

# **Quantum AI: The Next Leap in Physics Intelligence**

## **Research, Ecosystem, and Building Community**

**Dr. Taha Selim**  
**Director General MolKet**  
**Co-founder iQafé and Founder Quantum AI Lab**

## | Talk outline>

- **Short CV**
- **MolKet**
- **Quantum molecular dynamics & the JWST**
- **Simulating molecular collisions of CO<sub>2</sub> – He**
- **Overcoming computational challenges with AI**
- **GenAI applications**
- **Quantum AI community building**

## | Short CV >

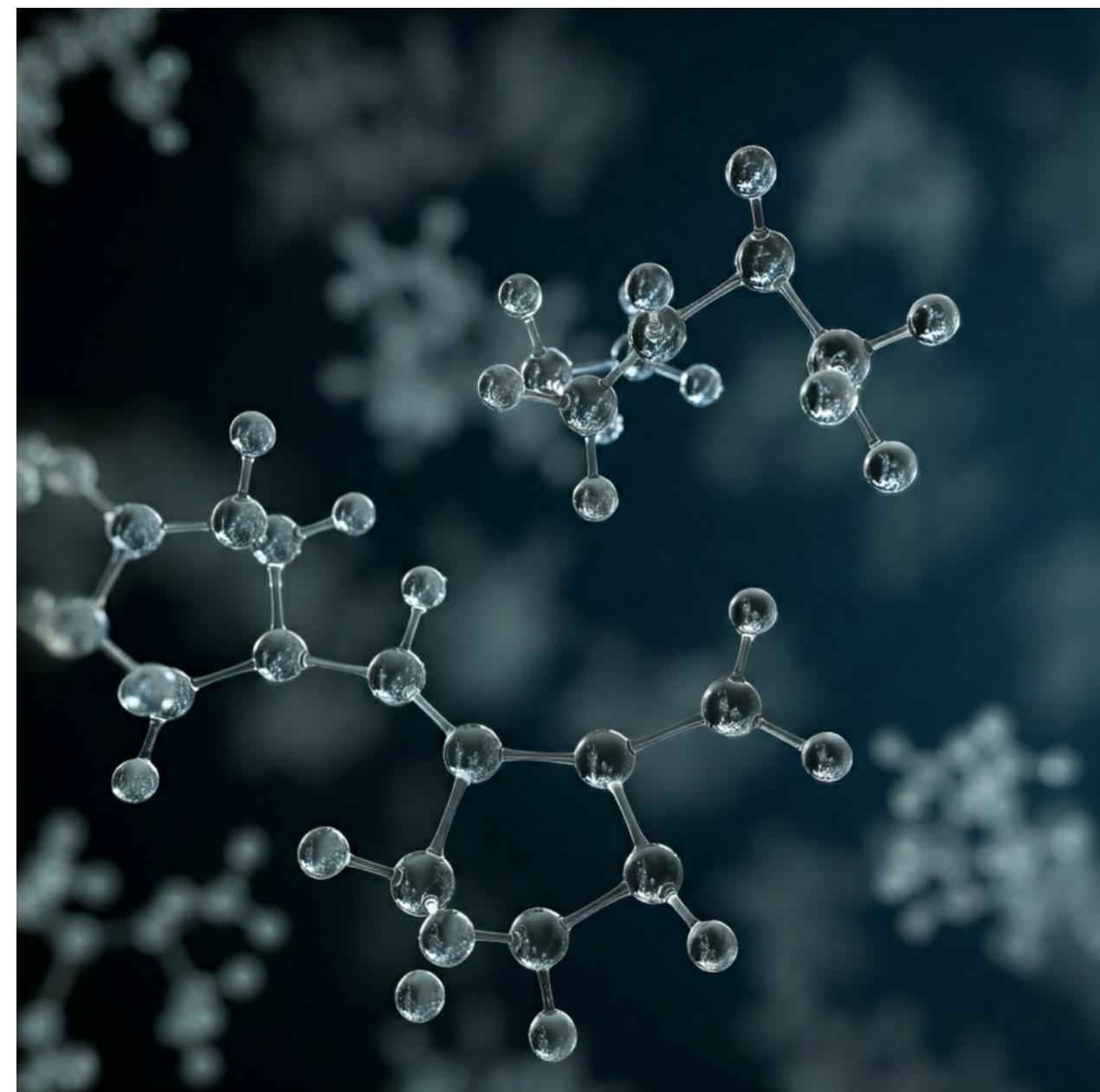
- **Researcher:** quantum information, quantum machine learning, and quantum chemistry.
- **Educator:** Quantum Education Officer at Amsterdam University of Applied Sciences and co-founder of iQafé, an online platform for teaching quantum computing and AI.
- **Entrepreneur:** General Manager of MolKet SAS, a company providing consulting and AI services for quantum technologies.
- **Science communicator:** Tech YouTuber, making complex topics accessible to a wide audience in English and Arabic.



