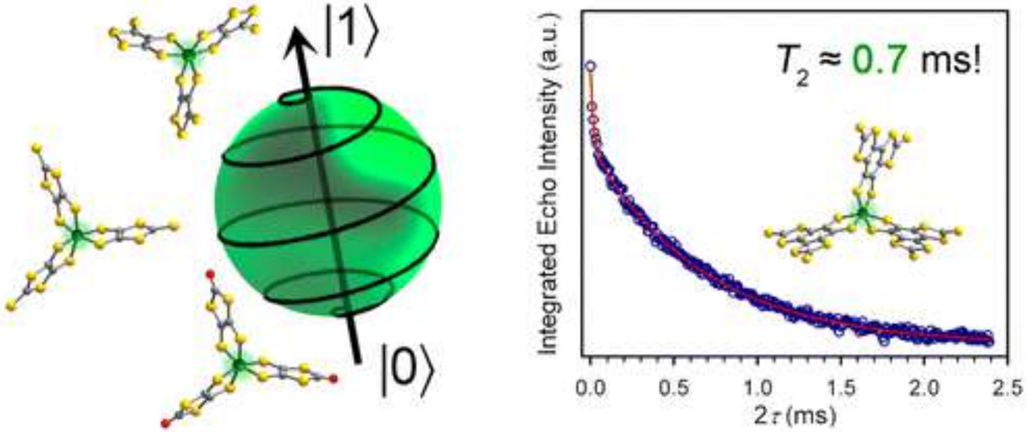


Long T_2

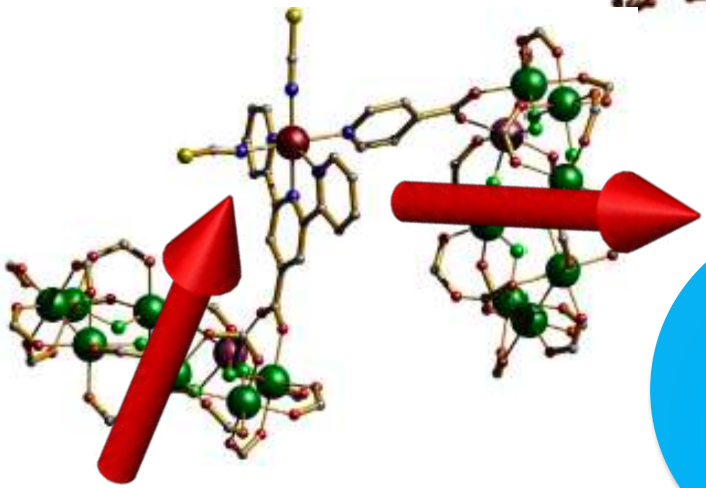
MNMs

Chemical tunability

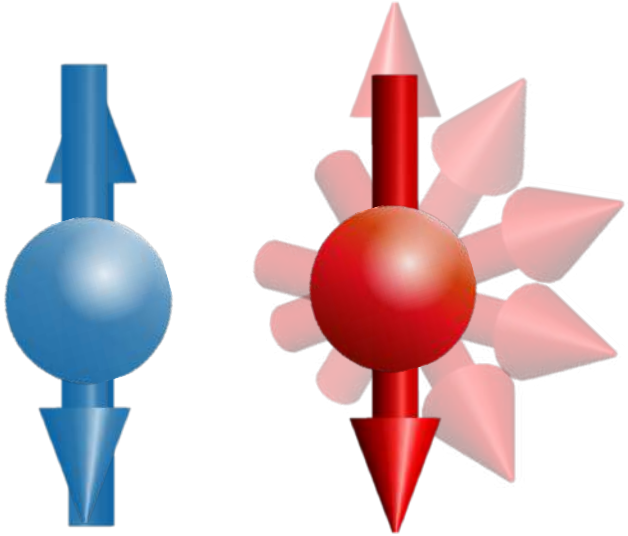
Multi-level structure



ACS Cent. Sci. **1**, 488 (2015)

