Qubits and Quantum Computing

Literature Presentation

15 March 2022

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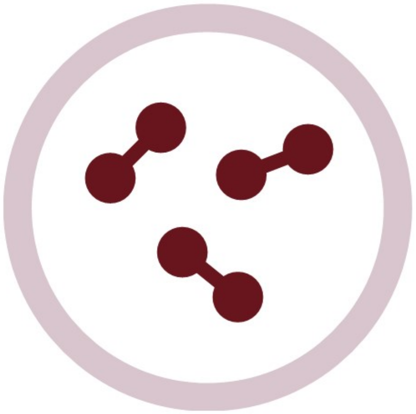
MacMillan Group

Princeton University

Quantum computing

Quantum computer: a machine that use the properties of quantum physics to store and process data



chemical dynamics

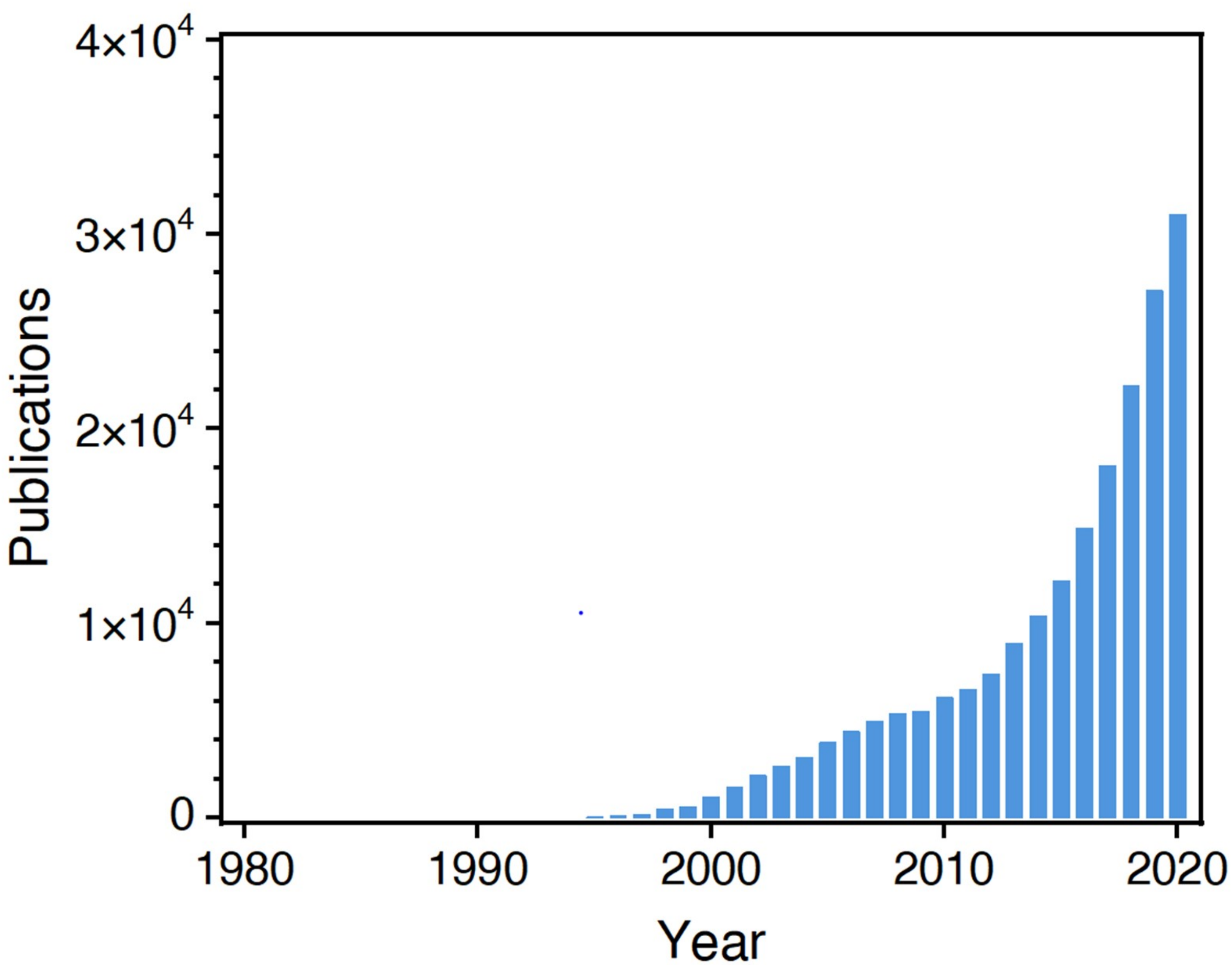
codebreaking

protein folding

artificial intelligence

Qubit research has grown exponentially over the past decade

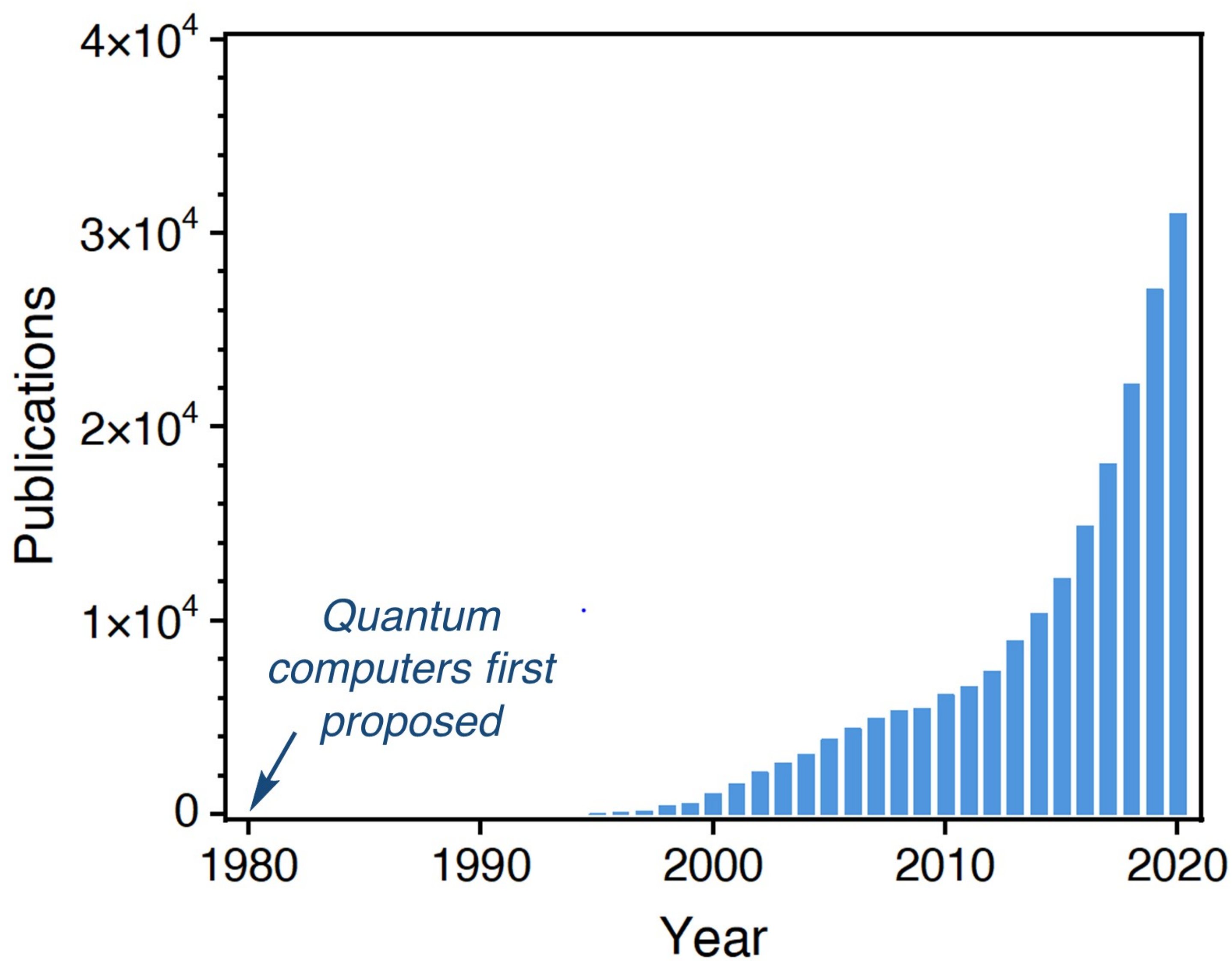
qubit: the basic unit of information in a quantum computer



Plot generated from a Google Scholar search for articles containing the term "qubit"

Qubit research has grown exponentially over the past decade

independently proposed by Feynman, Manin, and Benioff



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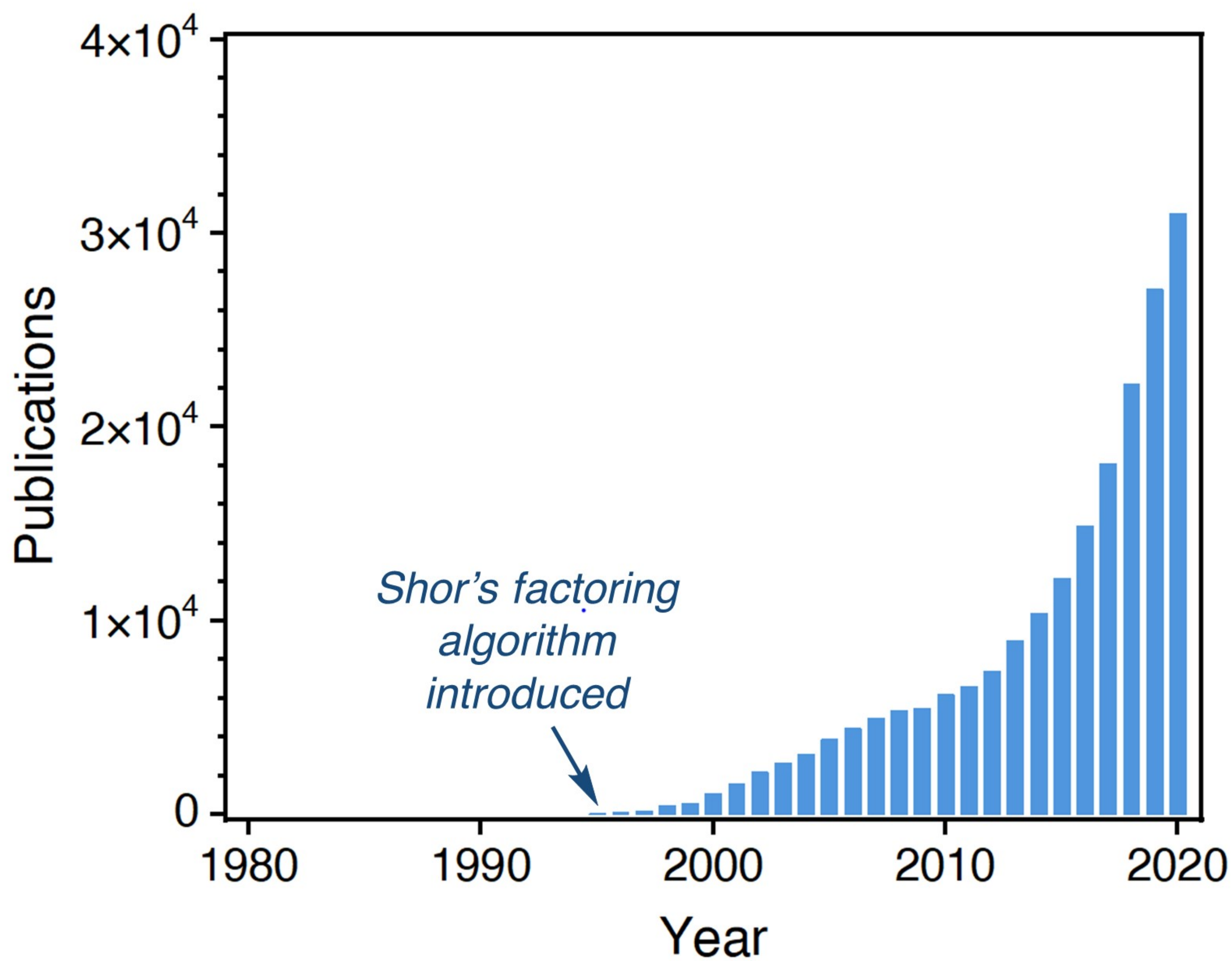
Qubit research has grown exponentially over the past decade

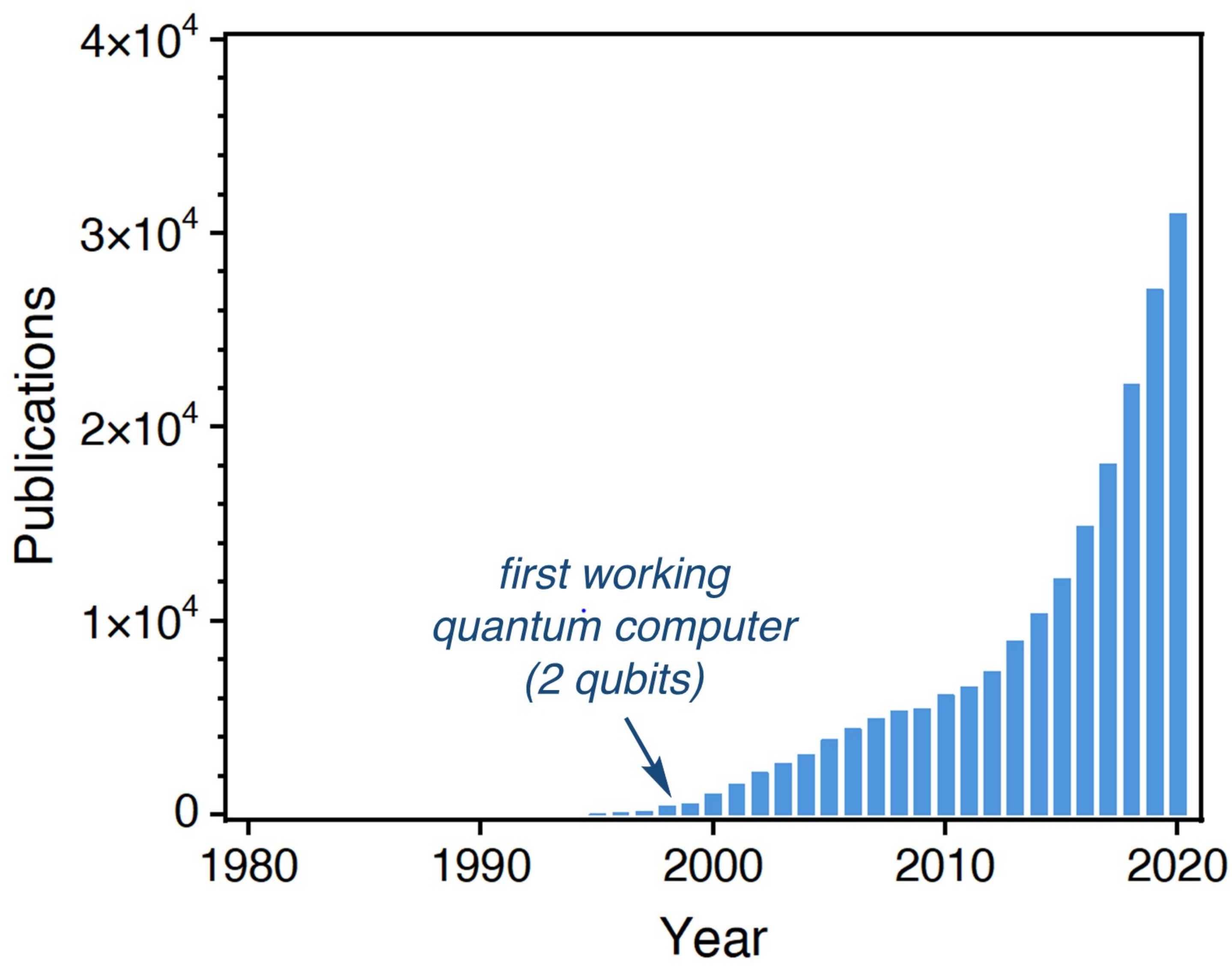
quantum computers could theoretically factor integers rapidly, which could undermine state-of-the-art encryption



Plot generated from a Google Scholar search for articles containing the term "qubit"

Qubit research has grown exponentially over the past decade

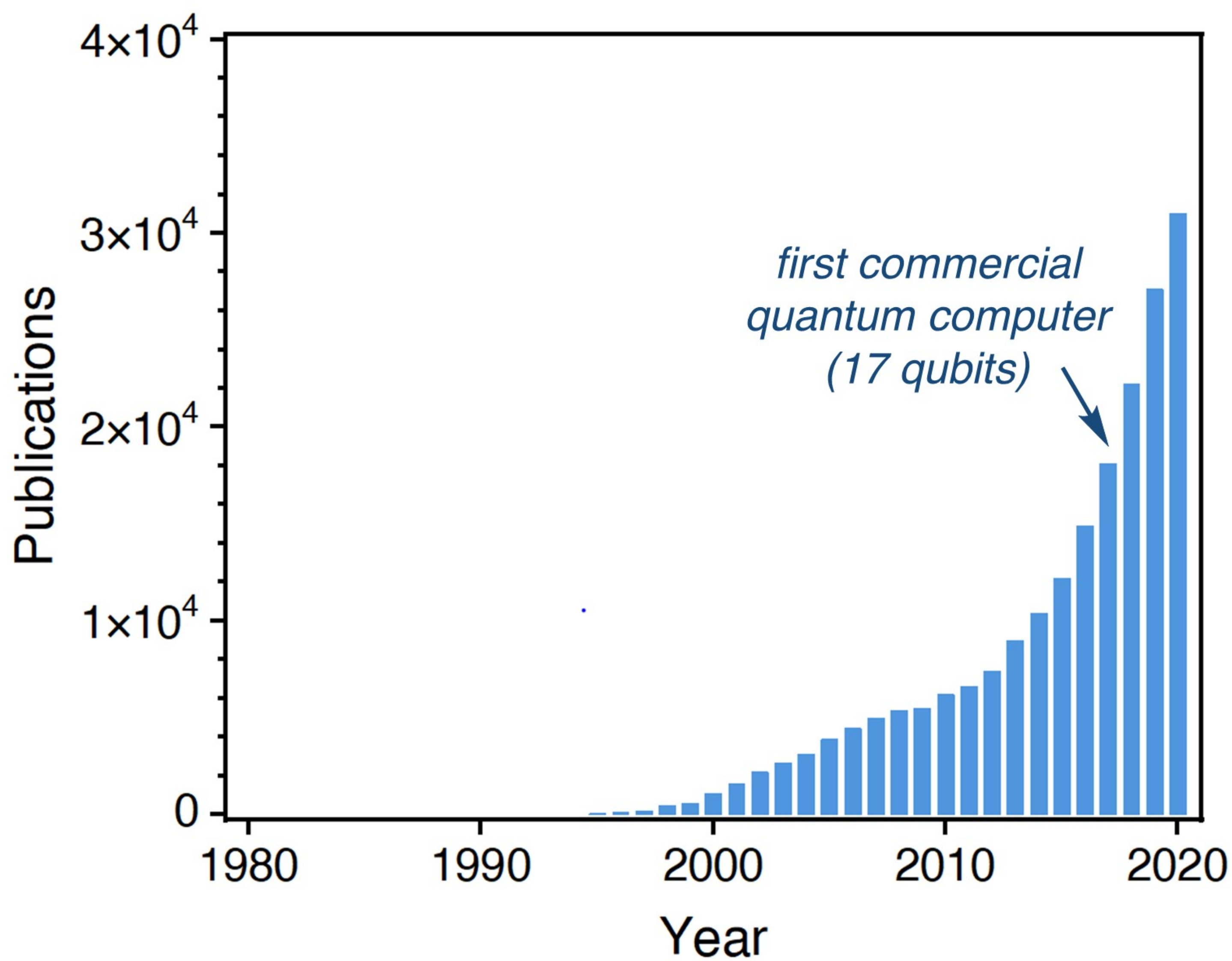
demonstration of simple quantum algorithm



Plot generated from a Google Scholar search for articles containing the term "qubit"

Qubit research has grown exponentially over the past decade

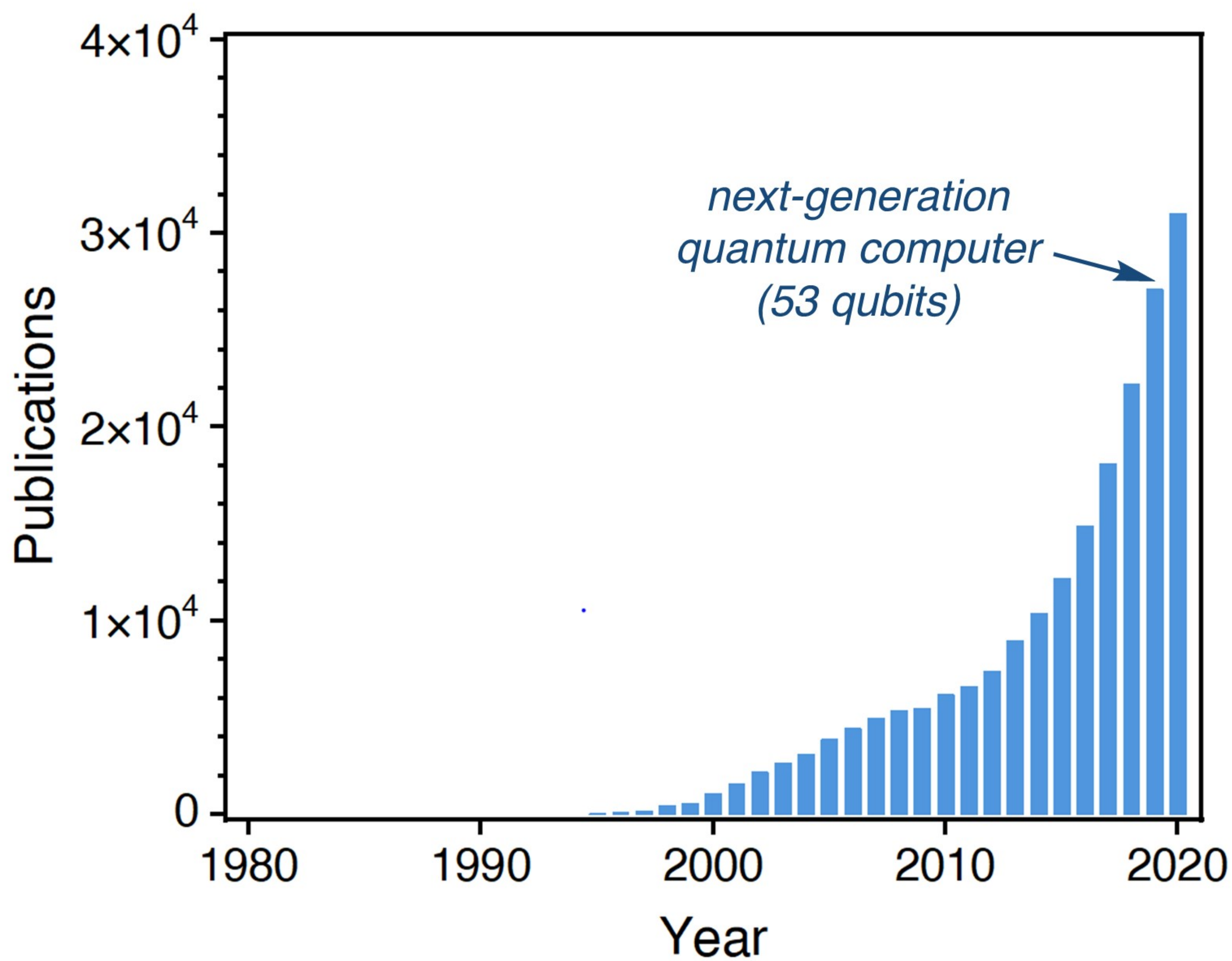
introduced by Quantum AI Lab (Google, NASA, etc.)