**Taha Selim**



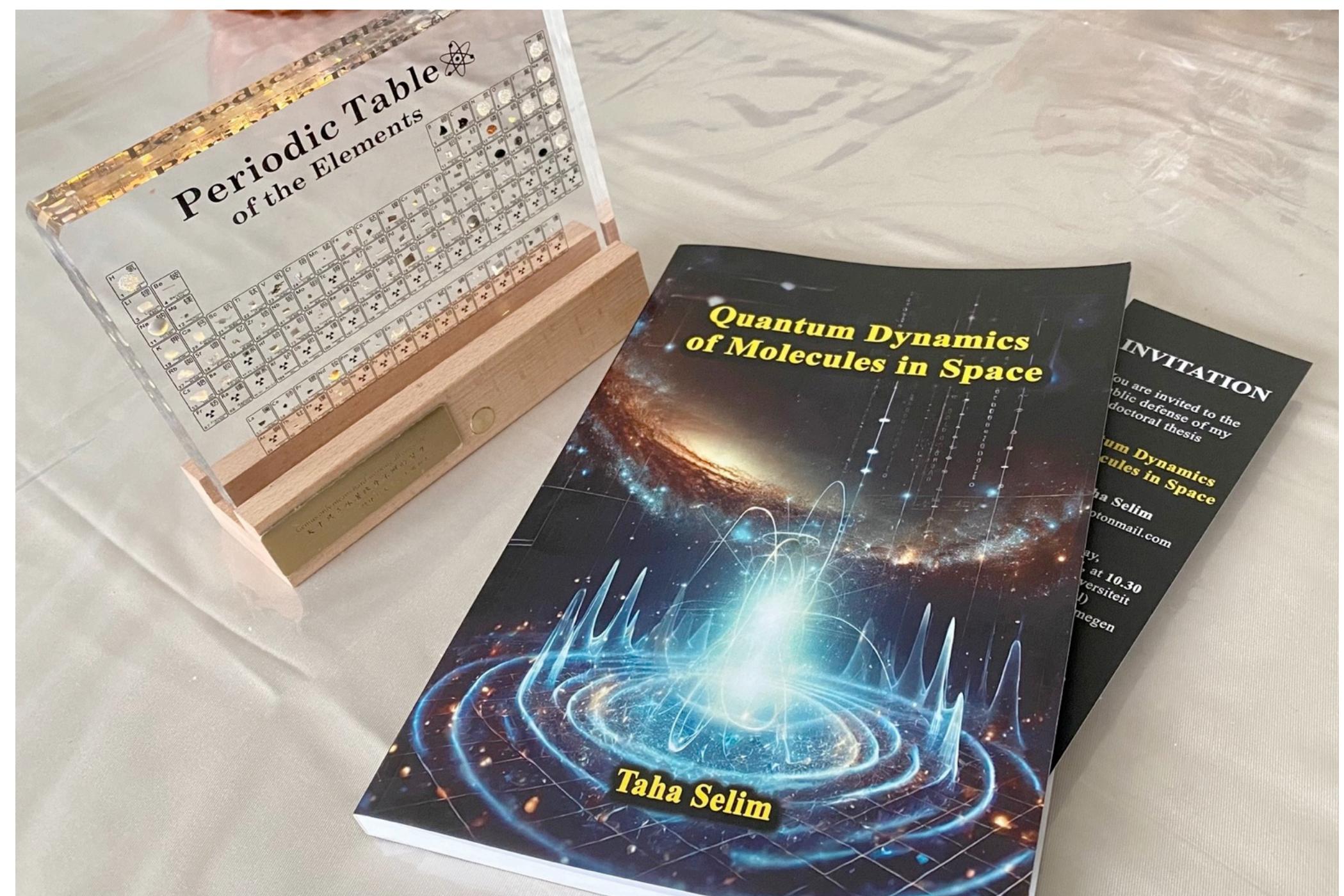
We propose leveraging AI to accelerate chemical design and quantum dynamical simulations. These AI applications can be trained on the inputs and outputs of quantum chemistry and dynamics algorithms, effectively replacing computationally expensive components. Furthermore, they can learn the scaling behavior of these algorithms, enabling extrapolation to larger systems.