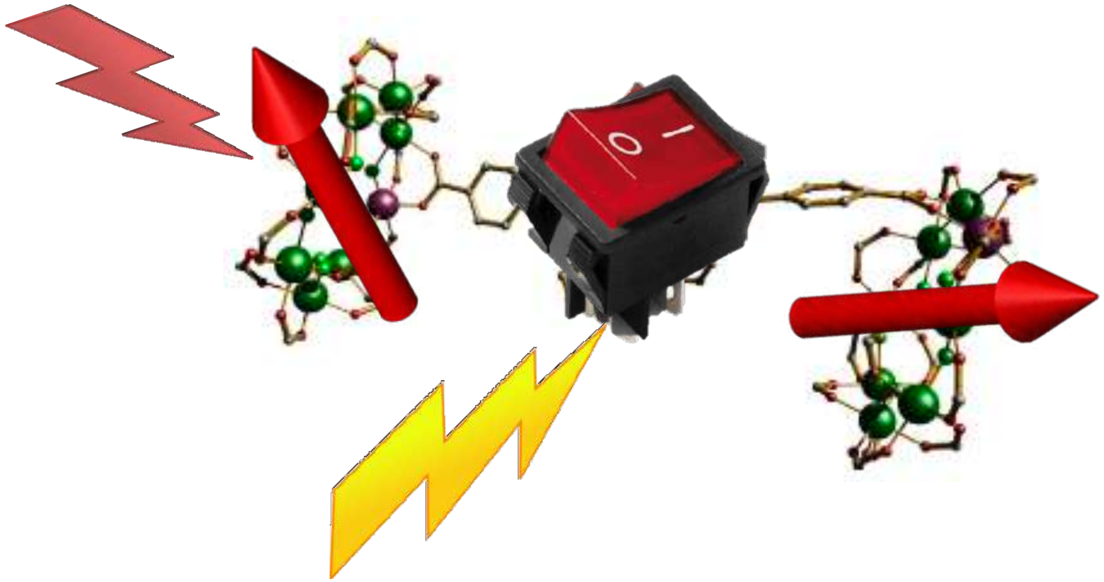


Nat. Commun. **7**, 11377 (2016)



J. Am. Chem. Soc. **140**, 9814 (2018)

Engineering the coupling between molecular qubits



- A **switchable** **QQ interaction** is mandatory to implement quantum simulations of interesting models, i.e. to implement both single- and two-qubit gates.

- Molecular qubits can be chemically tuned to effectively switch on/off the QQ coupling by **selectively exciting the switch**.

P. Santini, S. Carretta, F. Troiani and G. Amoretti, *Phys. Rev. Lett.* **107**, 230502 (2011).
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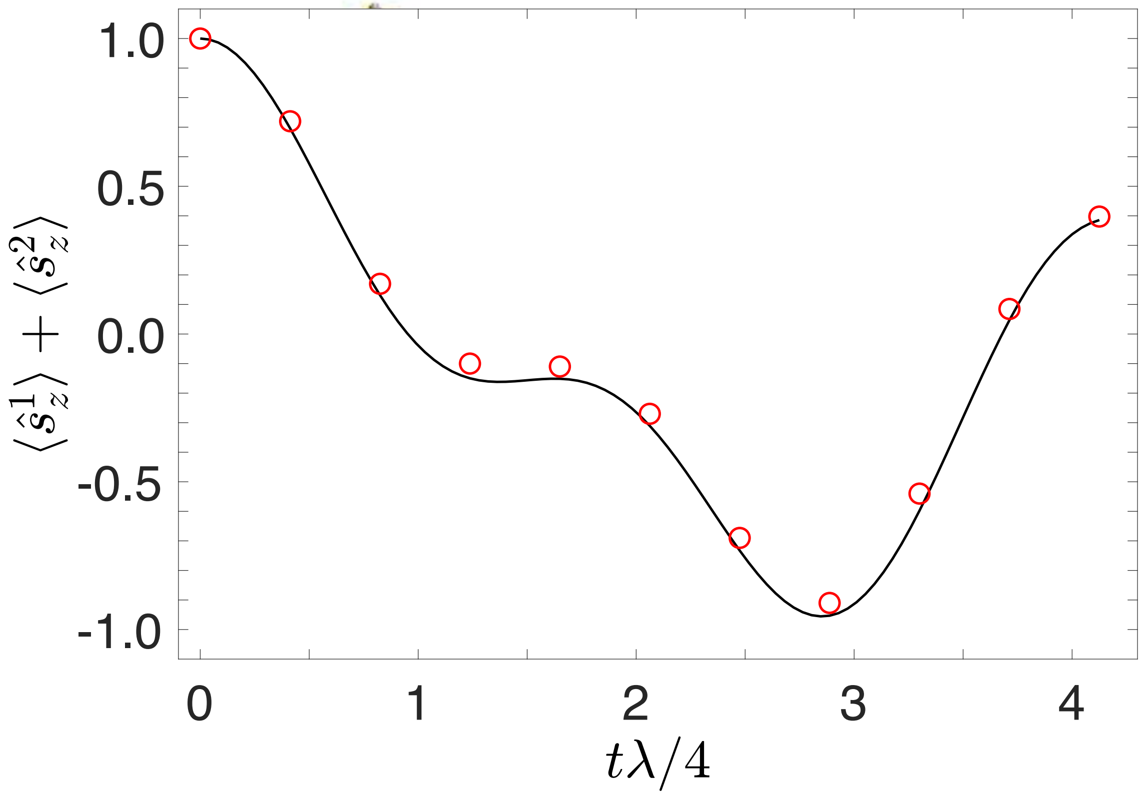
Engineering the coupling between molecular qubits