Plot generated from a Google Scholar search for articles containing the term "qubit"

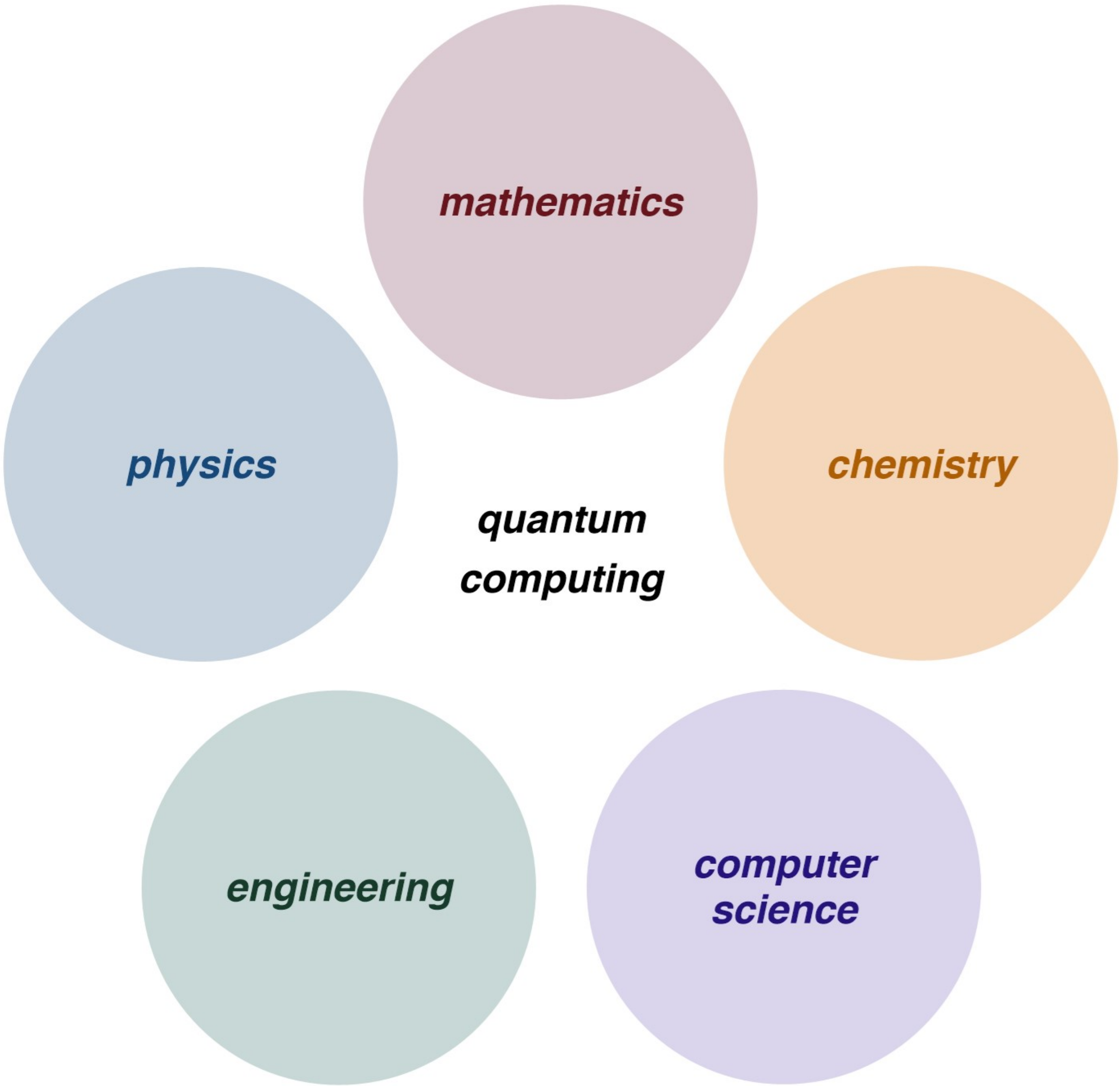
Qubit research has grown exponentially over the past decade

introduced by IBM



Plot generated from a Google Scholar search for articles containing the term "qubit"

Quantum computing research is highly interdisciplinary

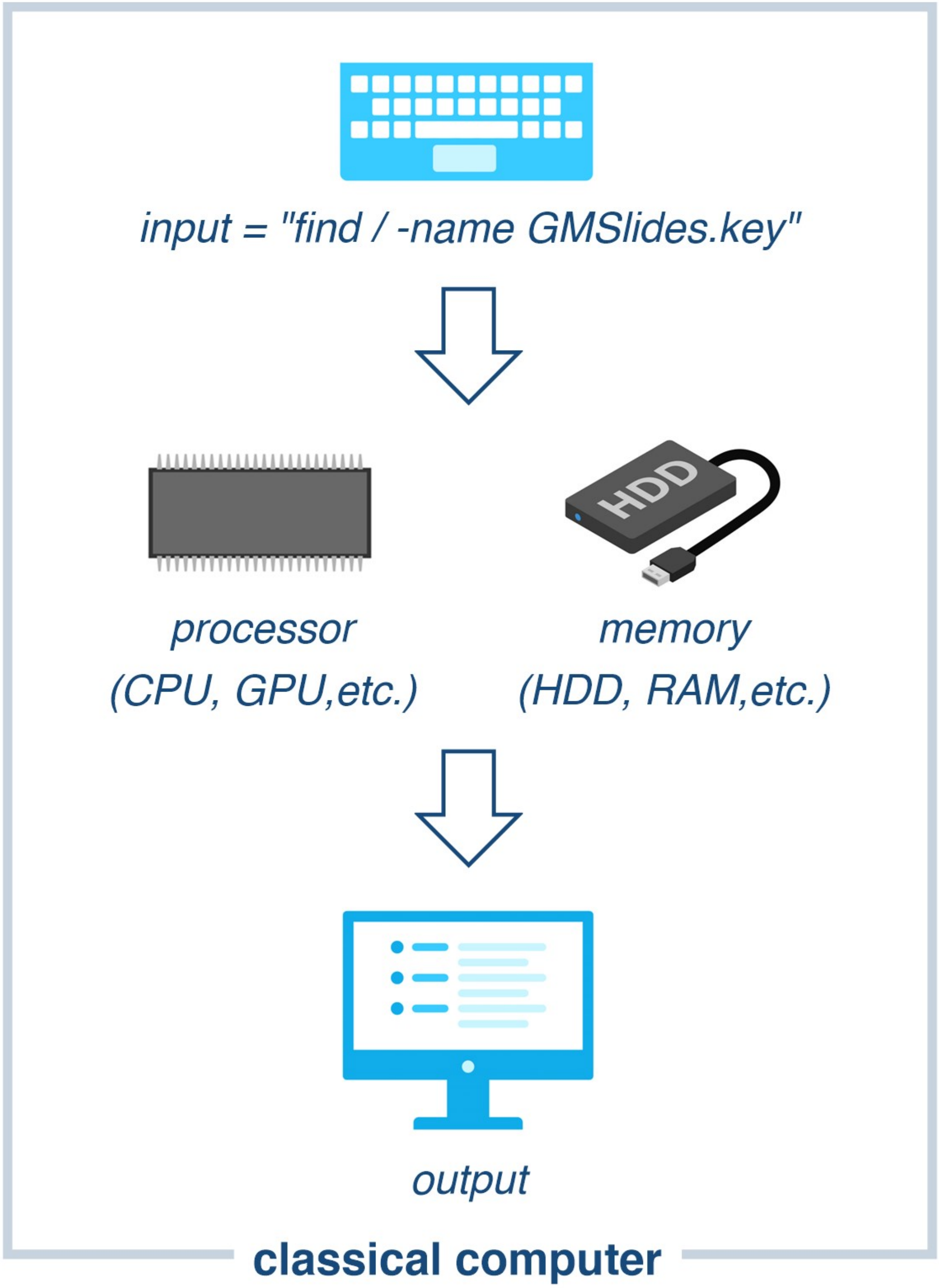


Goals for this literature review

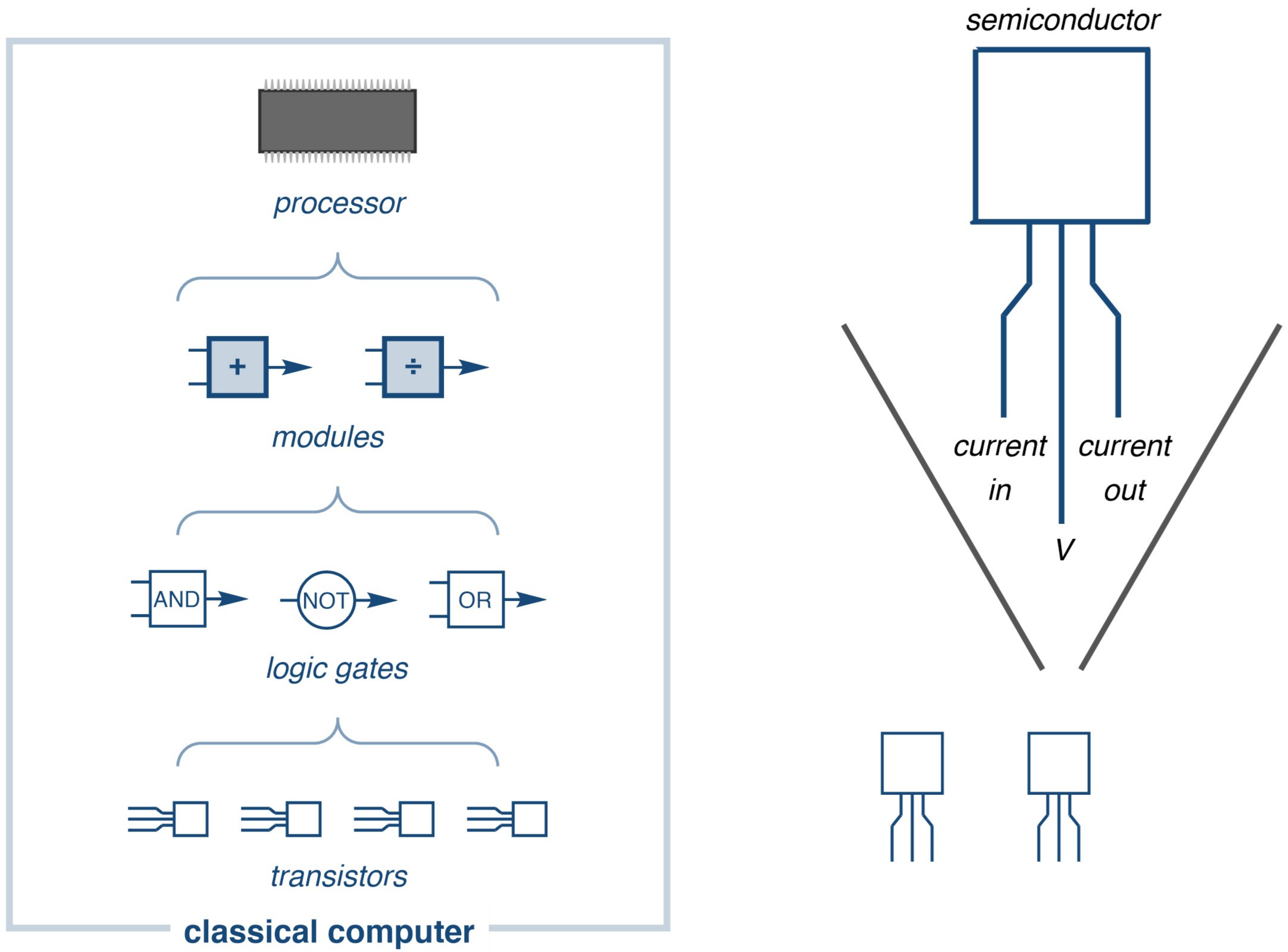
1) general introduction to quantum computing and qubits

2) highlight potential opportunities for chemists

Classical computers are based on binary units



Classical computers are based on binary units



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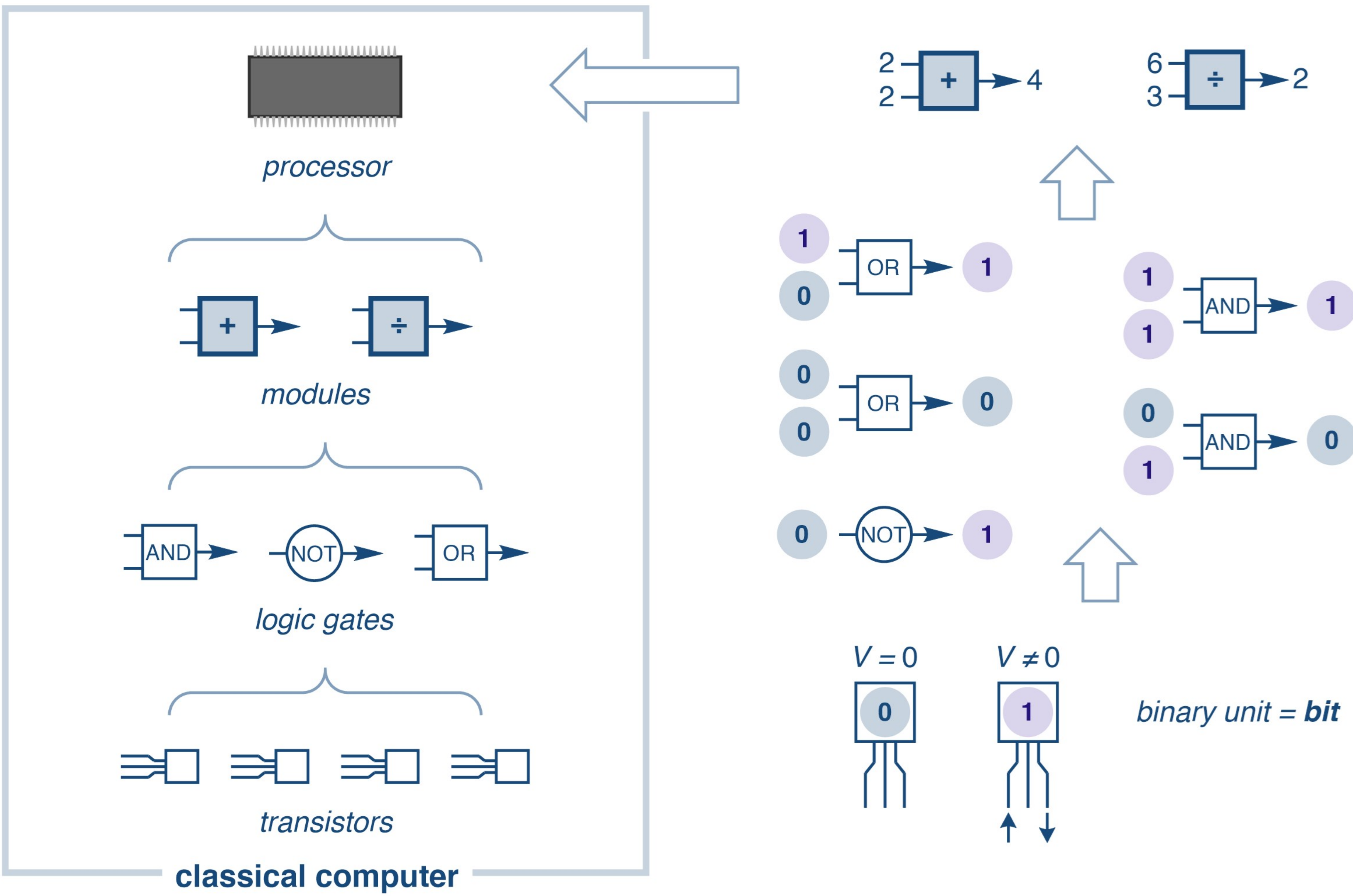

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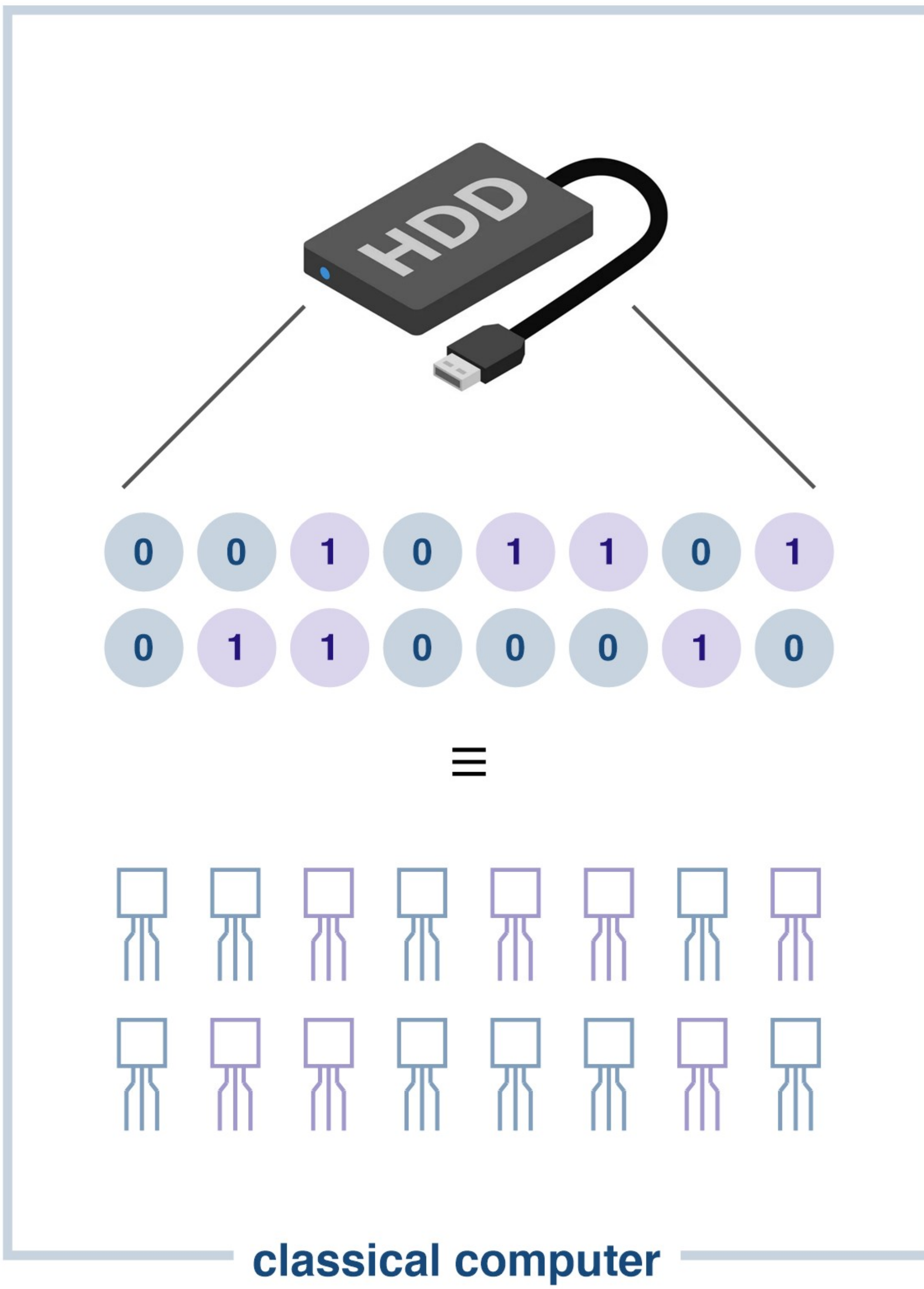