# | PhD publications >

This presentation is based on my PhD research, which is detailed in the following publications:

- Taha Selim. (2024). Quantum dynamics of molecules in space: Theoretical studies and efficient computational methods for collision-induced rovibrational transition rates in molecules. [Doctoral dissertation, Radboud University]. <https://repository.ubn.ru.nl/handle/2066/311101>
- Taha Selim, Arthur Christianen, Ad van der Avoird, & Gerrit C. Groenenboom. (2021). Multi-channel distorted-wave Born approximation for rovibrational transition rates in molecular collisions. *The Journal of Chemical Physics*, 155(3), 034105. <https://pubs.aip.org/aip/jcp/article-abstract/155/3/034105/200835/Multi-channel-distorted-wave-Born-approximation>
- Taha Selim, Ad van der Avoird, & Gerrit C. Groenenboom. (2022). Efficient computational methods for rovibrational transition rates in molecular collisions. *The Journal of Chemical Physics*, 157(6), 064105. <https://pubs.aip.org/aip/jcp/article/157/6/064105/2841671/Efficient-computational-methods-for-rovibrational>
- Taha Selim, Ad van der Avoird, & Gerrit C. Groenenboom. (2023). State-to-state rovibrational transition rates for CO<sub>2</sub> in the bend mode in collisions with He atoms. *The Journal of Chemical Physics*, 159(16), 164310. <https://pubs.aip.org/aip/jcp/article/159/16/164310/2918420/State-to-state-rovibrational-transition-rates-for>



| Deep Seek >

# Gemini

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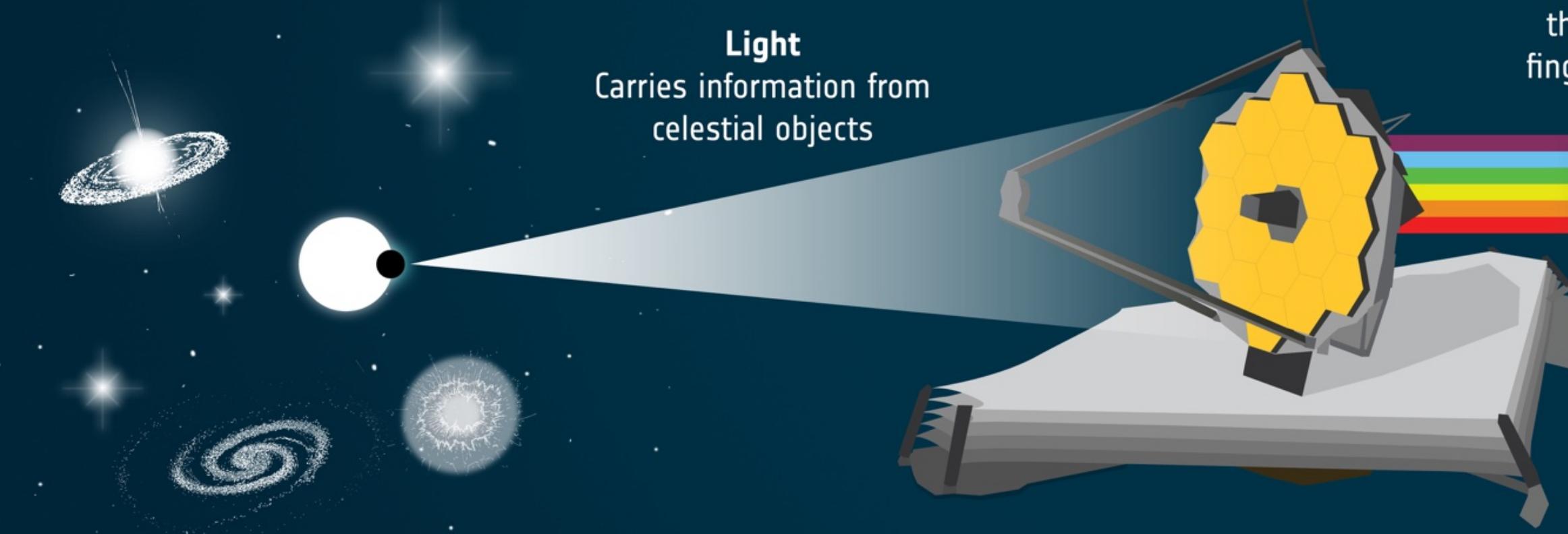