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- A **switchable QQ interaction** is mandatory to implement quantum simulations of interesting models, i.e. to implement both single- and two-qubit gates.
- Molecular qubits can be chemically tuned to effectively switch on/off the QQ coupling by **selectively exciting the switch**.
- Numerical simulations show that these systems are a very promising platform for QS.
- A scalable arrays can be envisaged.

$$\mathcal{H}_{\mathrm{TIM}} = \lambda \sum_{k=1}^{N-1} s_{kz} s_{(k+1)z} + b \sum_{k=1}^{N} s_{kx}$$


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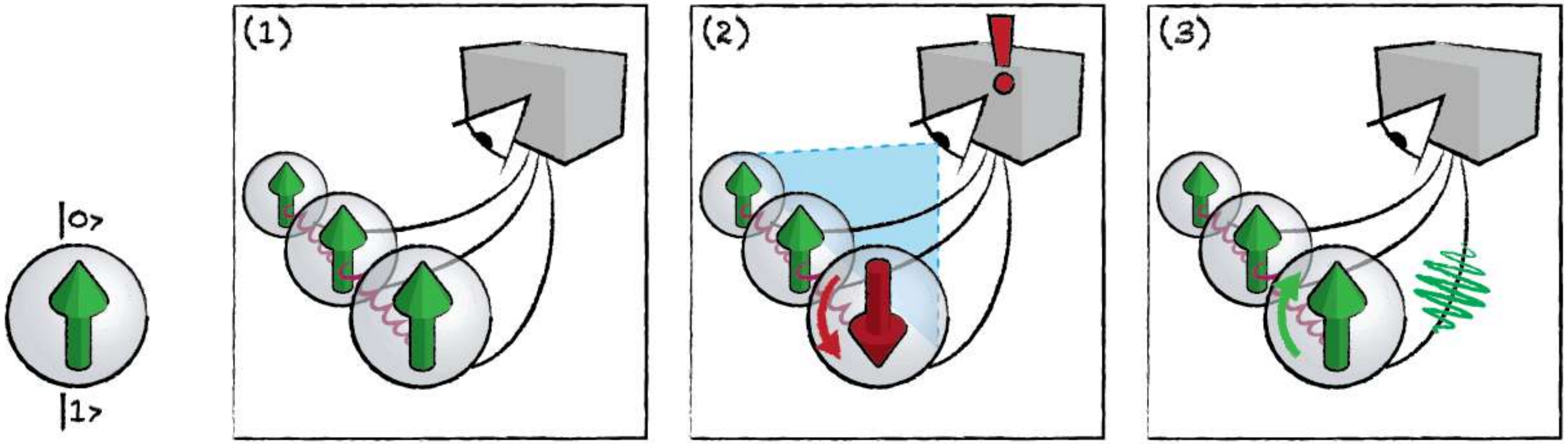
Molecular qubits with embedded error-correction



The easily accessible **multi-level structure** of molecular qubits can **embed** quantum error **correction** at the **single-molecule level**: errors lead outside from the computational subspace and hence can be detected and corrected, without requiring additional qubits resources.

Nature Nanotech. **9**, 171–176 (2014)

Molecular qubits with embedded error-correction

R. Hussain, G. Allodi, A. Chiesa, E. Garlatti, D. Mitcov, A. Konstantatos, K. S. Pedersen, R.De Renzi, S. Piligkos and S. Carretta, J. *Am. Chem. Soc.* **140**, 9814 (2018)