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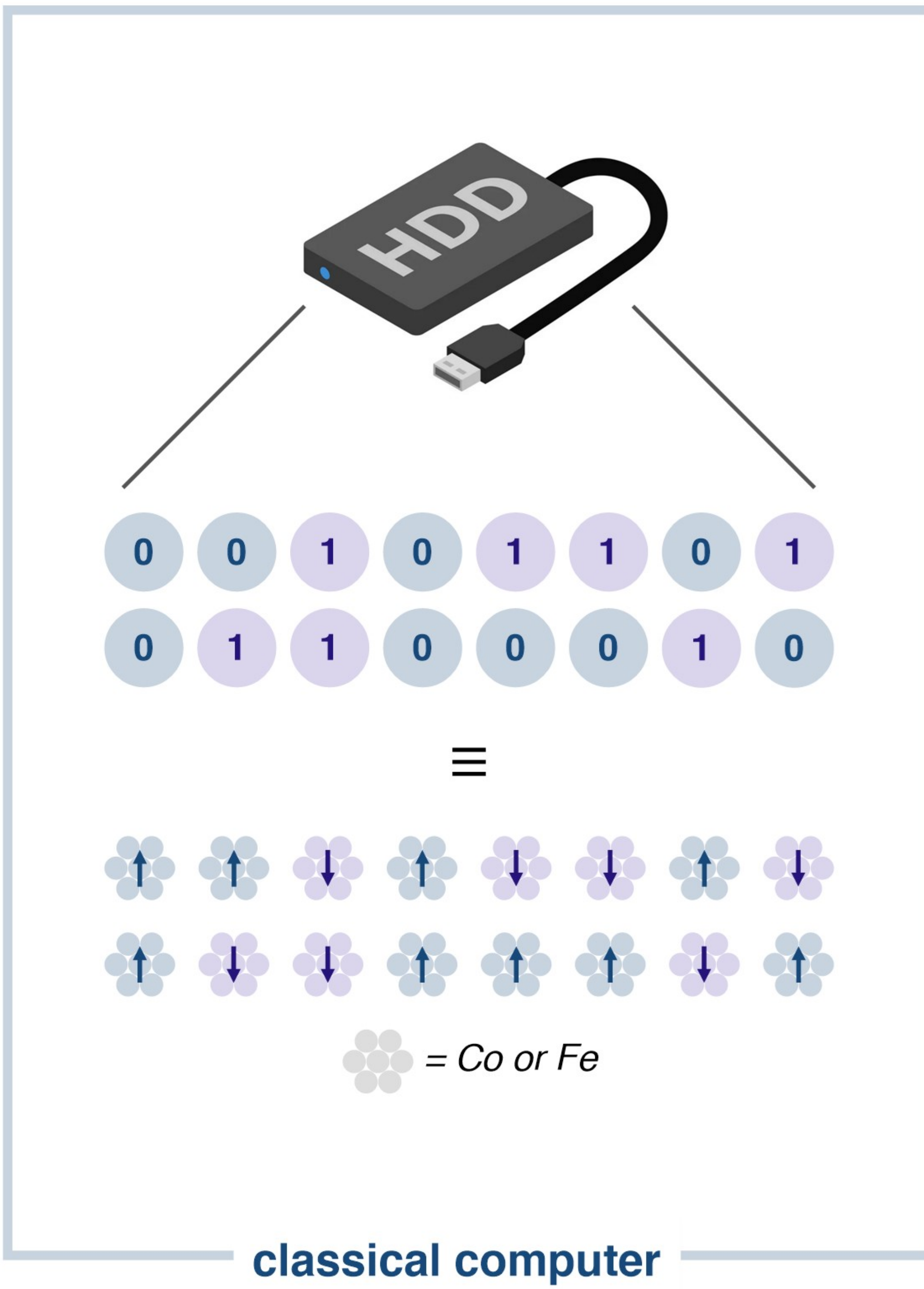
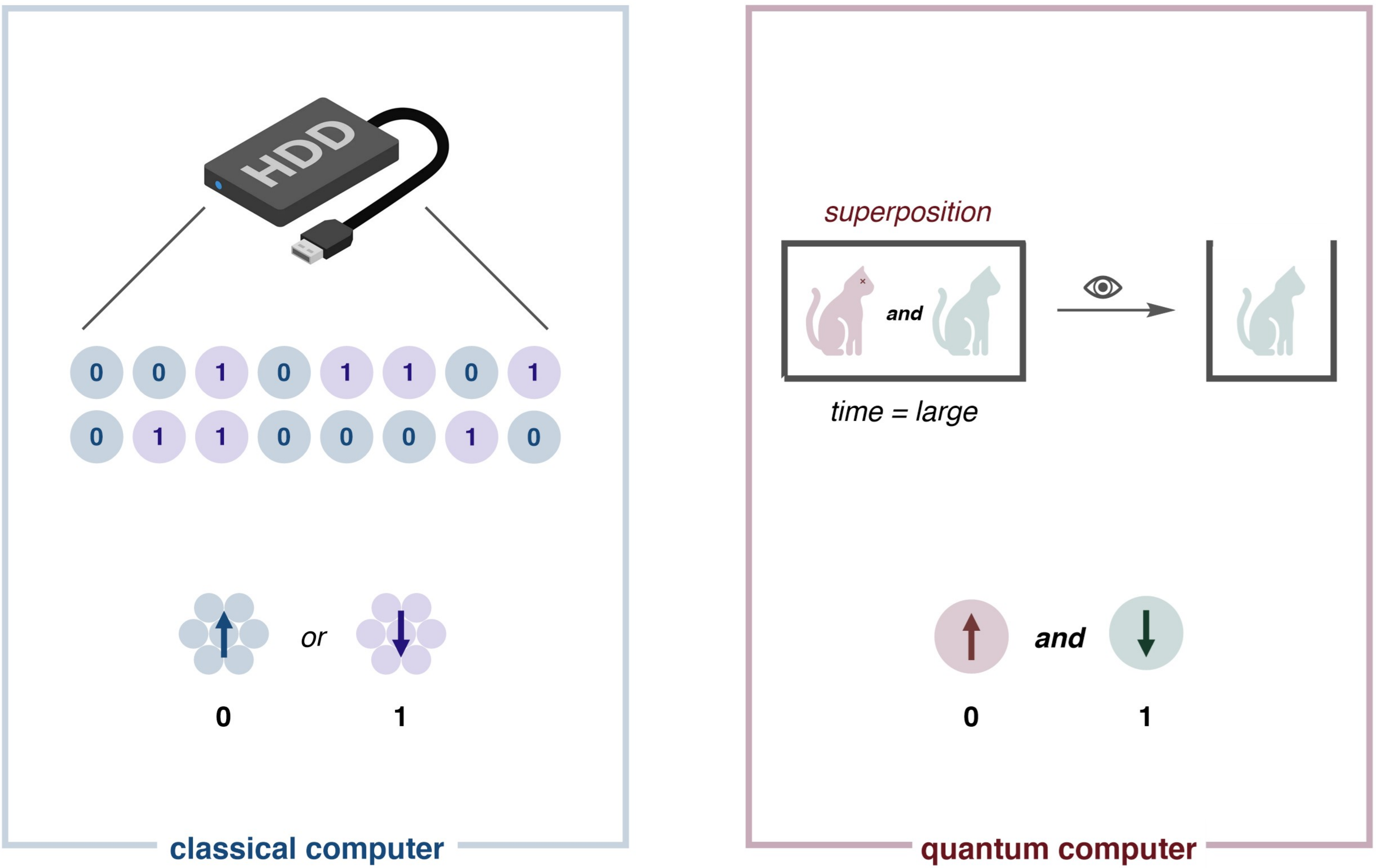


Qubits: a next-generation information storage technology



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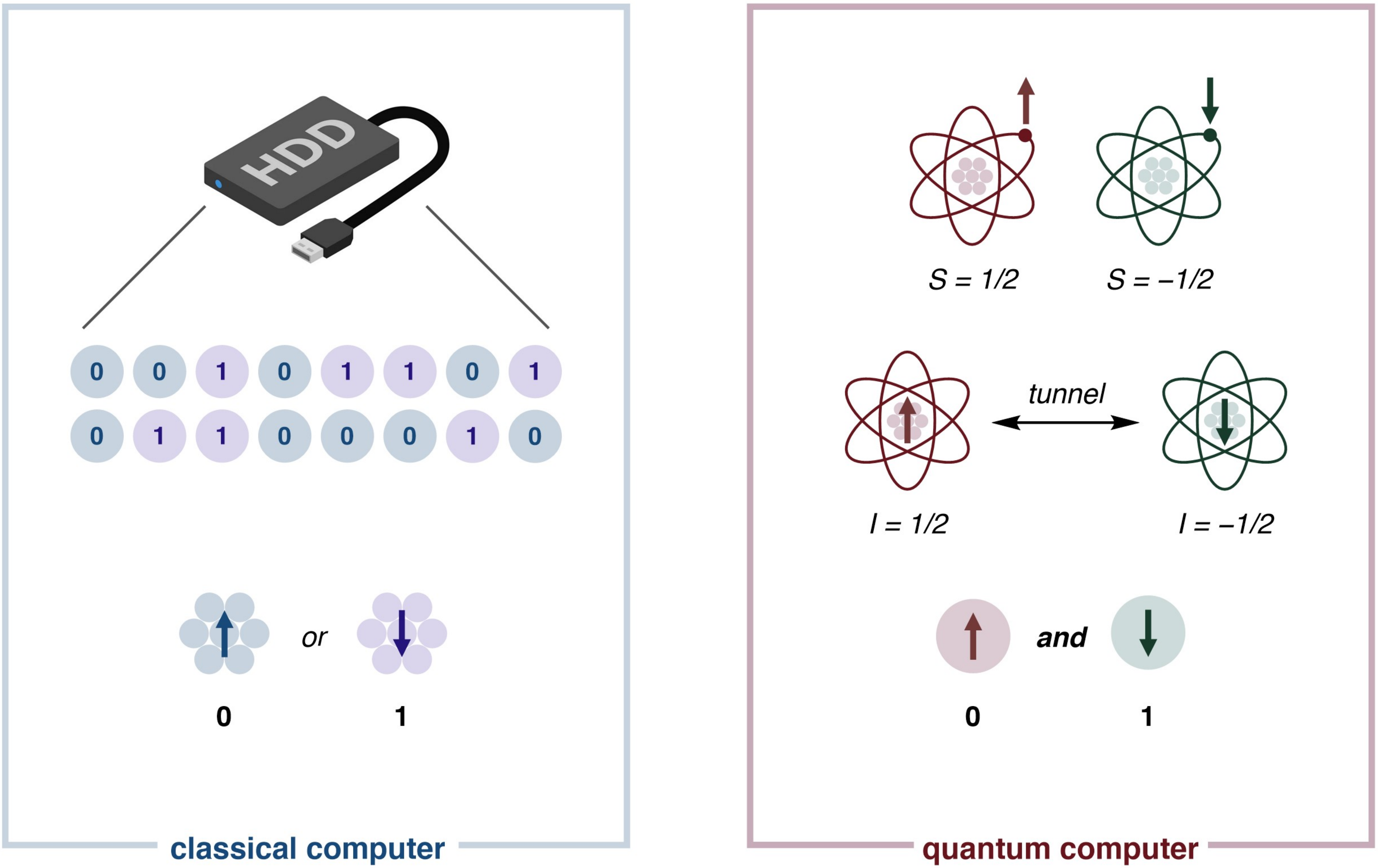

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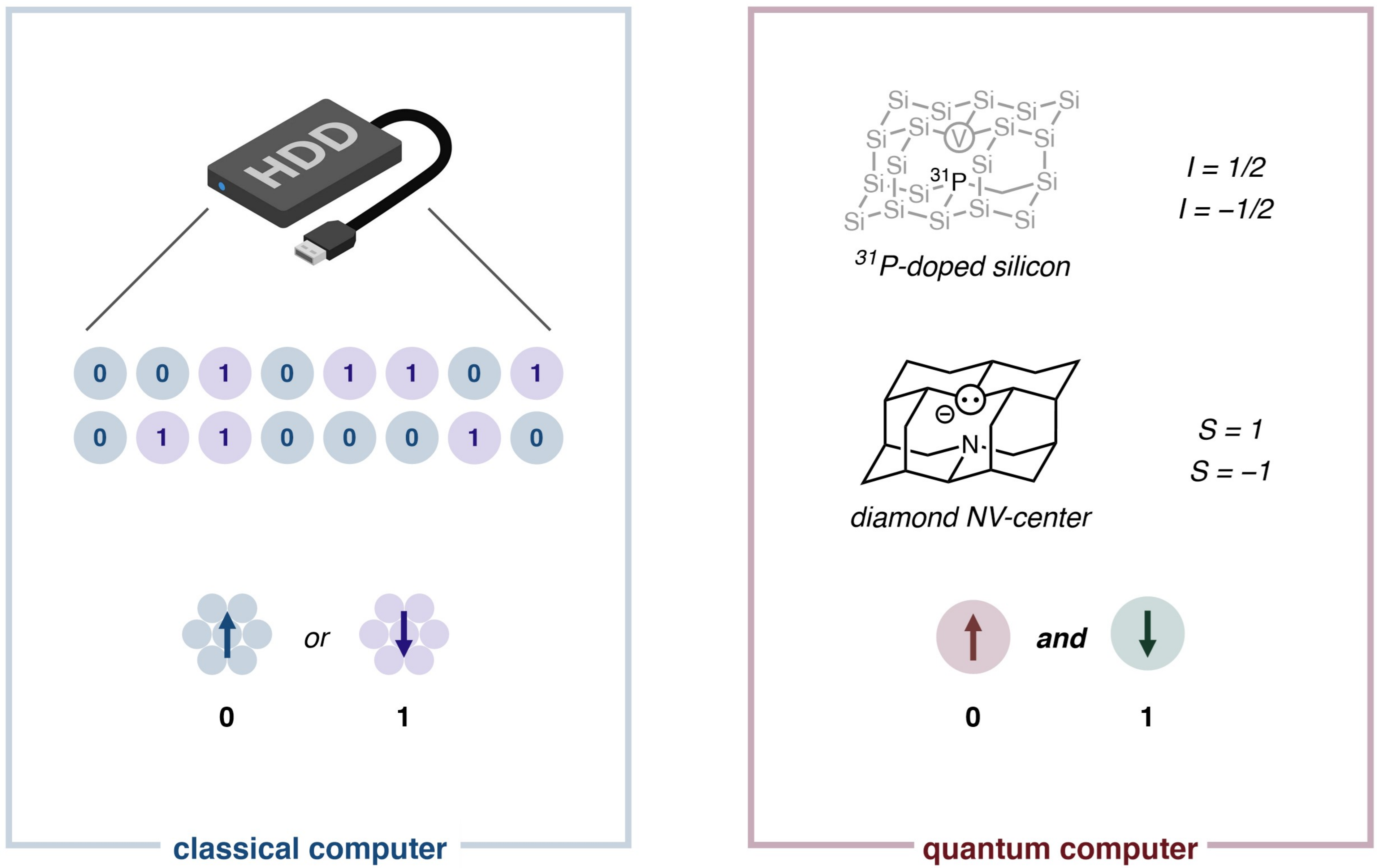

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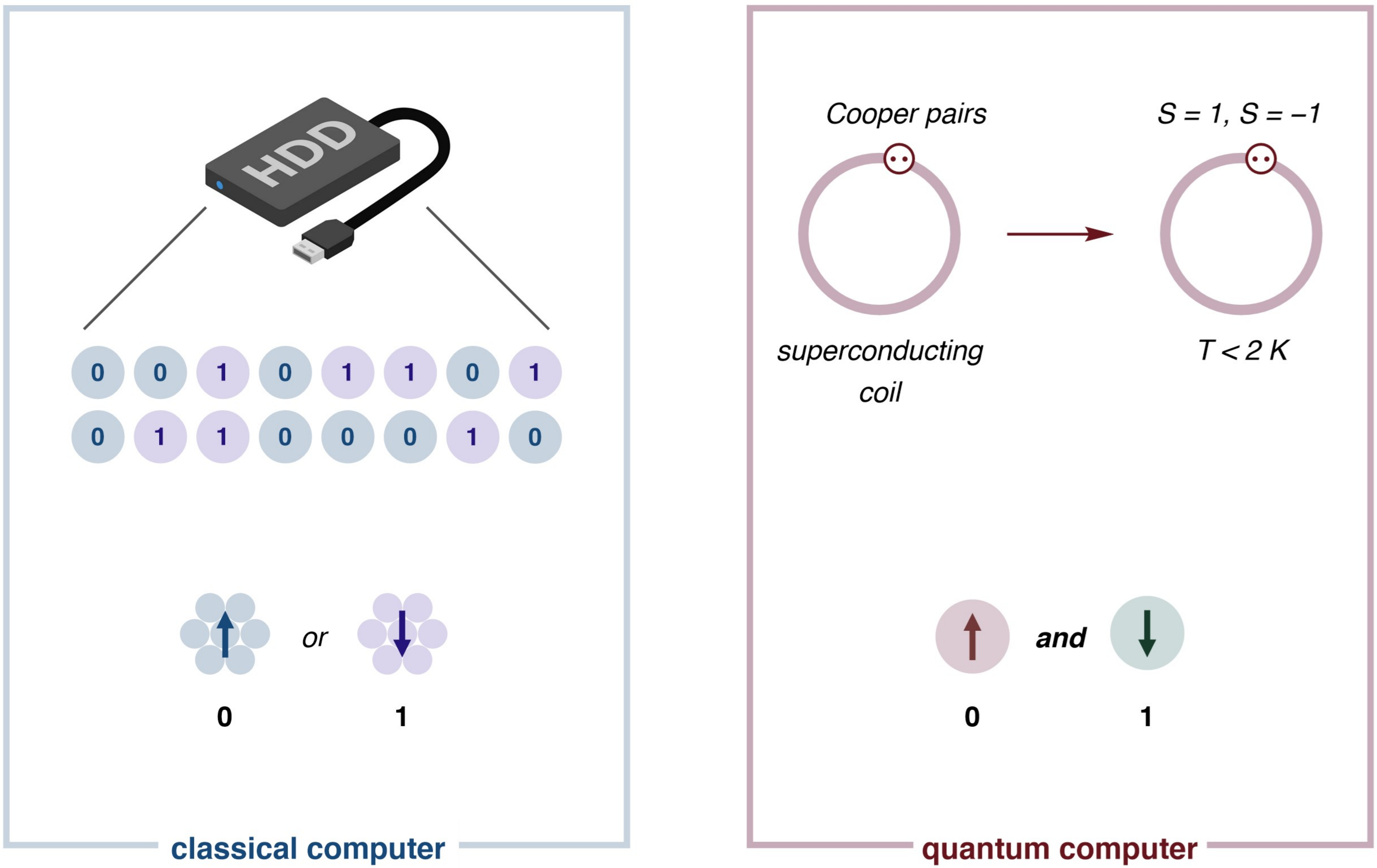