# ChatGPT

## | Quantum molecular dynamics & the JWST >

## SPECTROSCOPY WITH WEBB

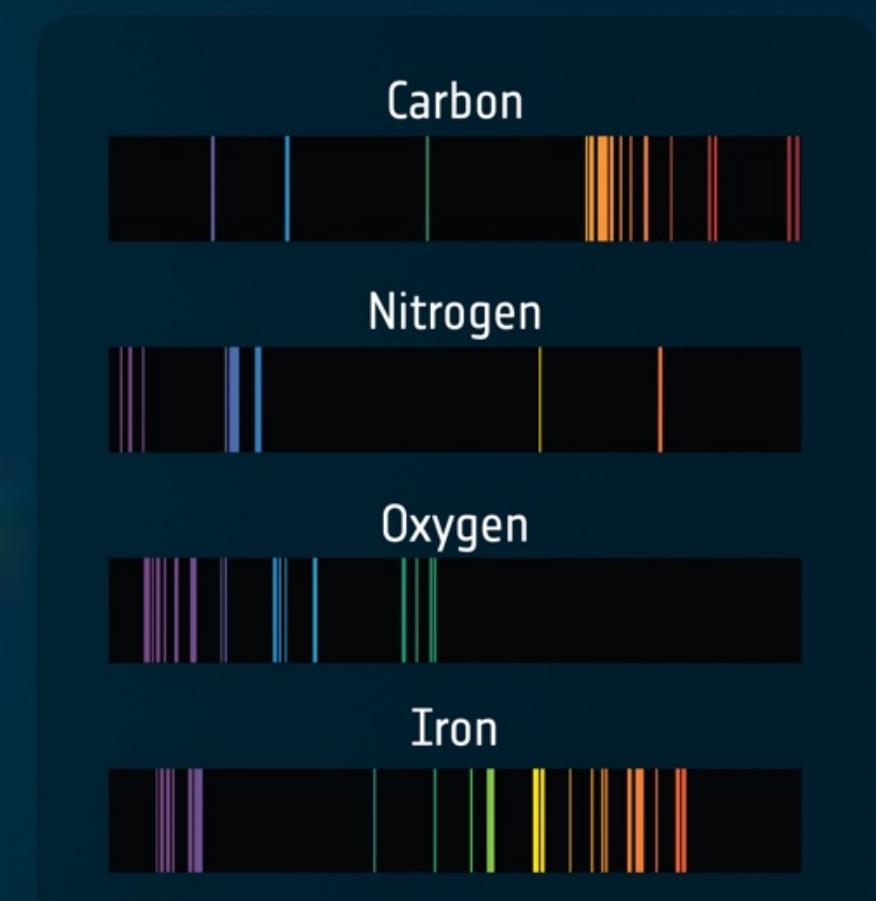
Spectroscopy is a tool that astronomers use to better understand the physics of objects in space. Like a prism splits white light from the Sun into its colour components (like a rainbow), Webb's spectrographs will dissect infrared light into its many wavelengths. This will provide detailed information about an object, such as how a galaxy moves or what molecules are present in an exoplanet's atmosphere.