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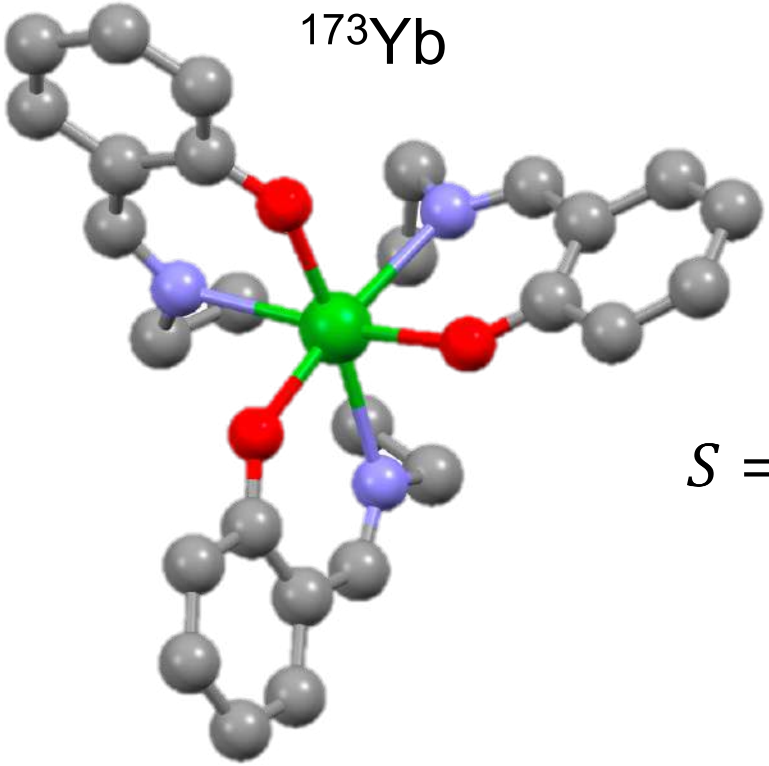
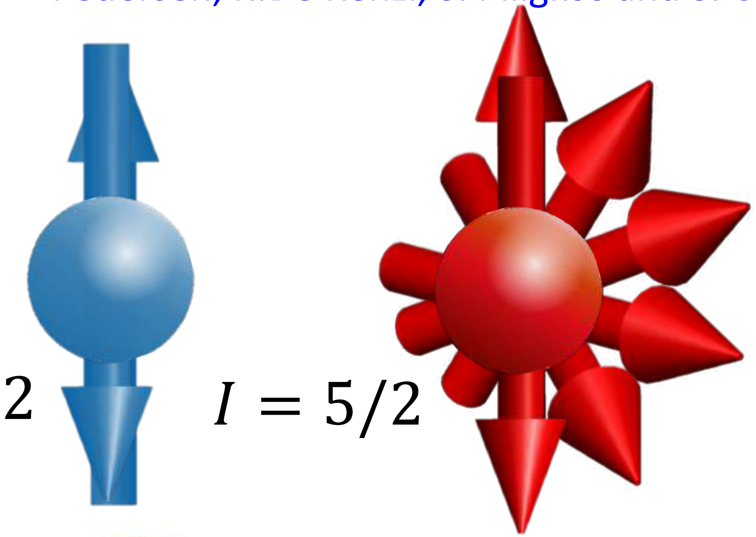
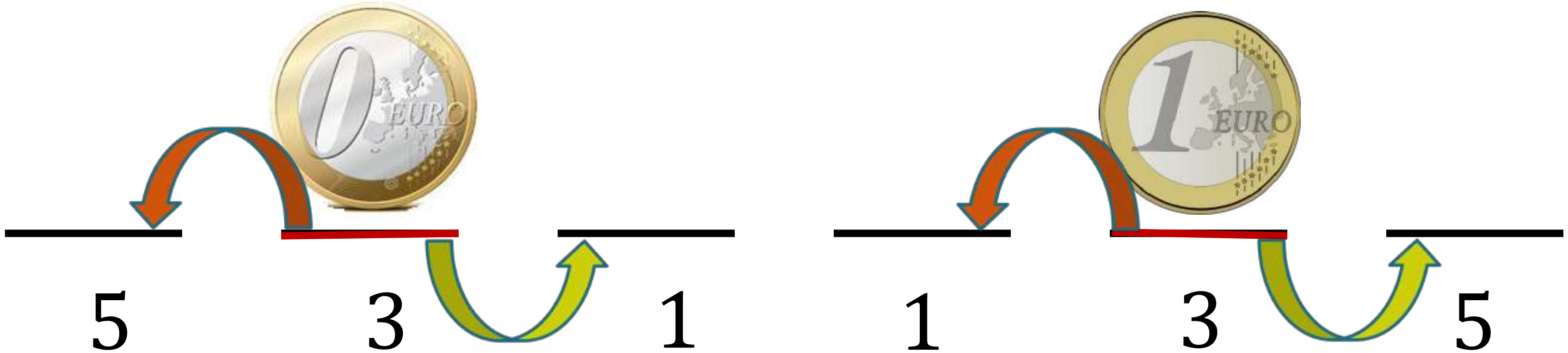