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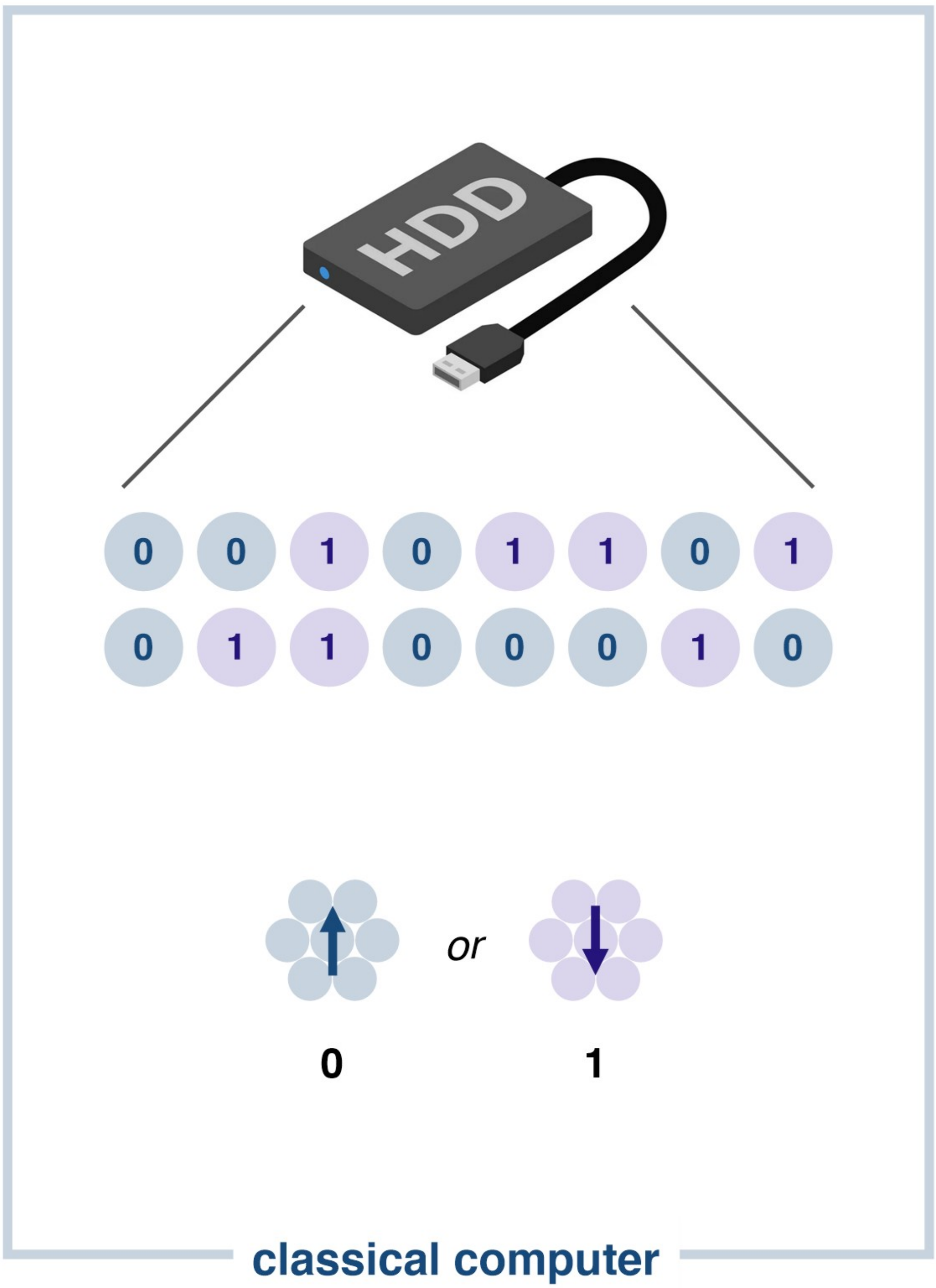
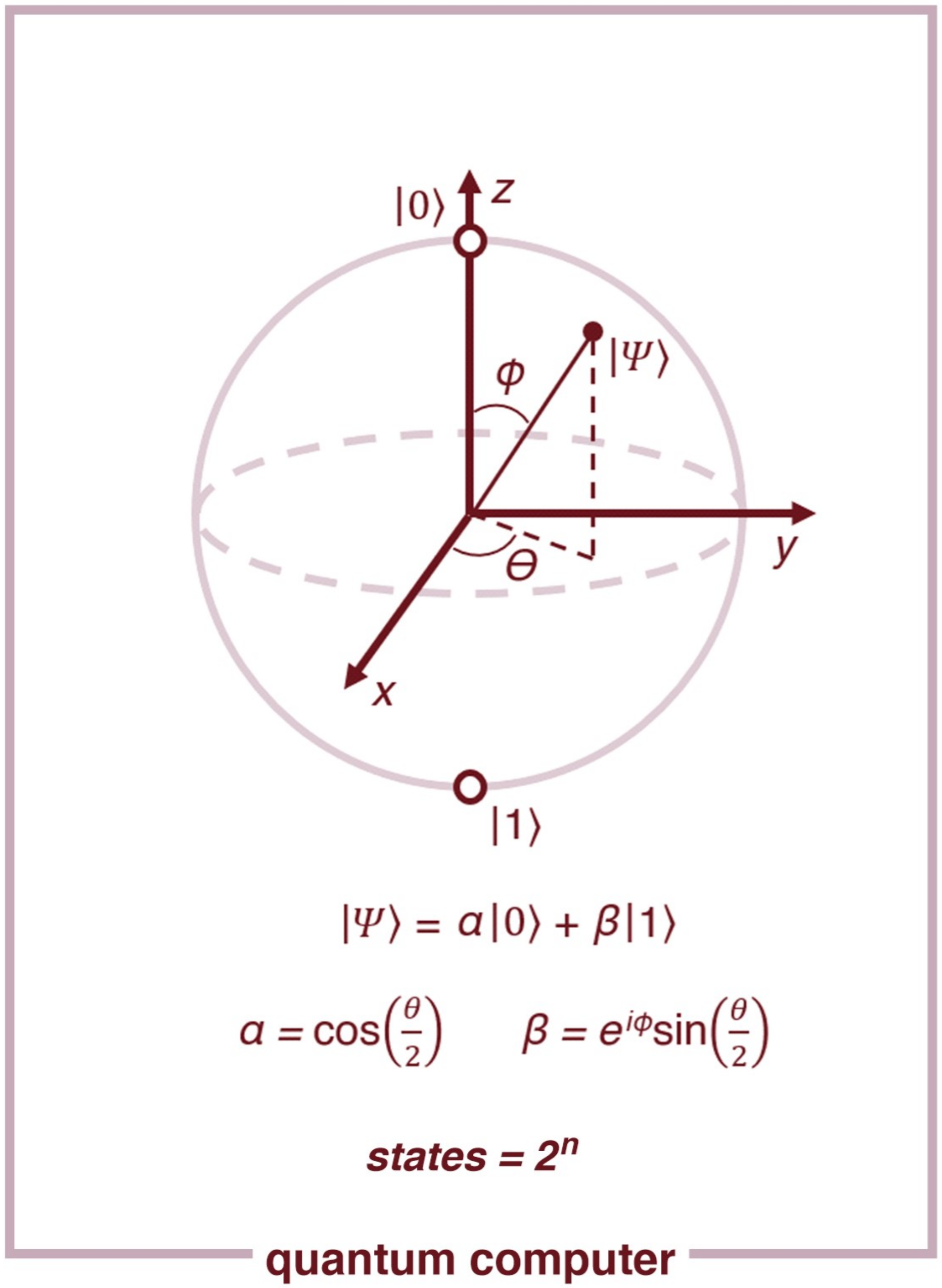
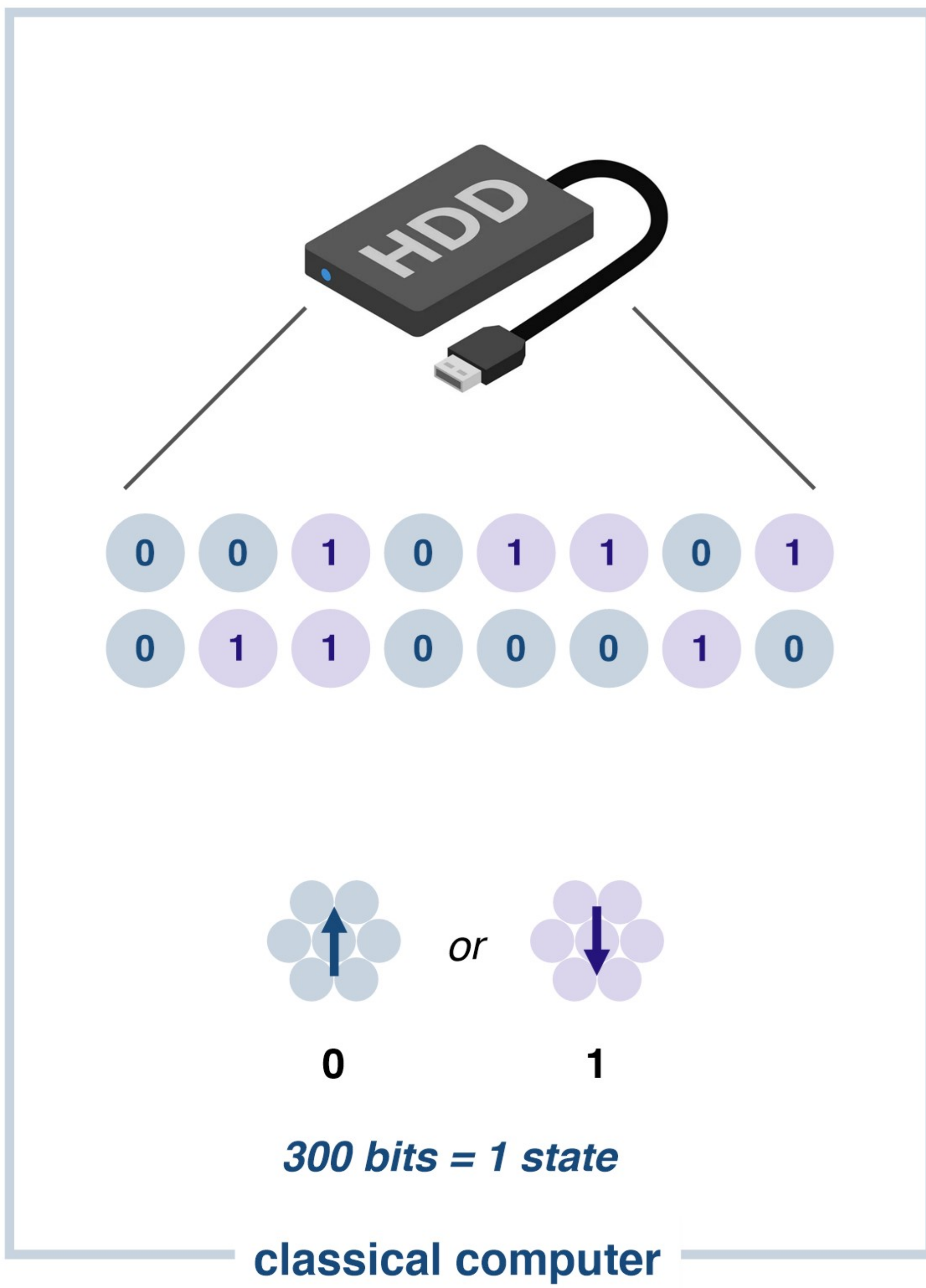
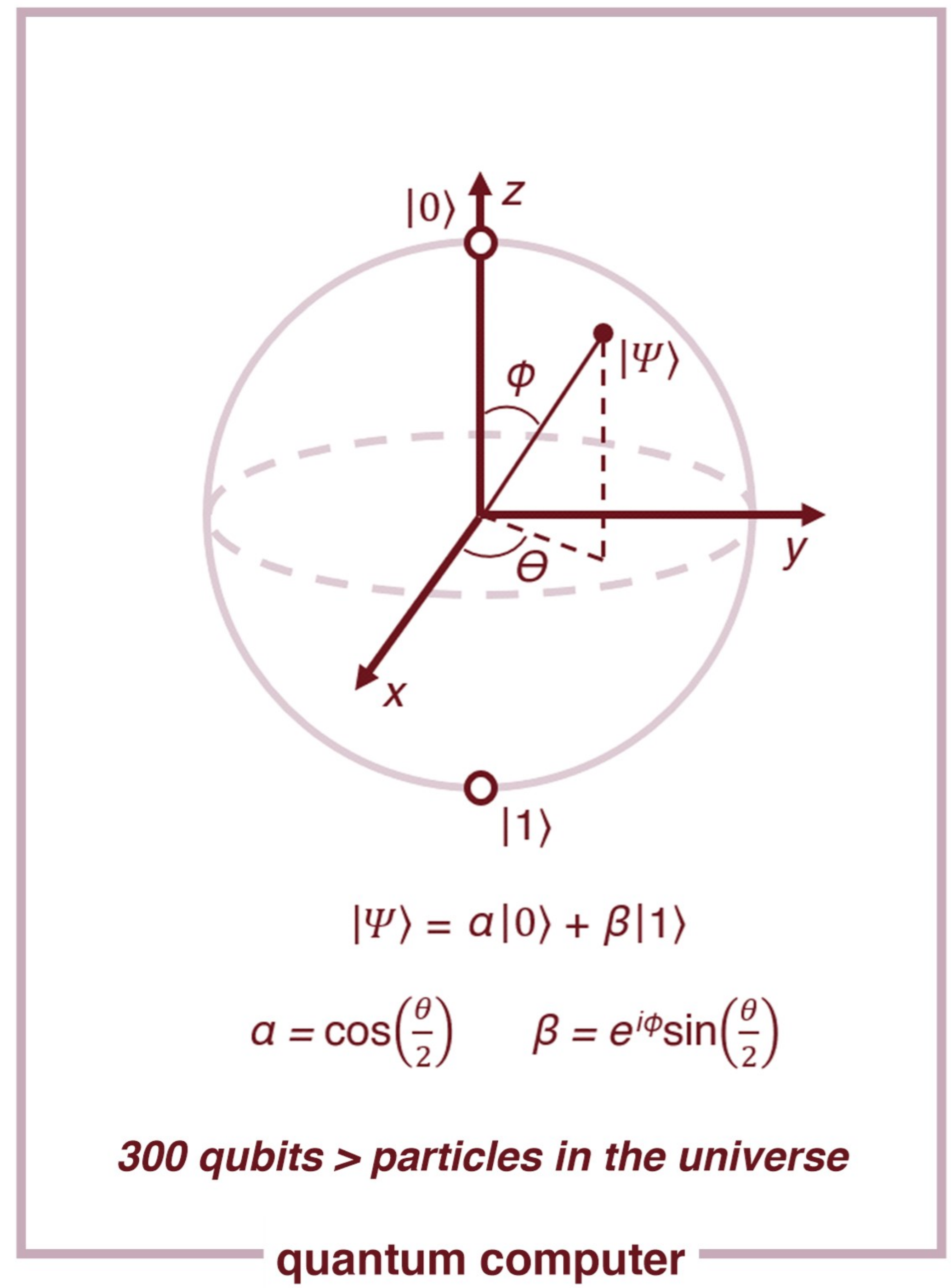




Qubits: a next-generation information storage technology





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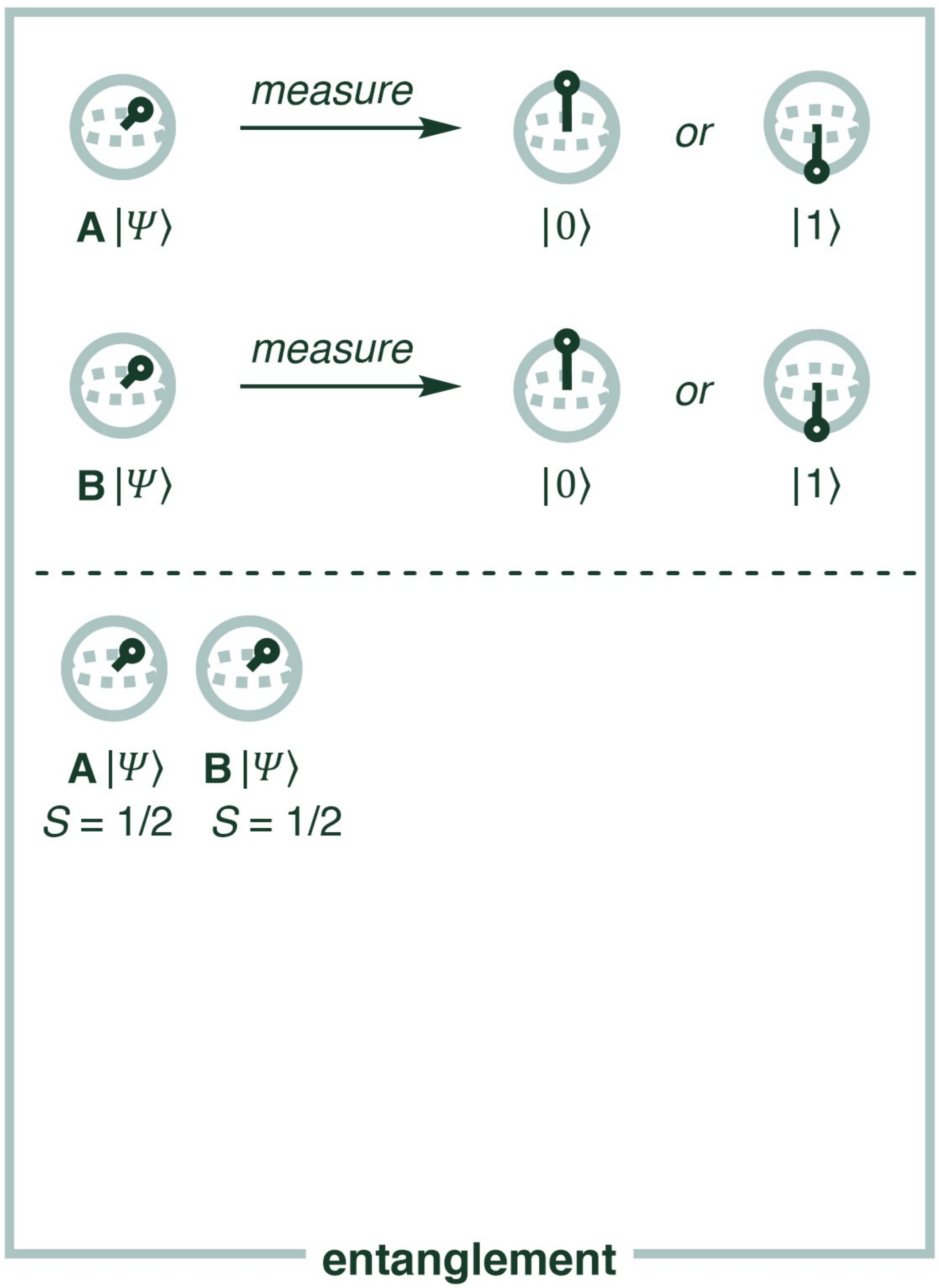