**Celestial objects**  
Stars, nebulae, exoplanet atmospheres, galaxies...

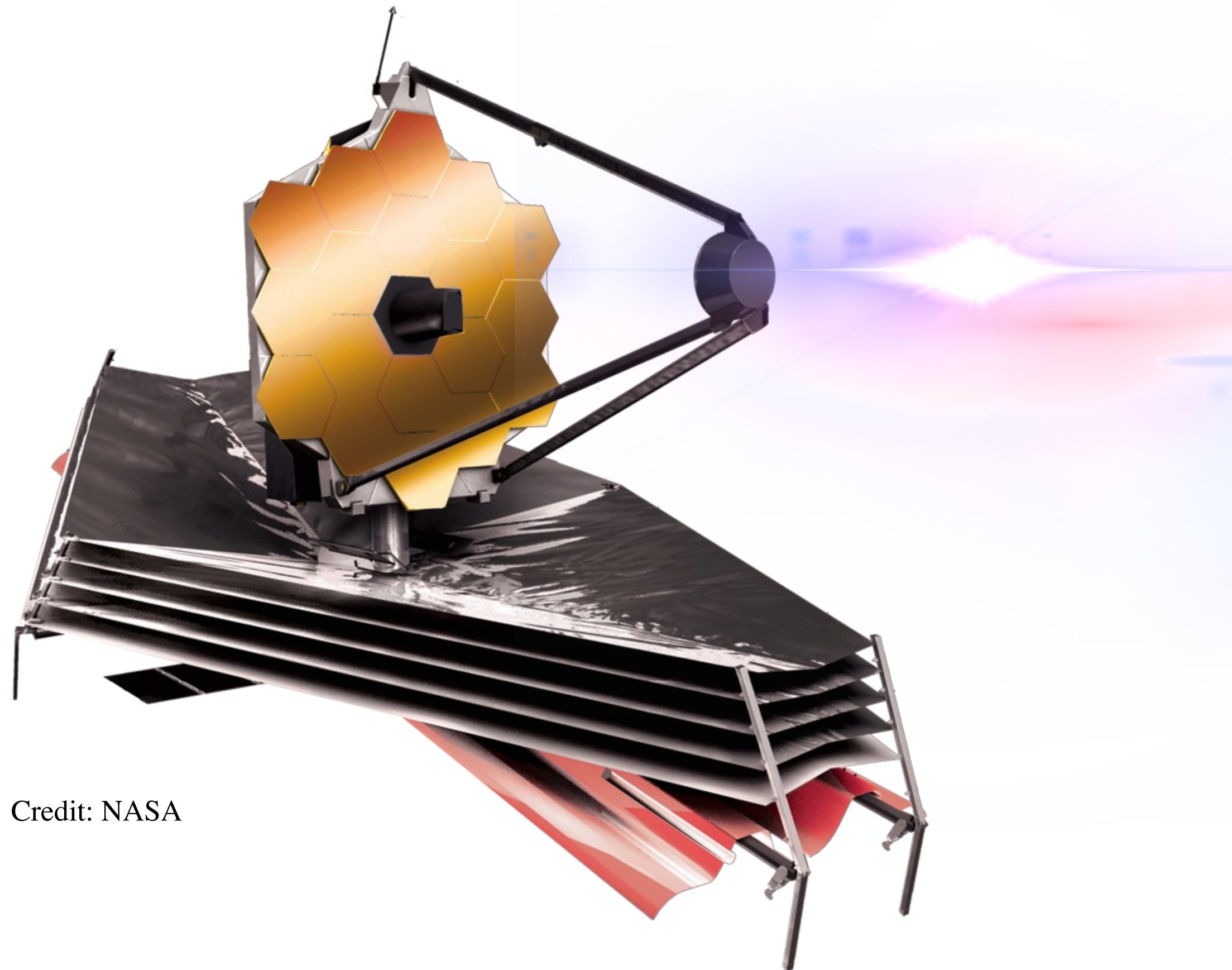
**Webb's instruments**  
Light is split into its different wavelengths and focused onto a detector, forming a spectrum