$S = 1/2$ $\qquad I = 5/2$



$|\bar{\psi}\rangle$

$m_I \qquad -\frac{5}{2} \qquad -\frac{3}{2} \qquad -\frac{1}{2} \qquad \frac{1}{2} \qquad \frac{3}{2} \qquad \frac{5}{2}$

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R. Hussain, G. Allodi, A. Chiesa, E. Garlatti, D. Mitcov, A. Konstantatos, K. S. Pedersen, R.De Renzi, S. Piligkos and S. Carretta, J. *Am. Chem. Soc.* **140**, 9814 (2018)

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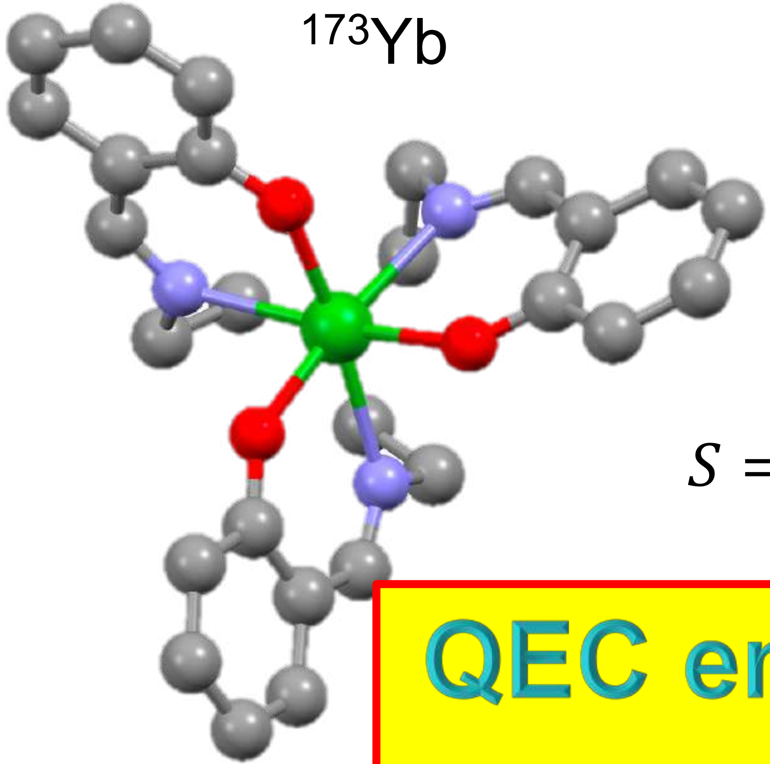
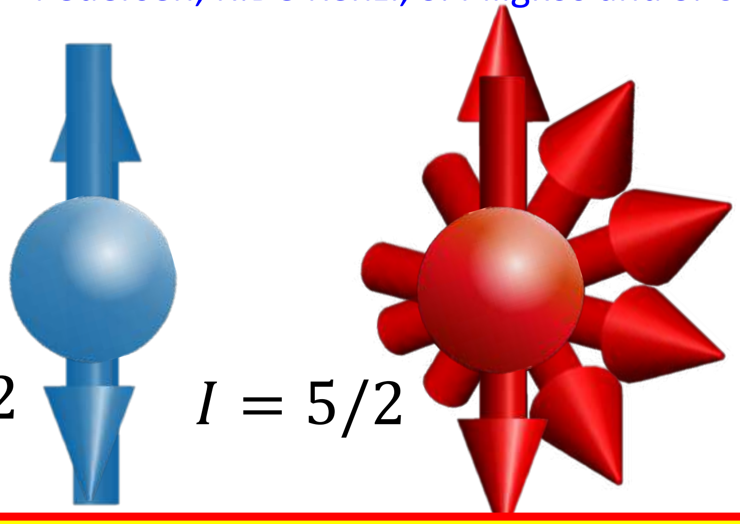




$S = 1/2$ $\quad I = 5/2$

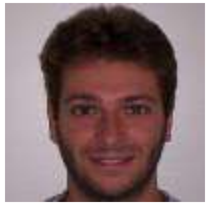
QEC embedded in a single molecule, without ancillae

$|\Psi\rangle$

$m_I \quad -\frac{5}{2} \quad -\frac{3}{2} \quad -\frac{1}{2} \quad \frac{1}{2} \quad \frac{3}{2} \quad \frac{5}{2}$

Collaborators


F. Tacchino


D. Gerace


I. Tavernelli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J. M. Skelton, D. P. Mills, N. F. Chilton, G. Timco, E. McInness, R. E. P. Winpenny

M. Atzori, L. Sorace, R. Sessoli

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E. Morra, M. Chiesa

Understanding → Design