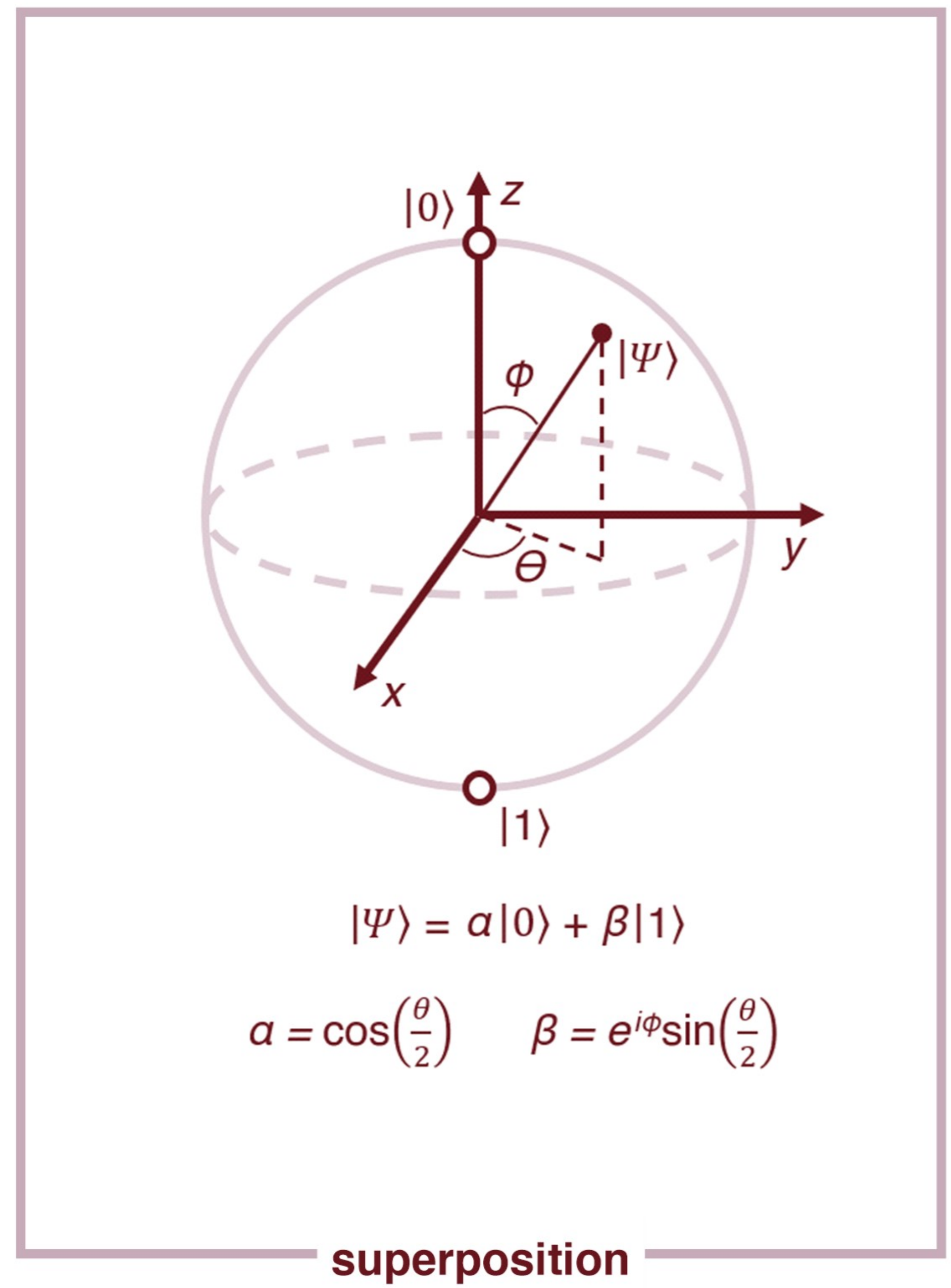

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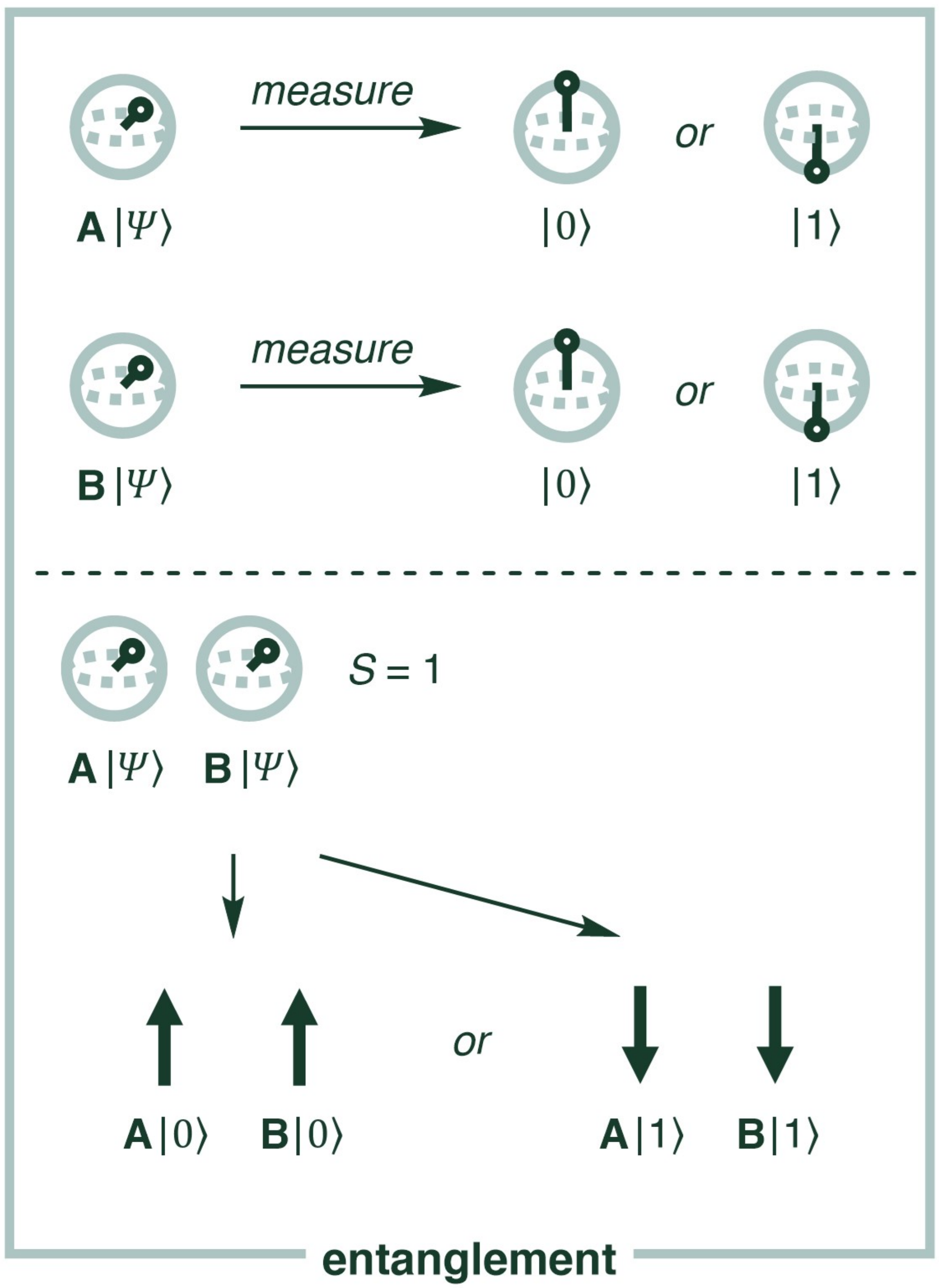
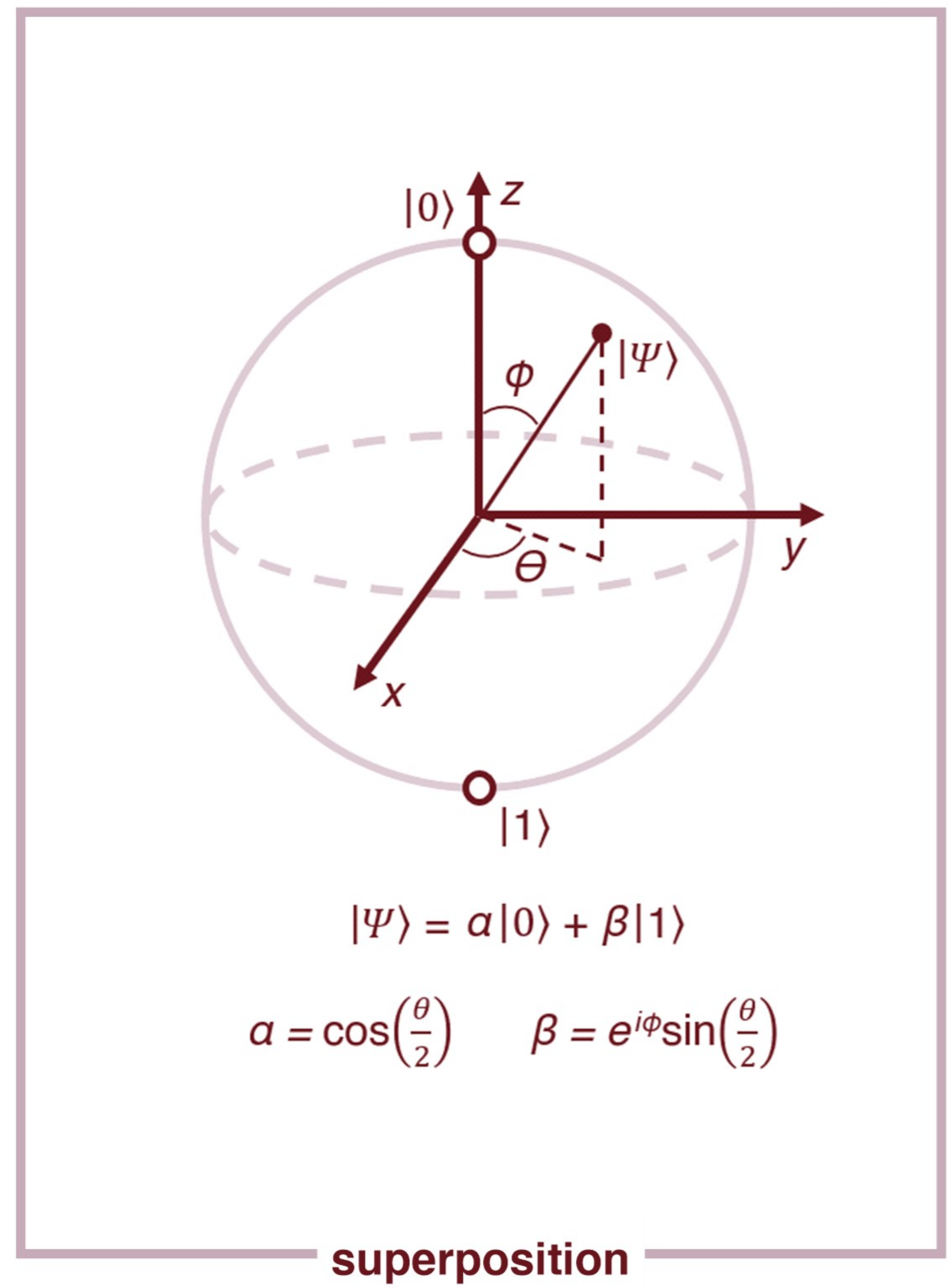
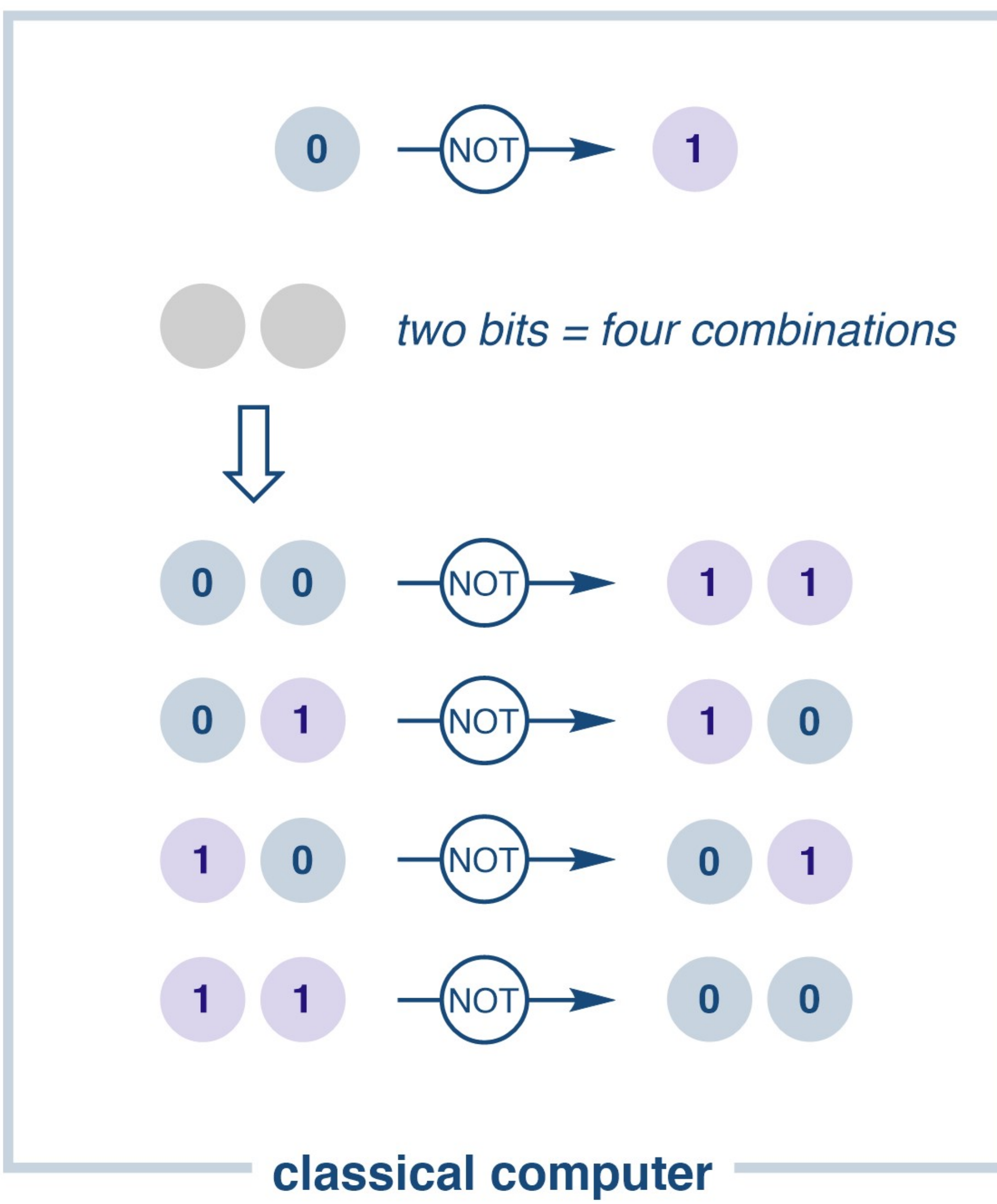
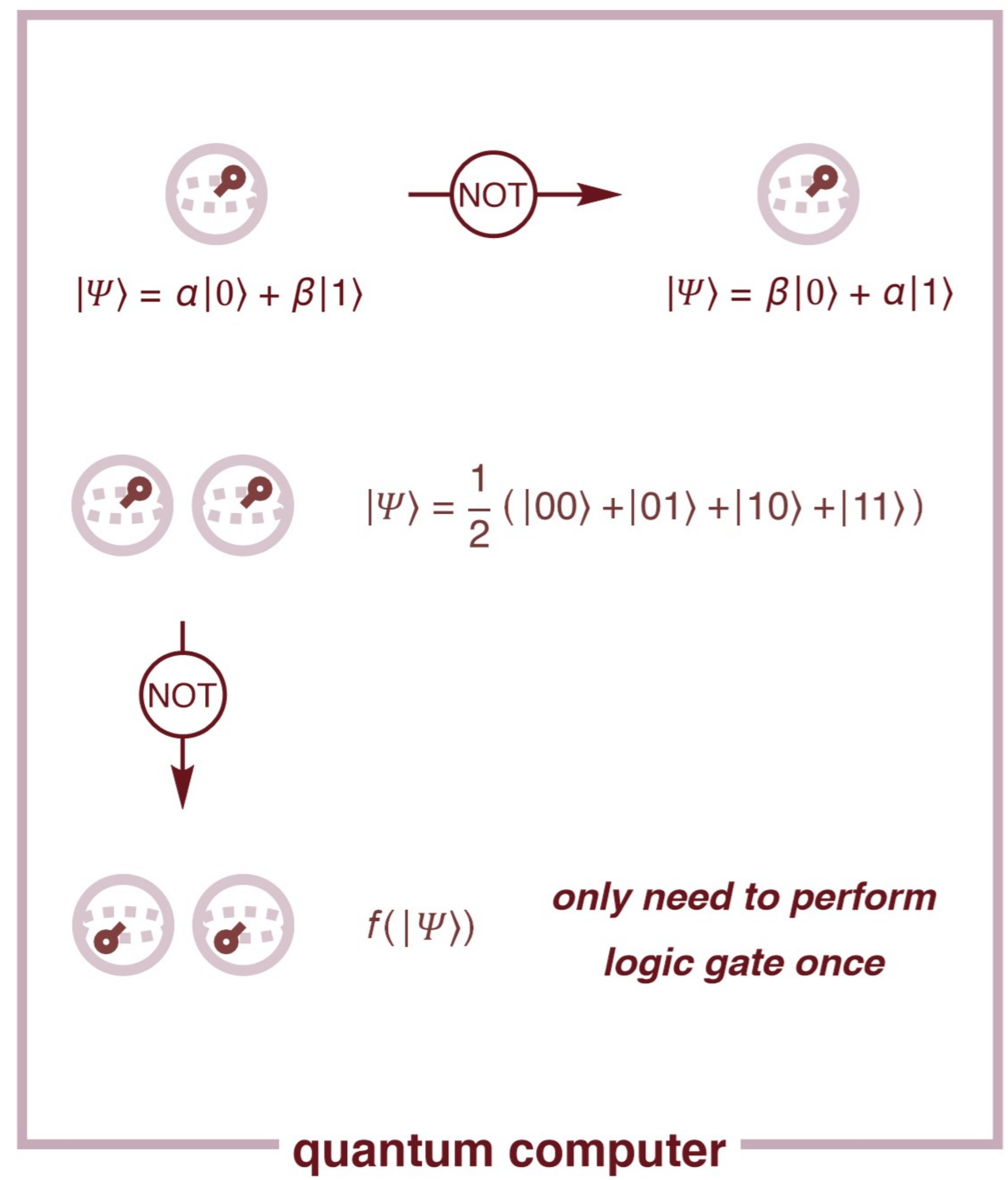




Faster processing speeds via quantum parallelism

Computers solve problems by operating on bits or qubits with logic gates





Applications of quantum computing

chemical dynamics

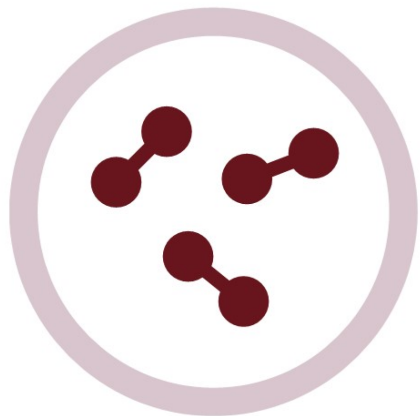
codebreaking

protein folding

artificial intelligence

Combinatorial optimization: a type of problem that deals with finding an optimal object from a finite set of objects

Applications of quantum computing



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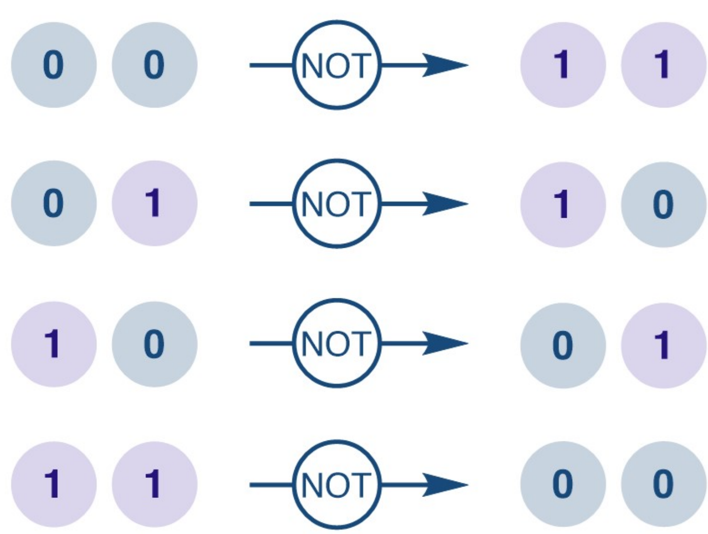
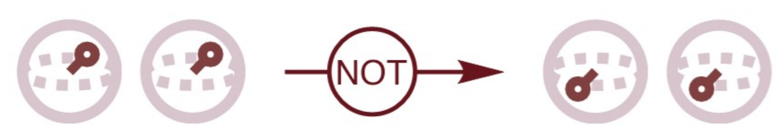
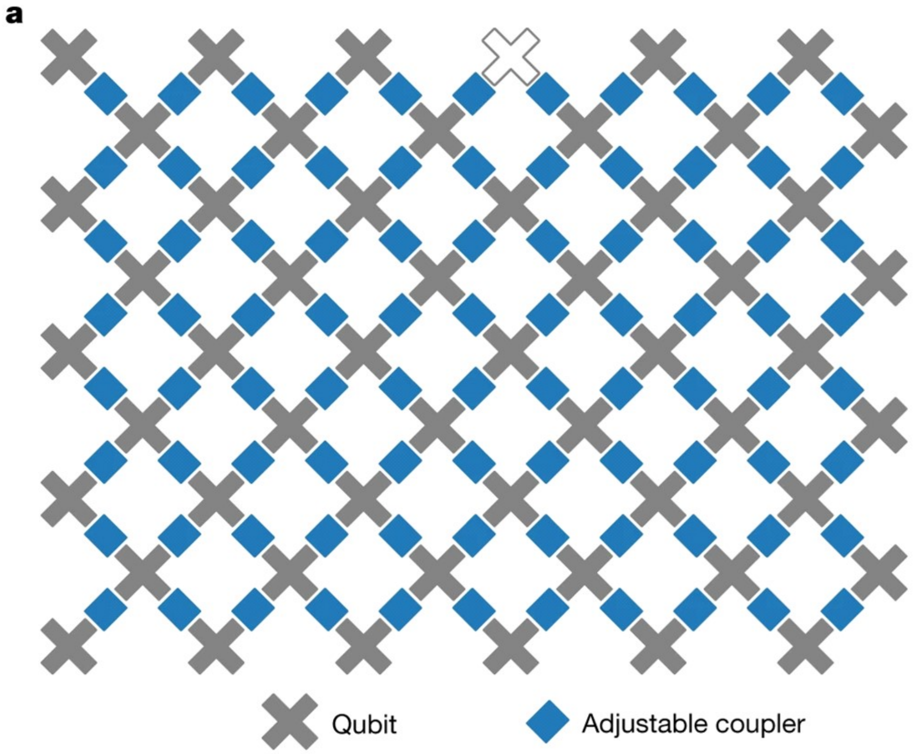


classic

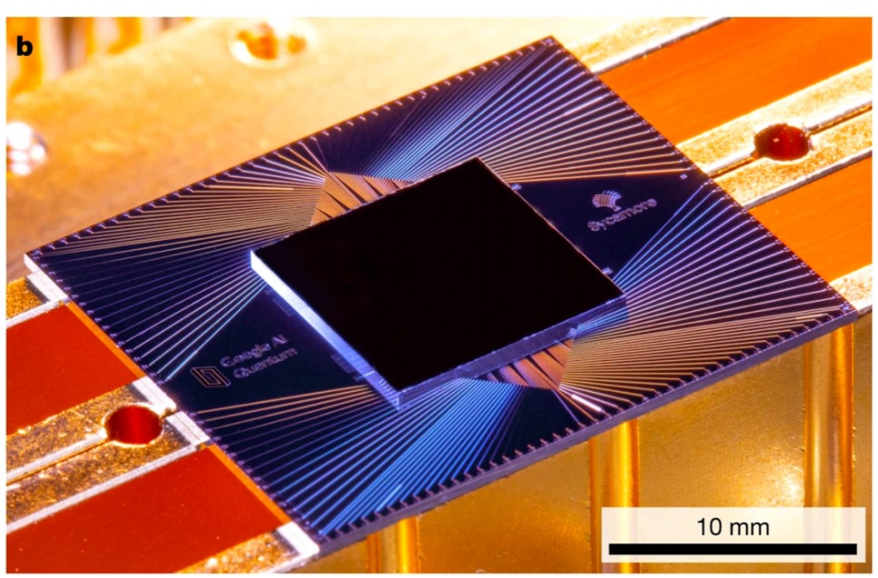


quantum

Google achieves "quantum supremacy"

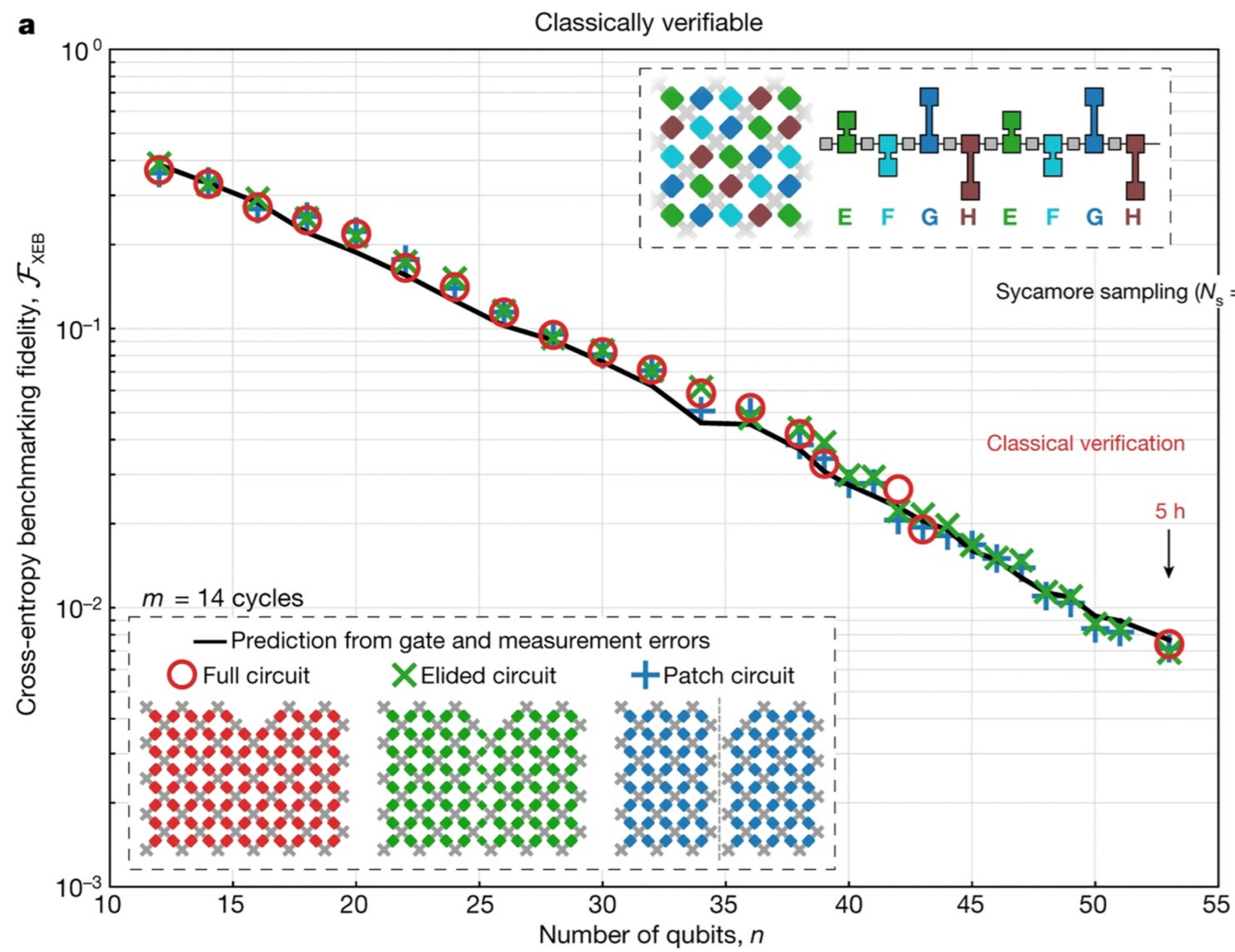


Sycamore quantum computer



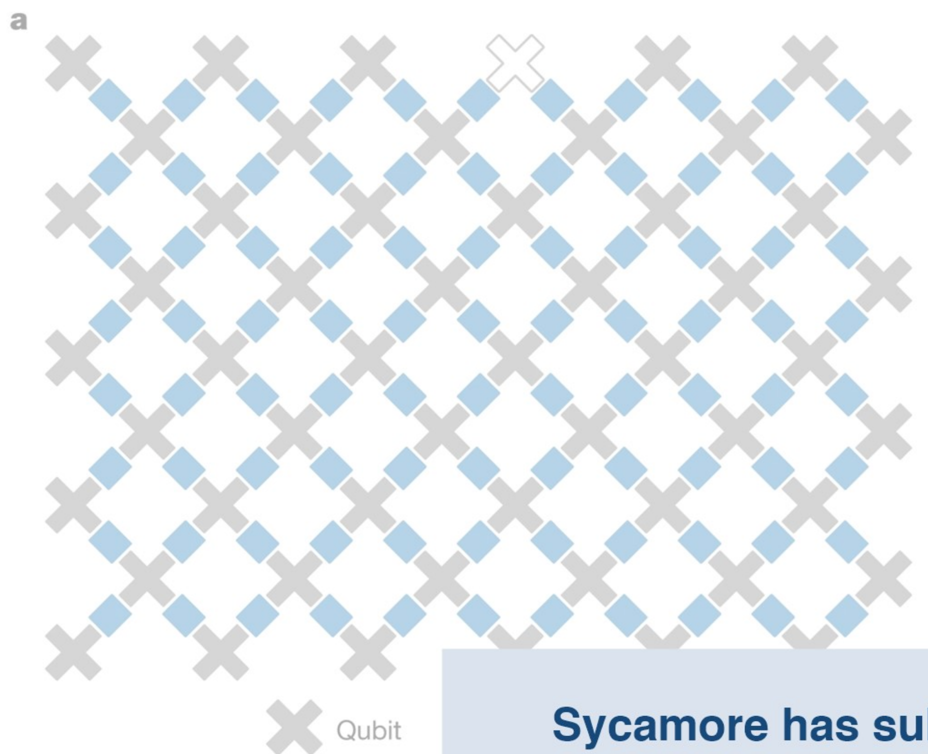
random quantum circuit → (*200 s*) *random bit string*

classical computer = 10,000 years



Martini, J. M. *et. al. Nature* **2019**, *574*, 505

Google achieves "quantum supremacy"



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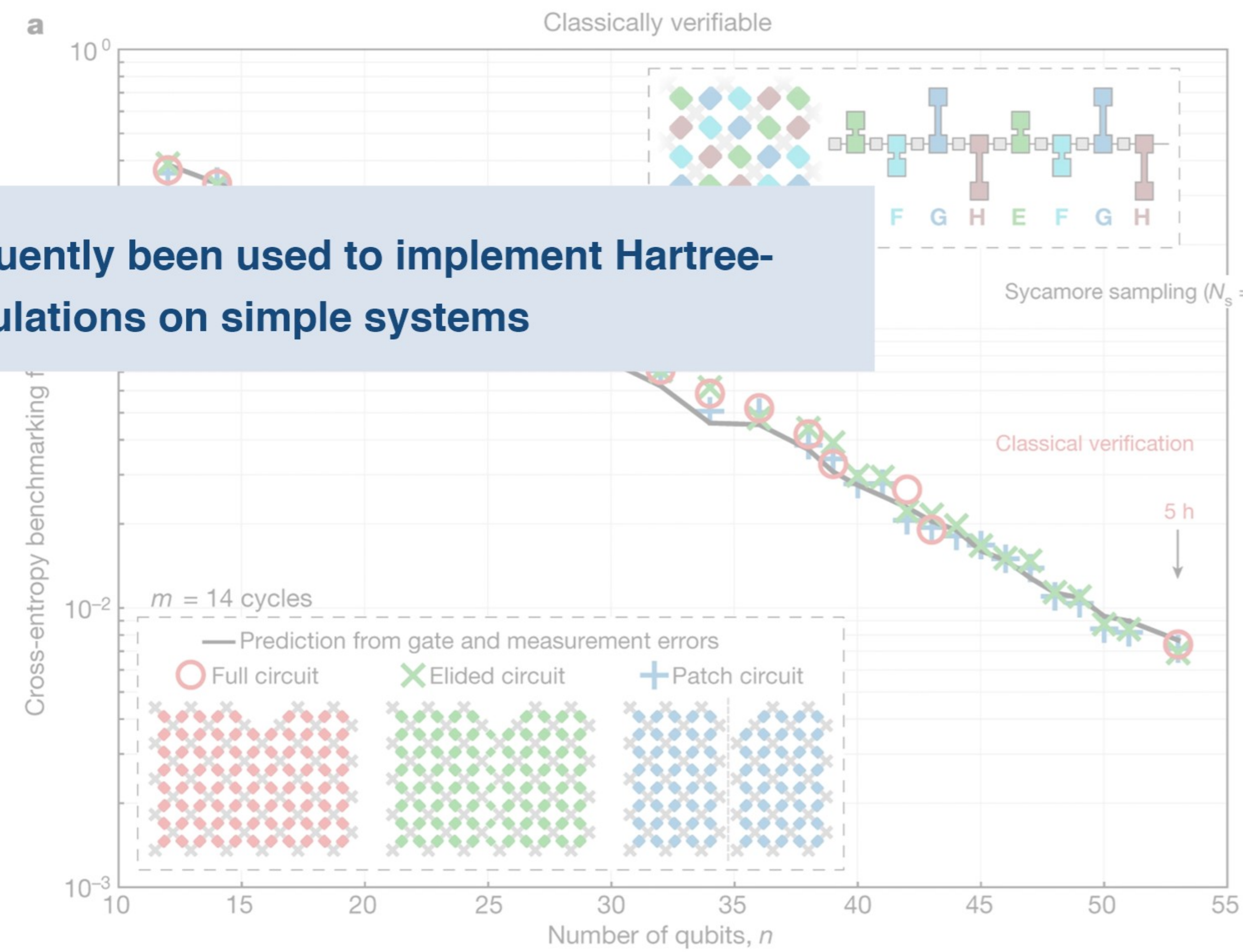
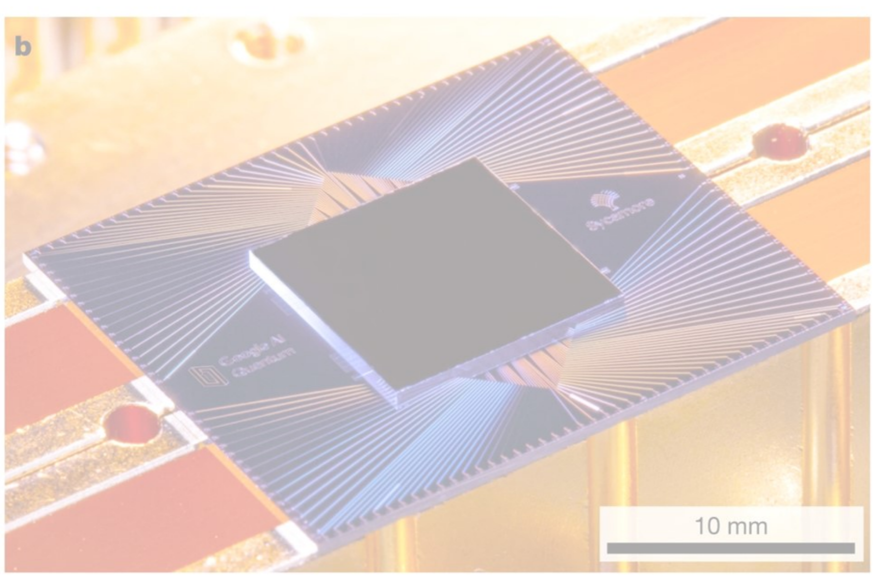


Sycamore has subsequently been used to implement Hartree-Fock calculations on simple systems

Sycamore quantum computer



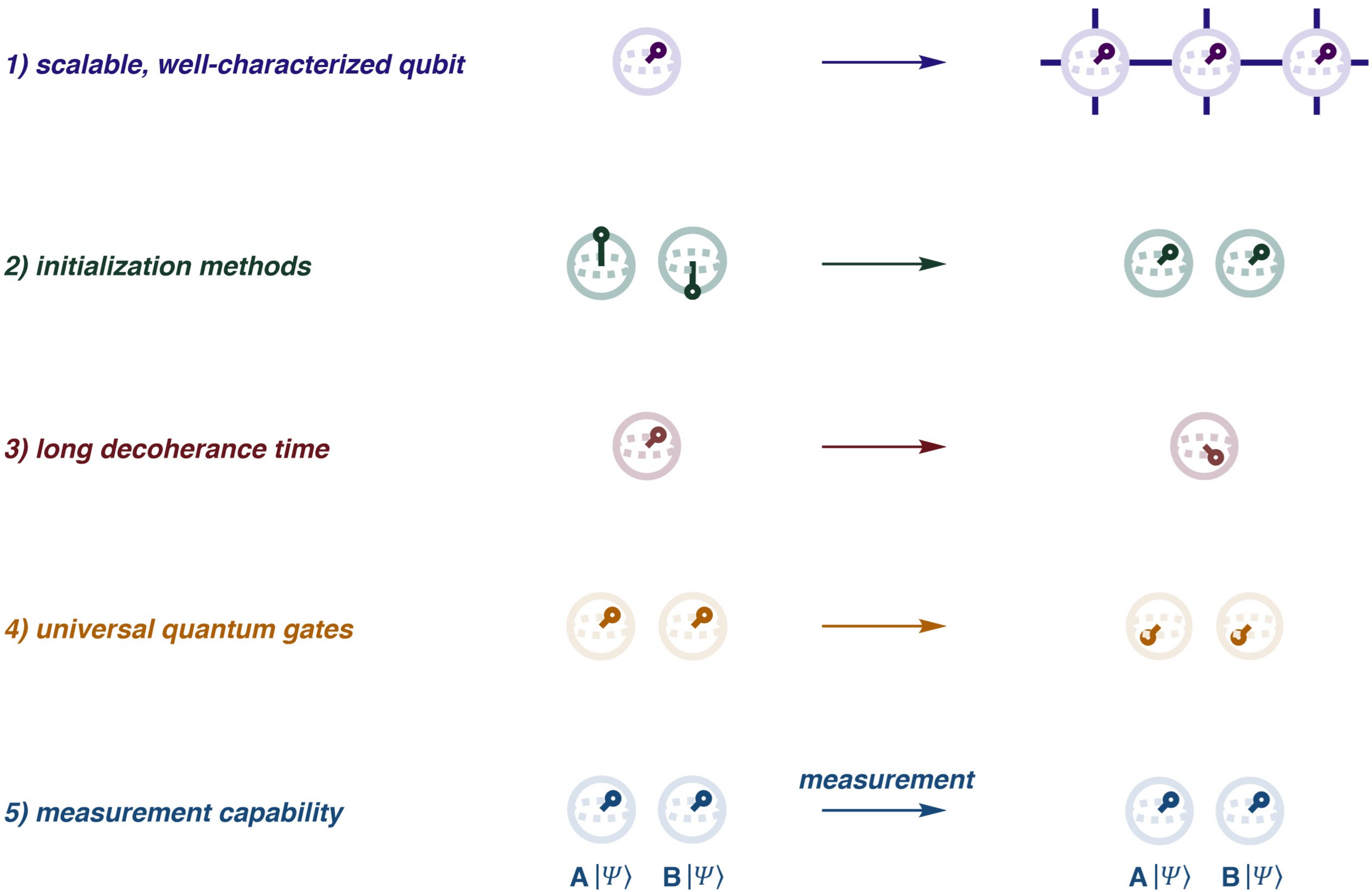
Martini, J. M. *et. al. Nature* **2019**, *574*, 505

Goals for this literature review

1) general introduction to quantum computing and qubits

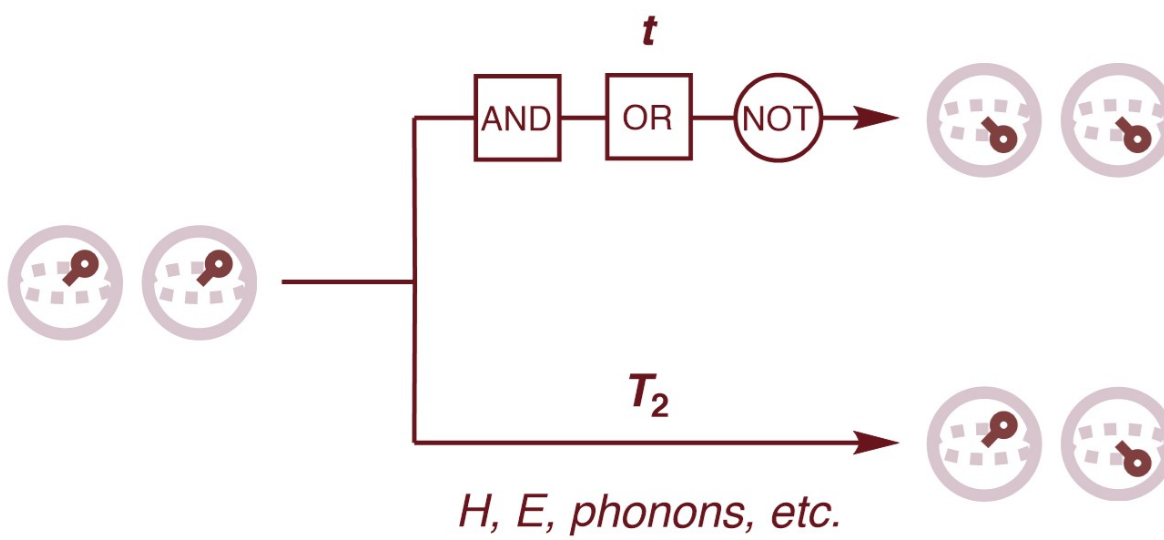
2) highlight potential opportunities for chemists

Necessary conditions for constructing a quantum computer

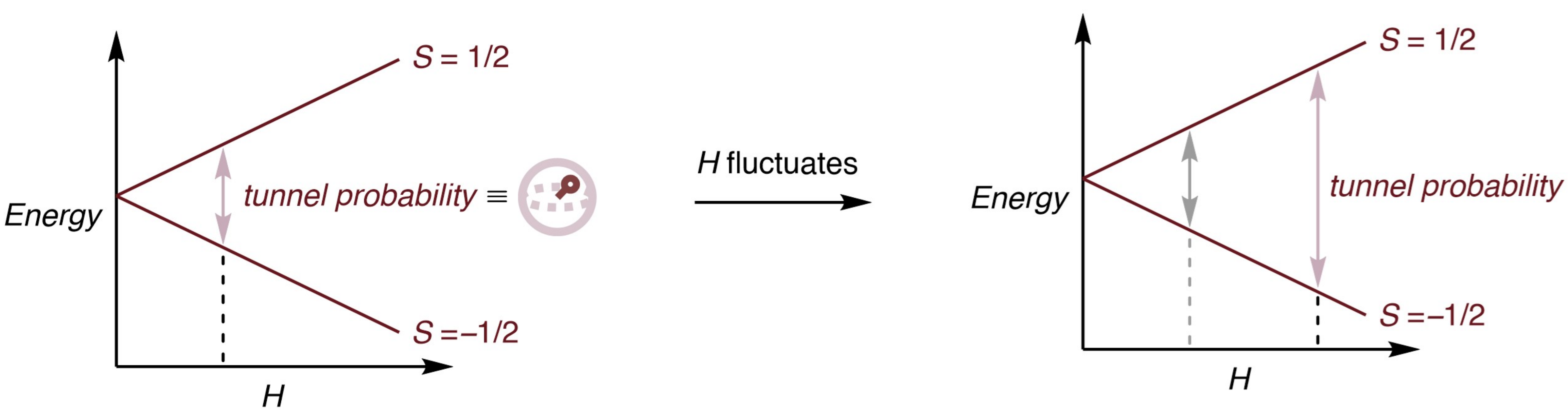


Achieving long decoherance times in molecular qubits

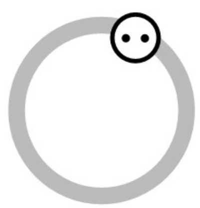
3) long decoherance time



required: $t > T_2$



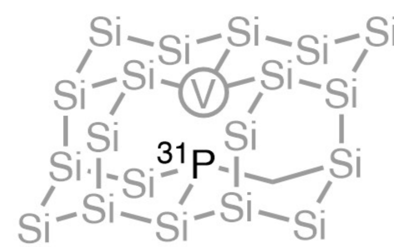
Achieving long decoherance times in molecular qubits



superconducting coil

T_2 ≤ 50 ms at 50 mK

liquid helium



^{31}P-doped silicon

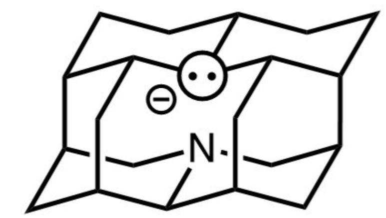
T_2 ~ 10 ms at 8 K

silicon isotopes:

^{28}Si (92%), I = 0

^{29}Si (5%), I = 1/2

semi-rigid lattice



diamond NV-center

T_2 ~ 0.5 s at 77 K

liquid nitrogen

carbon isotopes:

^{12}C (99%), I = 0

^{13}C (1%), I = 1/2

rigid lattice

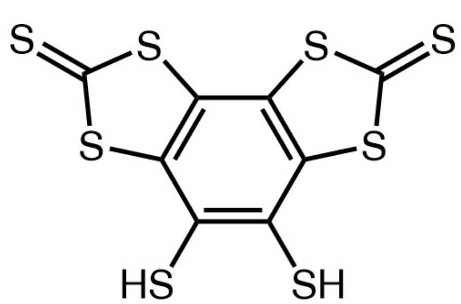
eliminate low E phonons

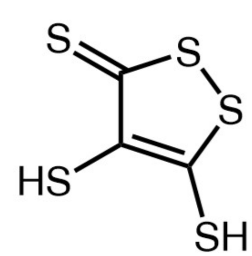
Can we use molecular design to achieve long T_2?

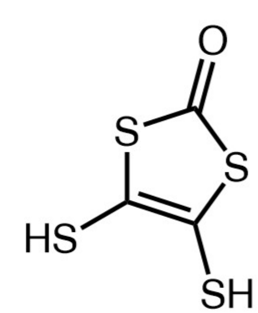
Achieving long decoherance times in molecular qubits

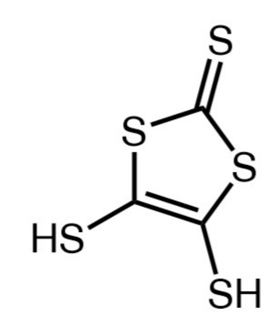
H ^{1}H (99%) S = 1/2				
	C ^{12}C (99%) S = 0	**N** ^{14}N (99%) S = 1	**O** ^{16}O (99%) S = 0	**F** ^{19}F (100%) S = 1/2
	Si ^{28}Si (92%) S = 0	**P** ^{31}P (100%) S = 1/2	**S** ^{32}S (95%) S = 0	**Cl** ^{35}Cl (76%) S = 3/2

Careful choice of elements in ligands could potentially eliminate nuclear spins



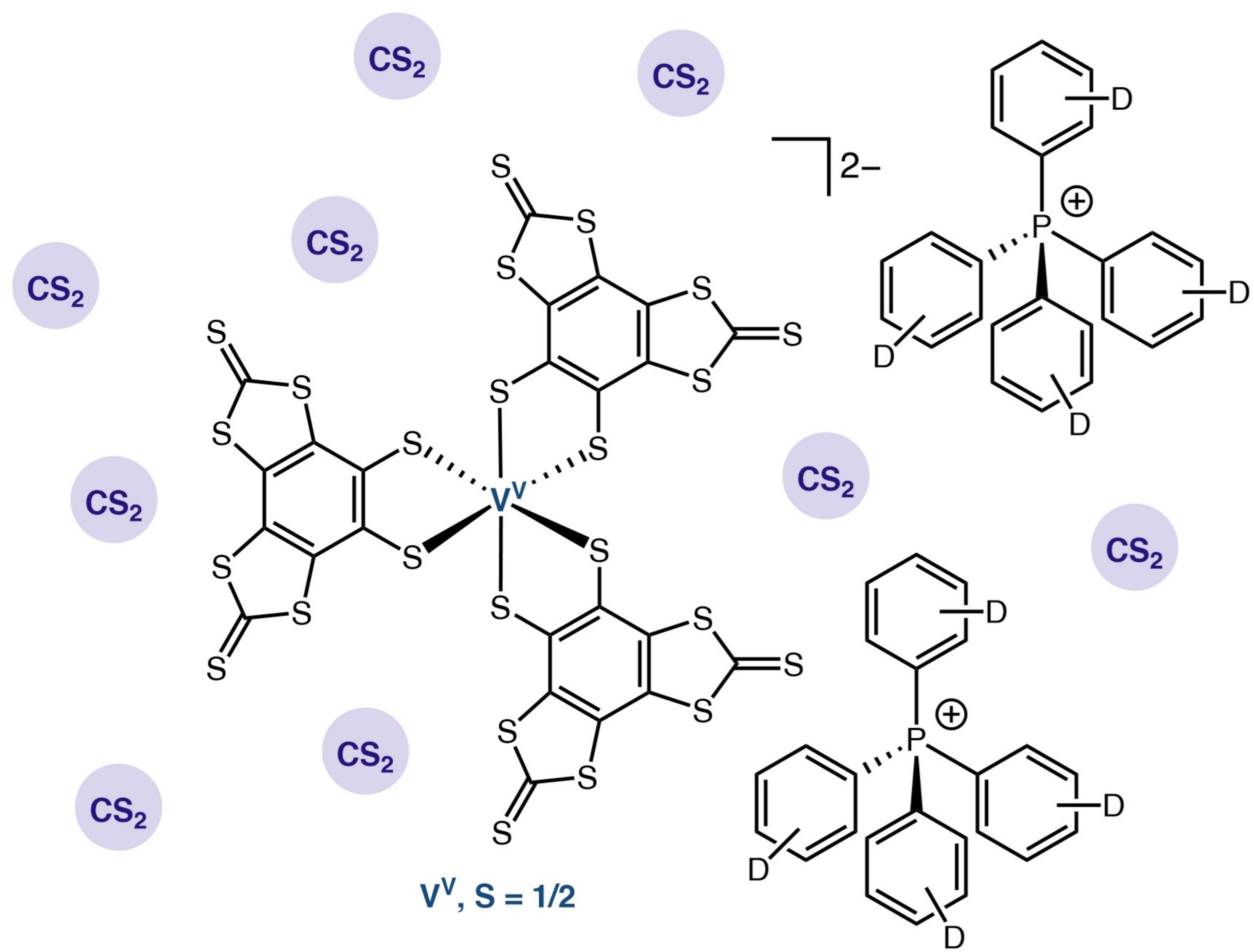






Yu, Graham, Zadrozny, Niklas, Krzyaniak, Wasielewski, Poluektov, Freedman, *J. Am. Chem. Soc.* **2016**, *138*, 14678

Achieving long decoherance times in molecular qubits



Zadrozny, Niklas, Poluektov, Freedman, *ACS Cent. Sci.* **2015**, *9*, 488

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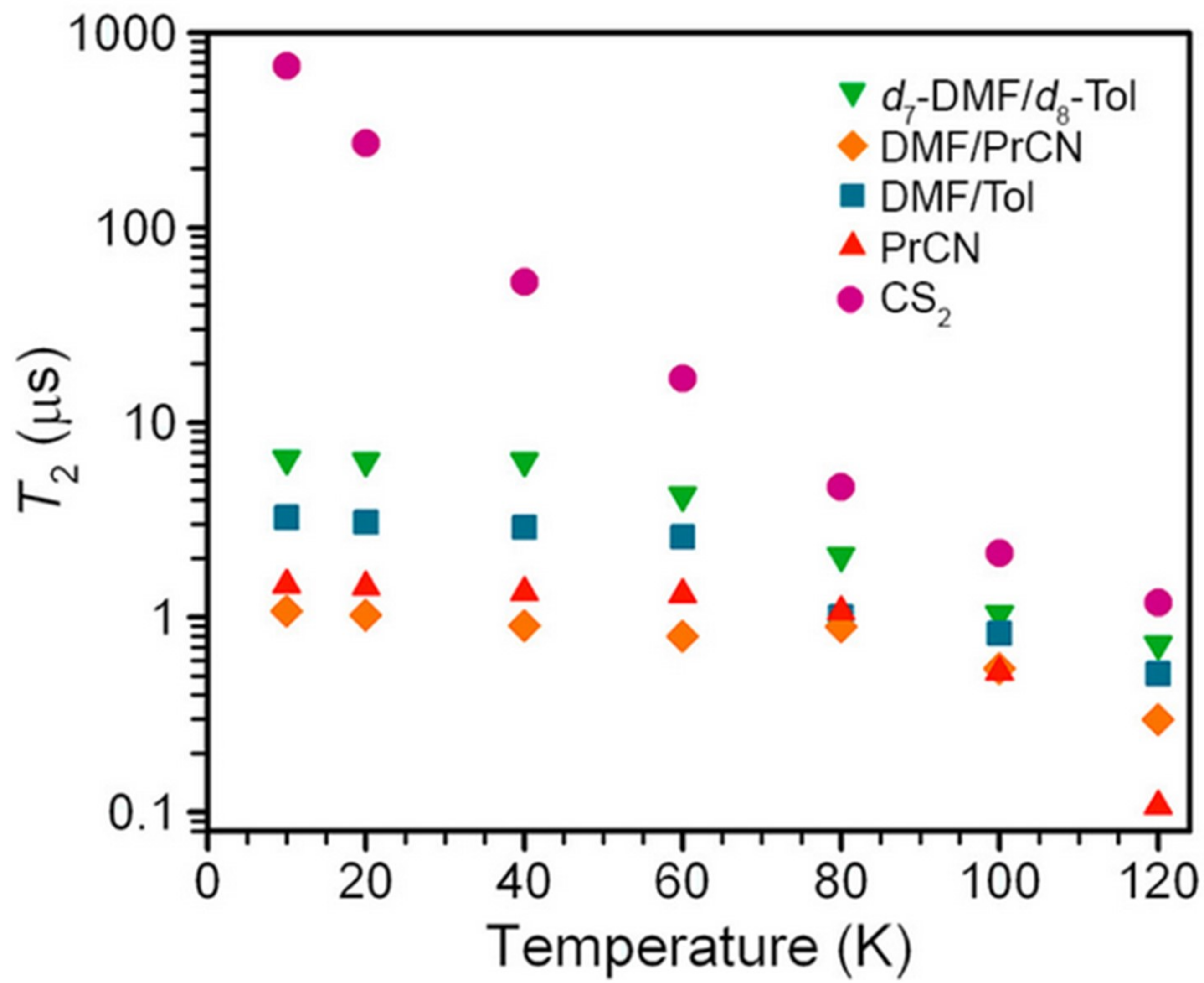

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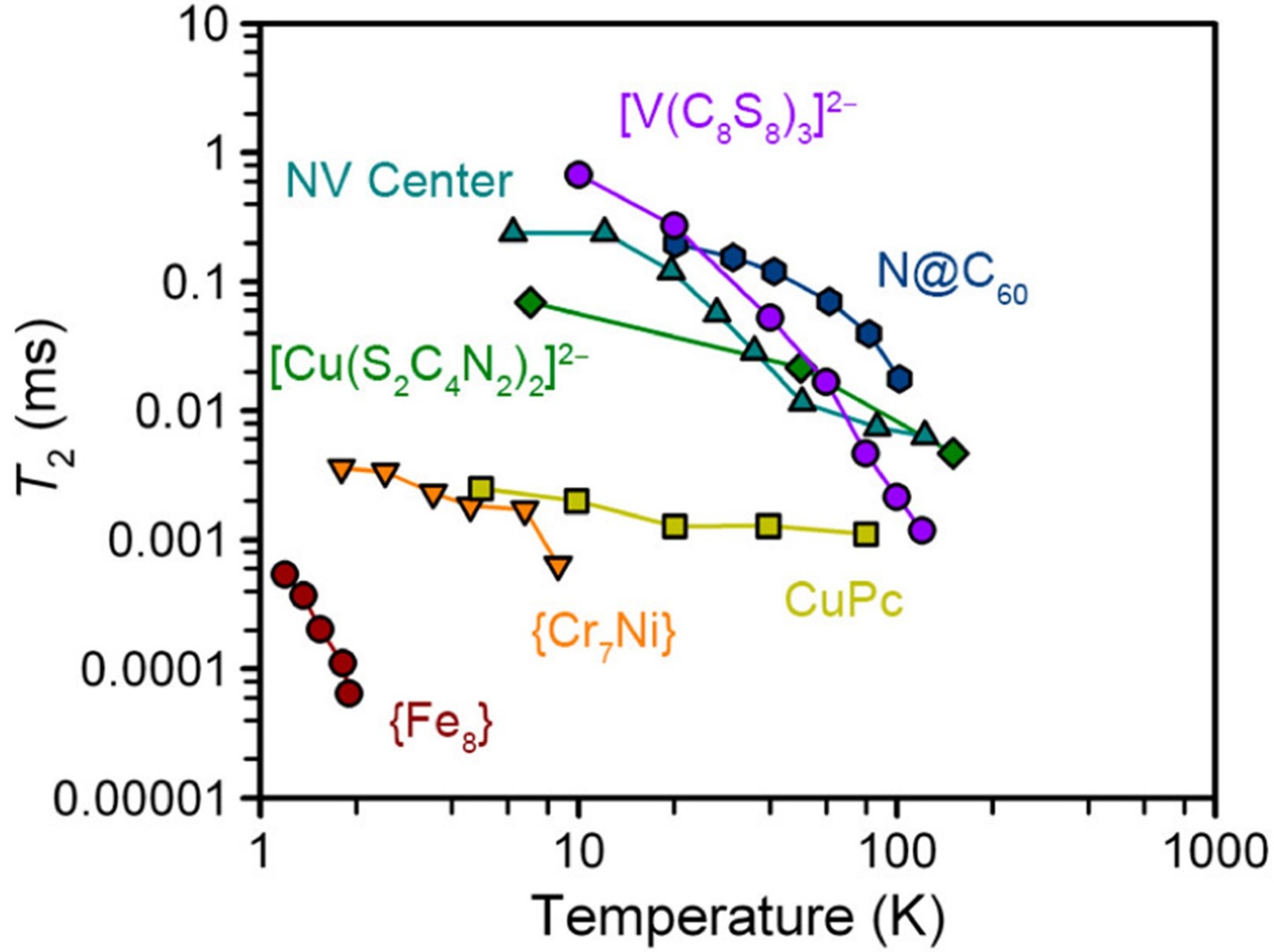
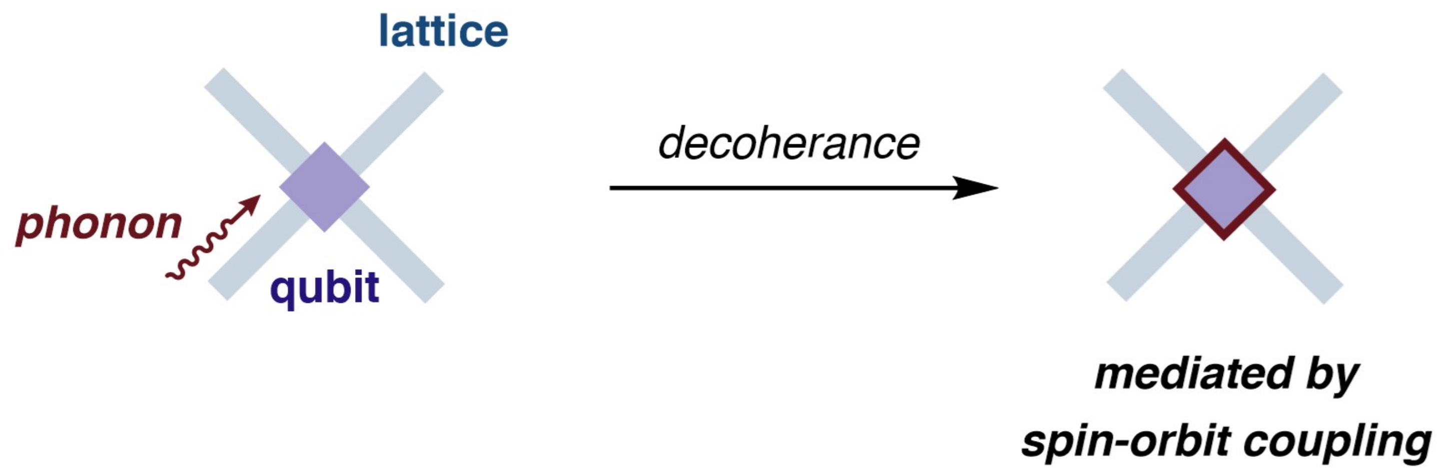
Achieving long decoherance times in molecular qubits

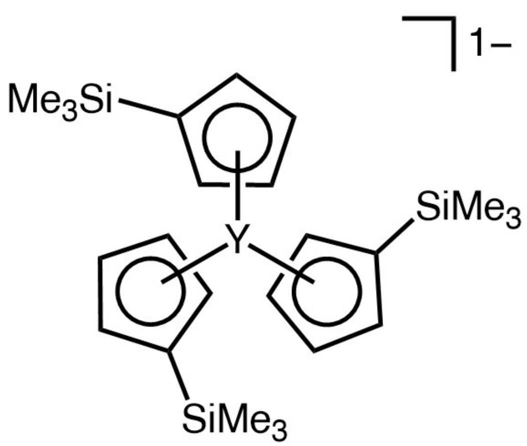


order of magnitude improvement over previous molecular qubits

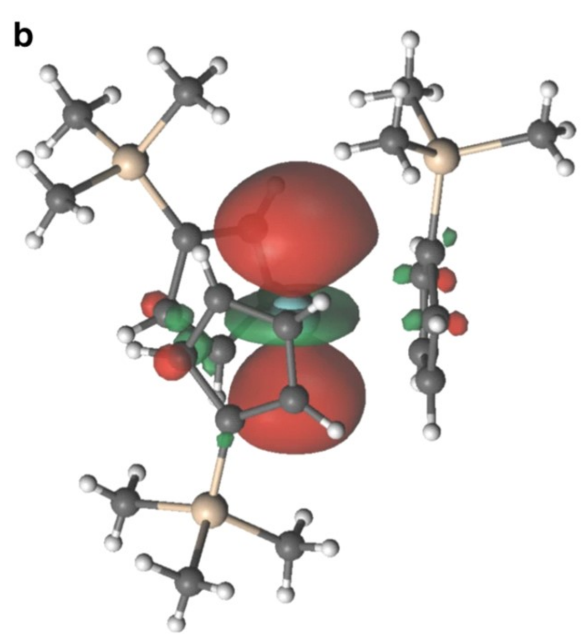
Zadrozny, Niklas, Poluektov, Freedman, *ACS Cent. Sci.* **2015**, *9*, 488

Isotropy promotes longer decoherance times at high temperature



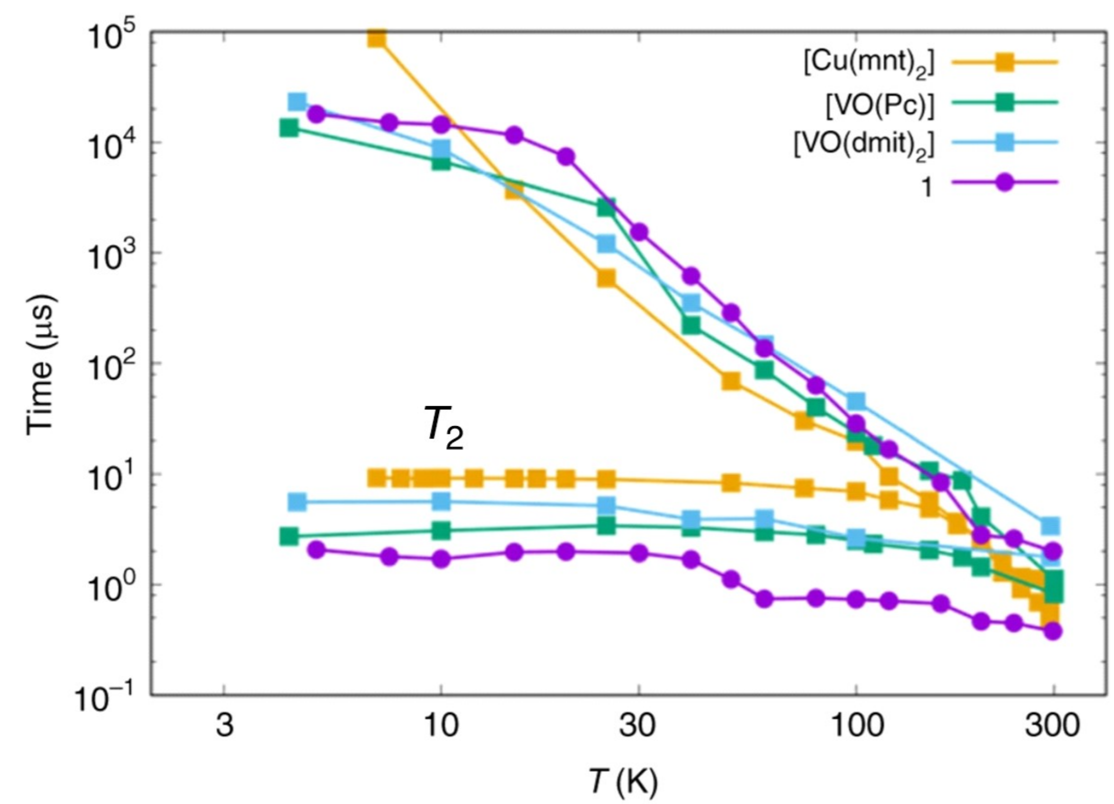


$[Y(Cp^{SiMe3})_3]^-$



92% $4dz^2$

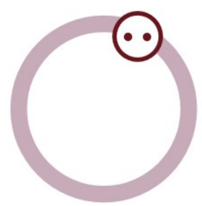
8% 5s, $L = 0$



Ariciu, Woen, Huh, Nodaraki, Kostopoulos, Goodwin, Chilton, McInnes, Winpenny, Evans, Tuna, *Nat. Commun.* **2019**, *10*, 3330

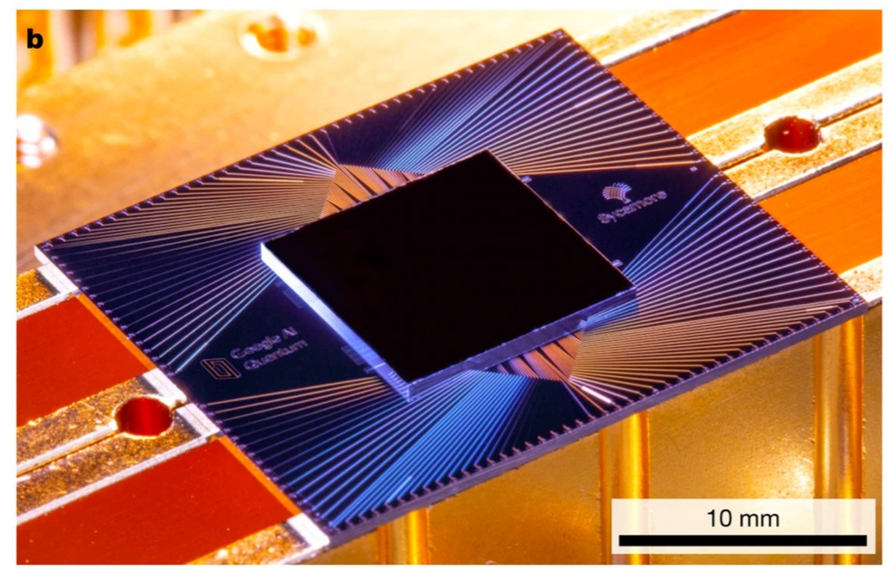
Bottom-up assembly could achieve well-ordered arrays of qubits

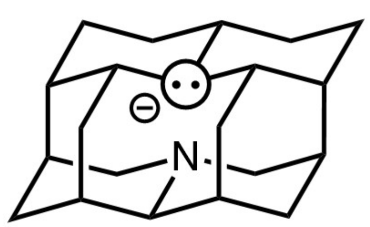
1) scalable, well-characterized qubit



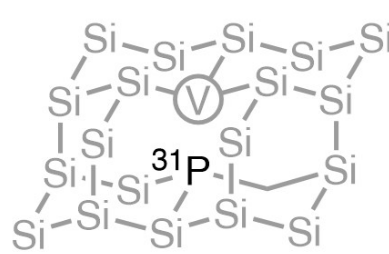
superconducting coil

scalable, BUT long T_2 only at mK temperatures



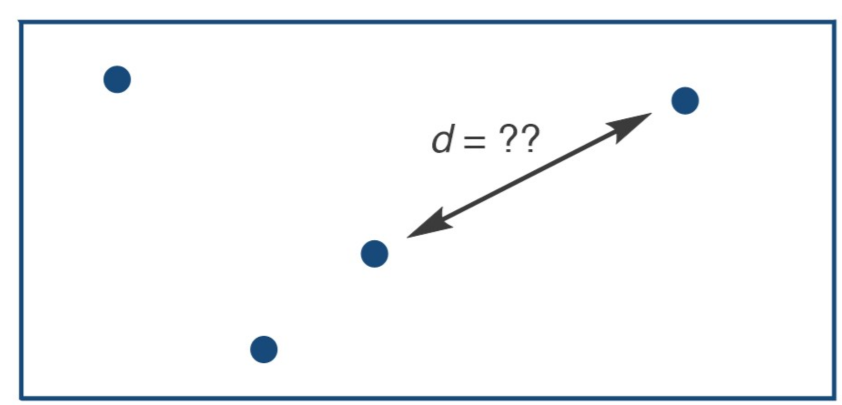


diamond NV-center



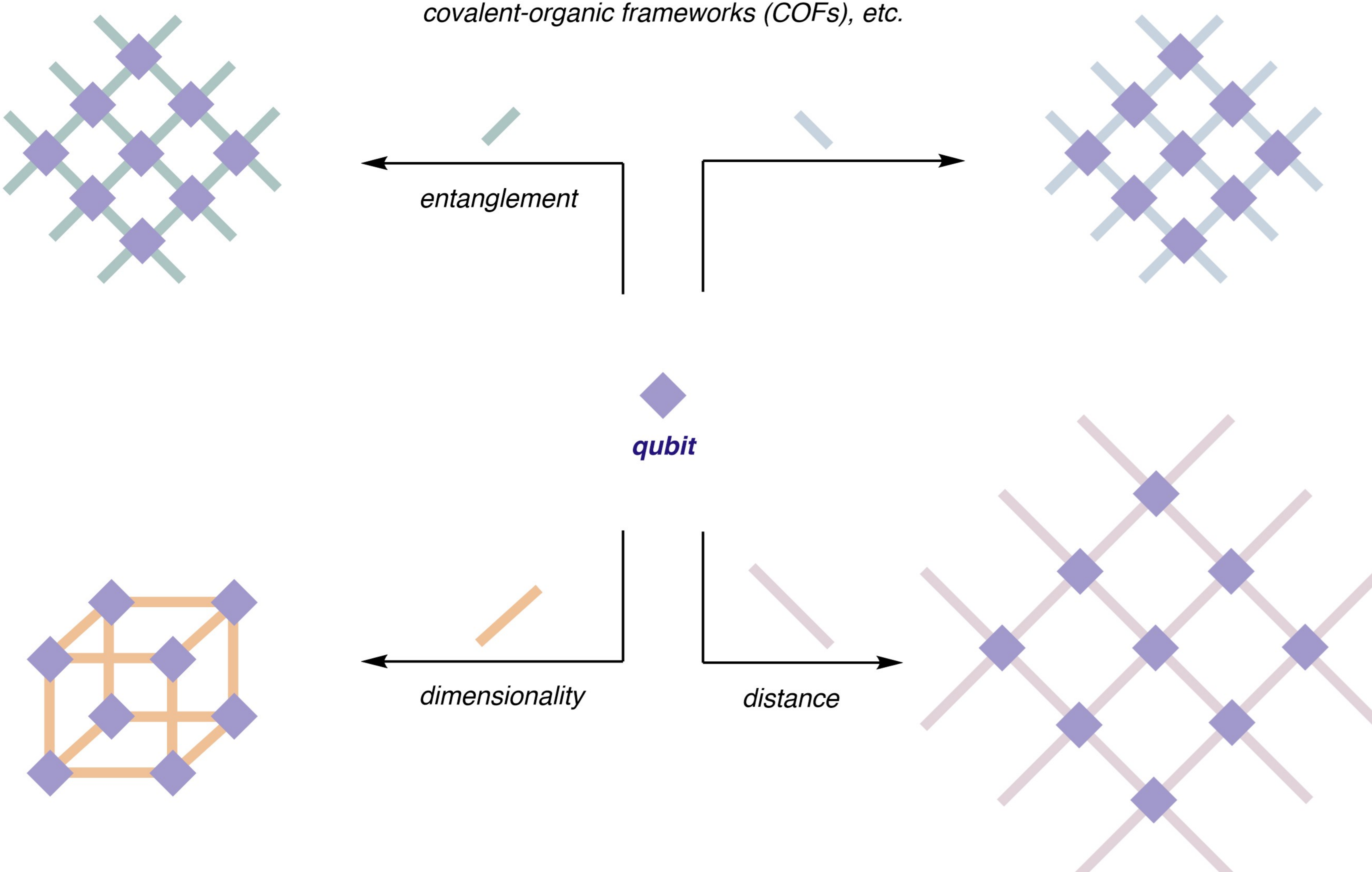
^{31}P-doped silicon

long T_2, but not scalable

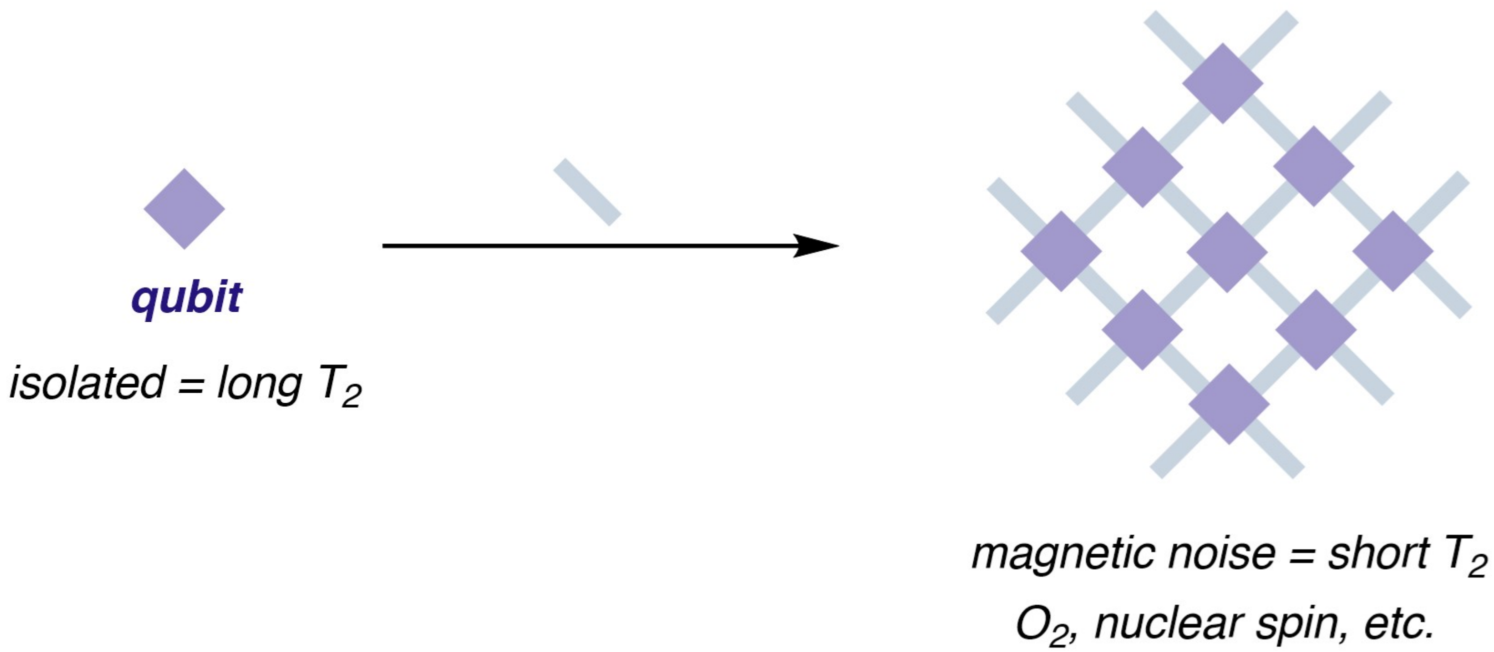


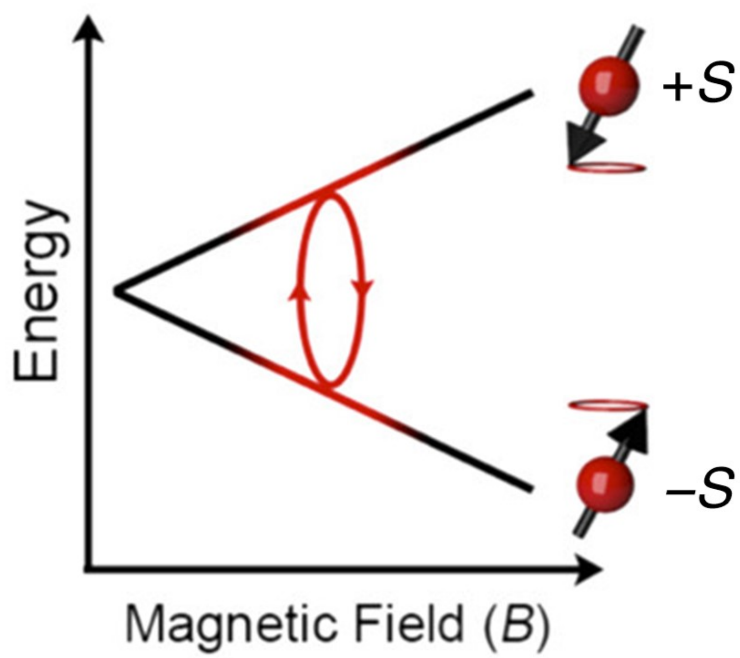
Bottom-up assembly could achieve well-ordered arrays of qubits

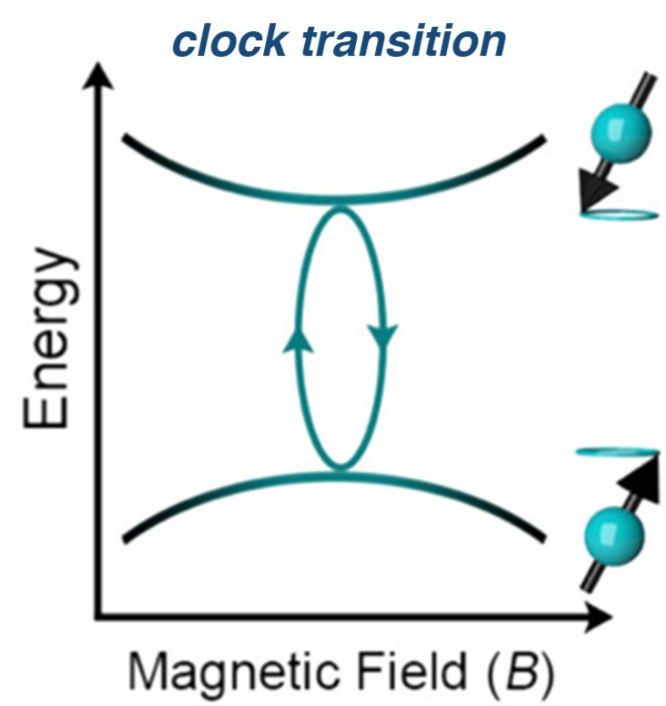
Bottom-up assembly is well studied in metal-organic frameworks (MOFs), covalent-organic frameworks (COFs), etc.



A porous array of clock qubits

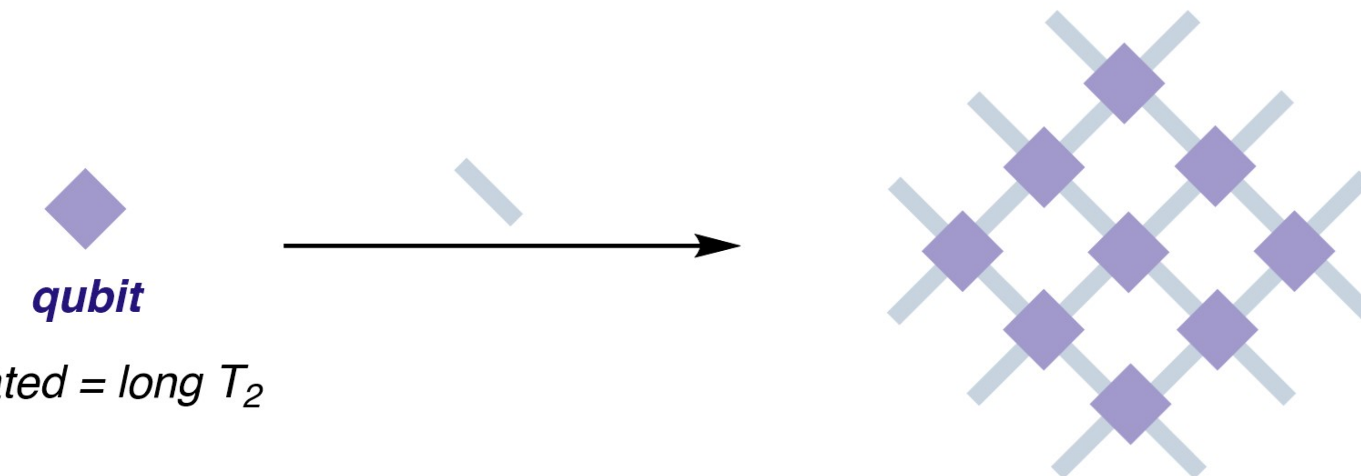






Zadrozny, Gallagher, Harris, Freedman *J. Am. Chem. Soc.* **2017**, *139,* 7809

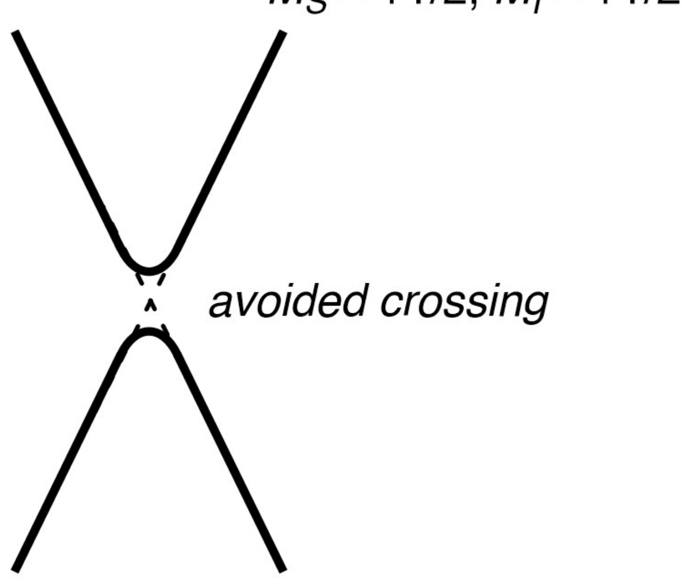
A porous array of clock qubits



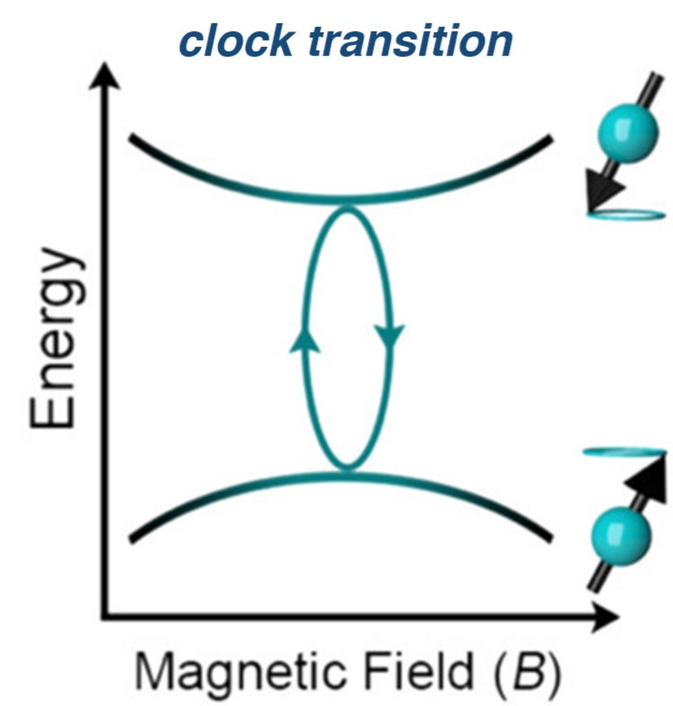
isolated = long T_2

magnetic noise = short T_2

O_2, nuclear spin, etc.



induced by strong hyperfine coupling



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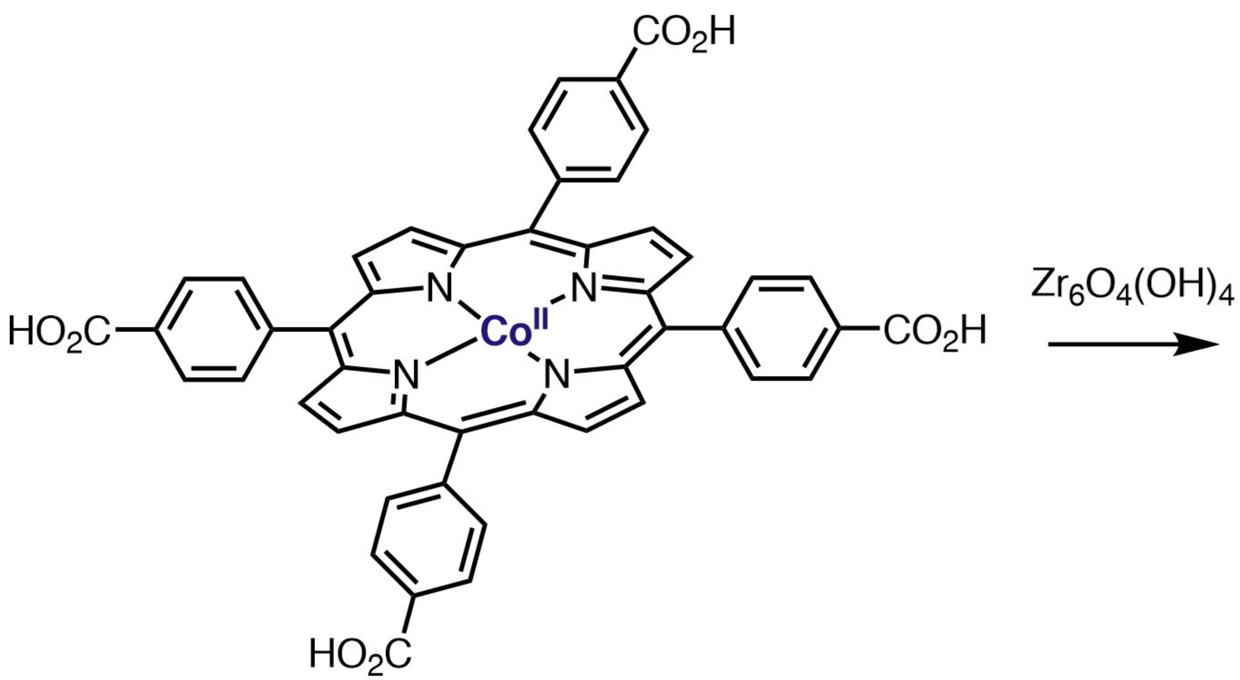
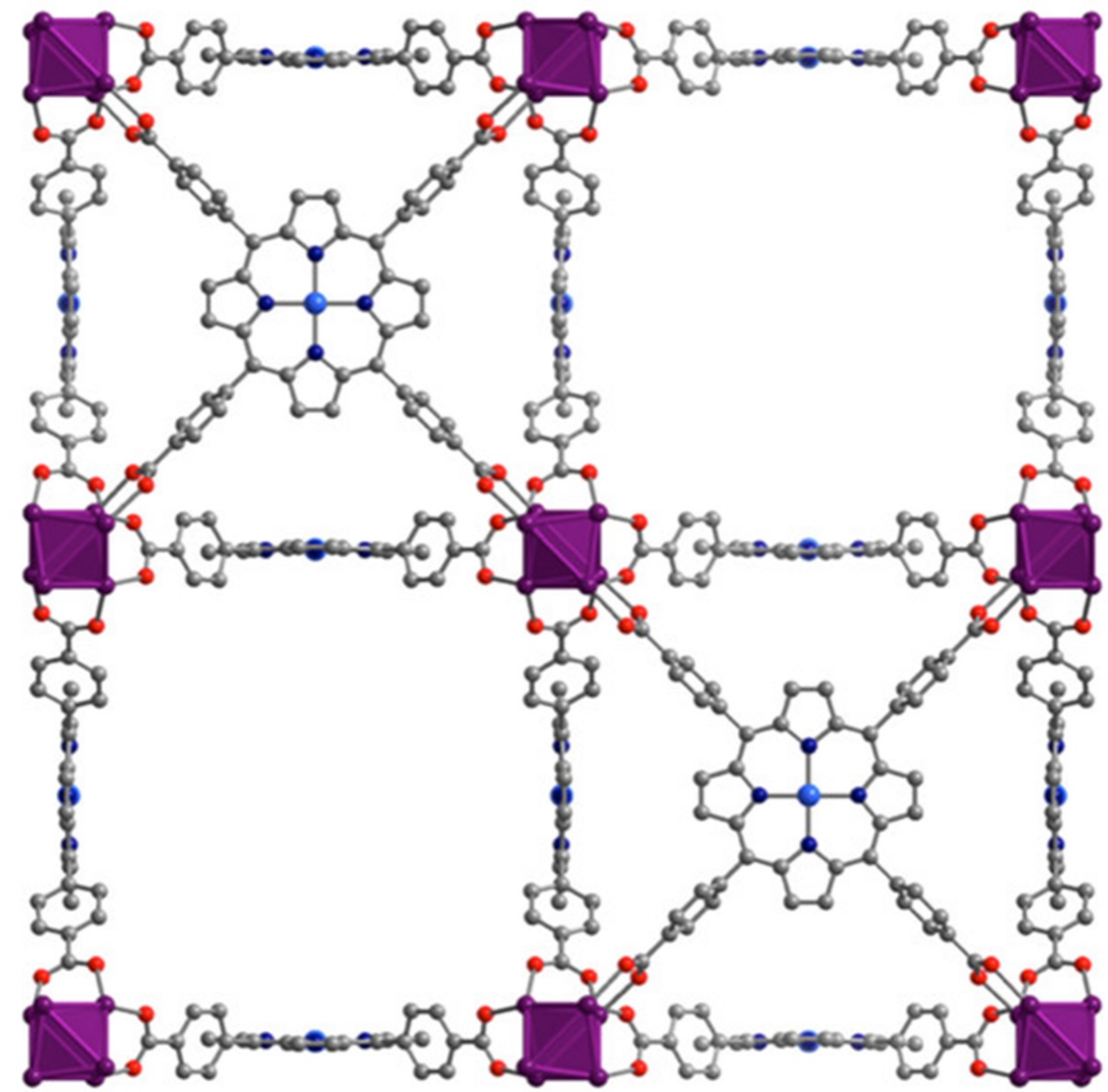
A porous array of clock qubits



Low spin $^{59}Co^{II}$

$S = 1/2$

$I = 7/2$



$[(TCPP)Co_{0.07}Zn_{0.93}]_3[Zr_6O_4(OH)_4(H_2O)_6]_2$

T_2 = 15 μs at 5 K

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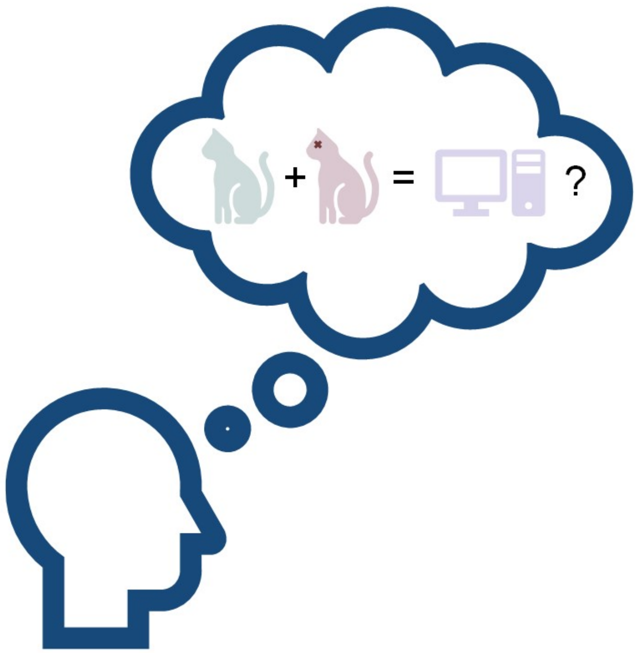
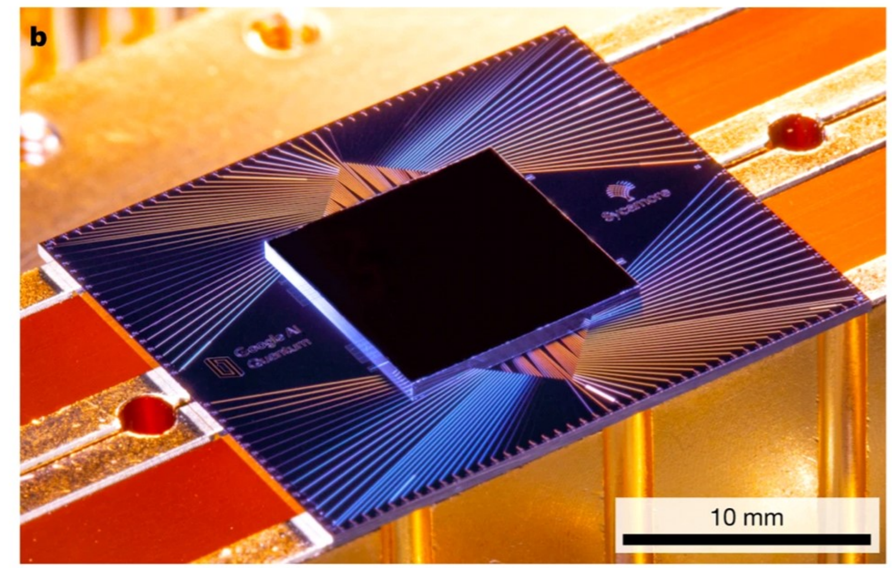
Conclusions



~40 years



chemical dynamics

codebreaking

protein folding

artificial intelligence

Conclusions

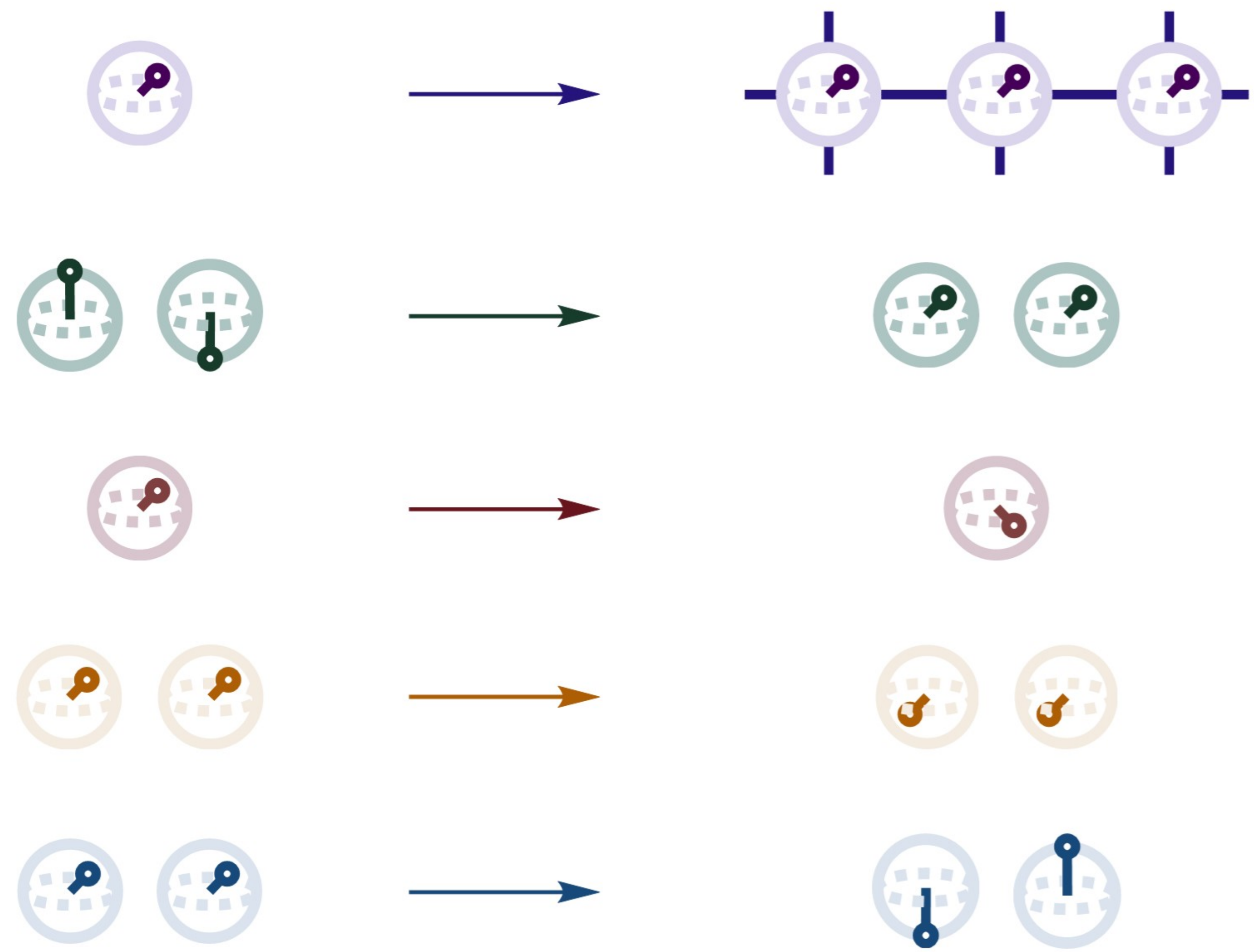
1) scalable, well-characterized qubit

2) initialization methods

3) long decoherance time

4) universal quantum gates

5) measurement capability



Chemistry enables fine control over qubit properties and spatial arrangement