**Spectrum**  
Atoms and molecules stamp their unique properties as fingerprints on the spectrum

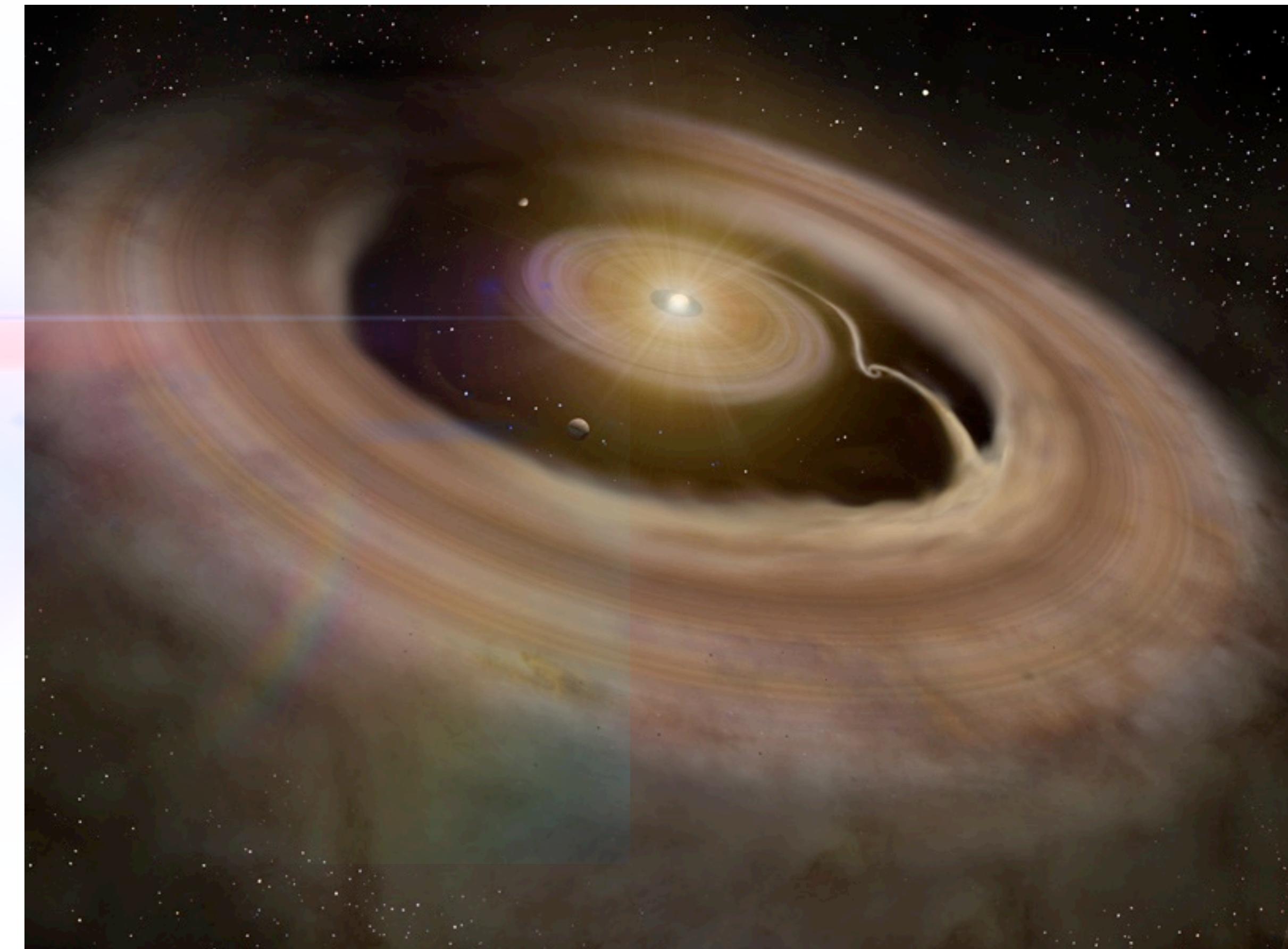


**Spectra detectives**  
Scientists study spectra to analyse what atoms and molecules are present in the source. Spectra also reveal the temperature, density and motion of the objects

## | James Webb Space Telescope (JWST) >



Credit: NASA



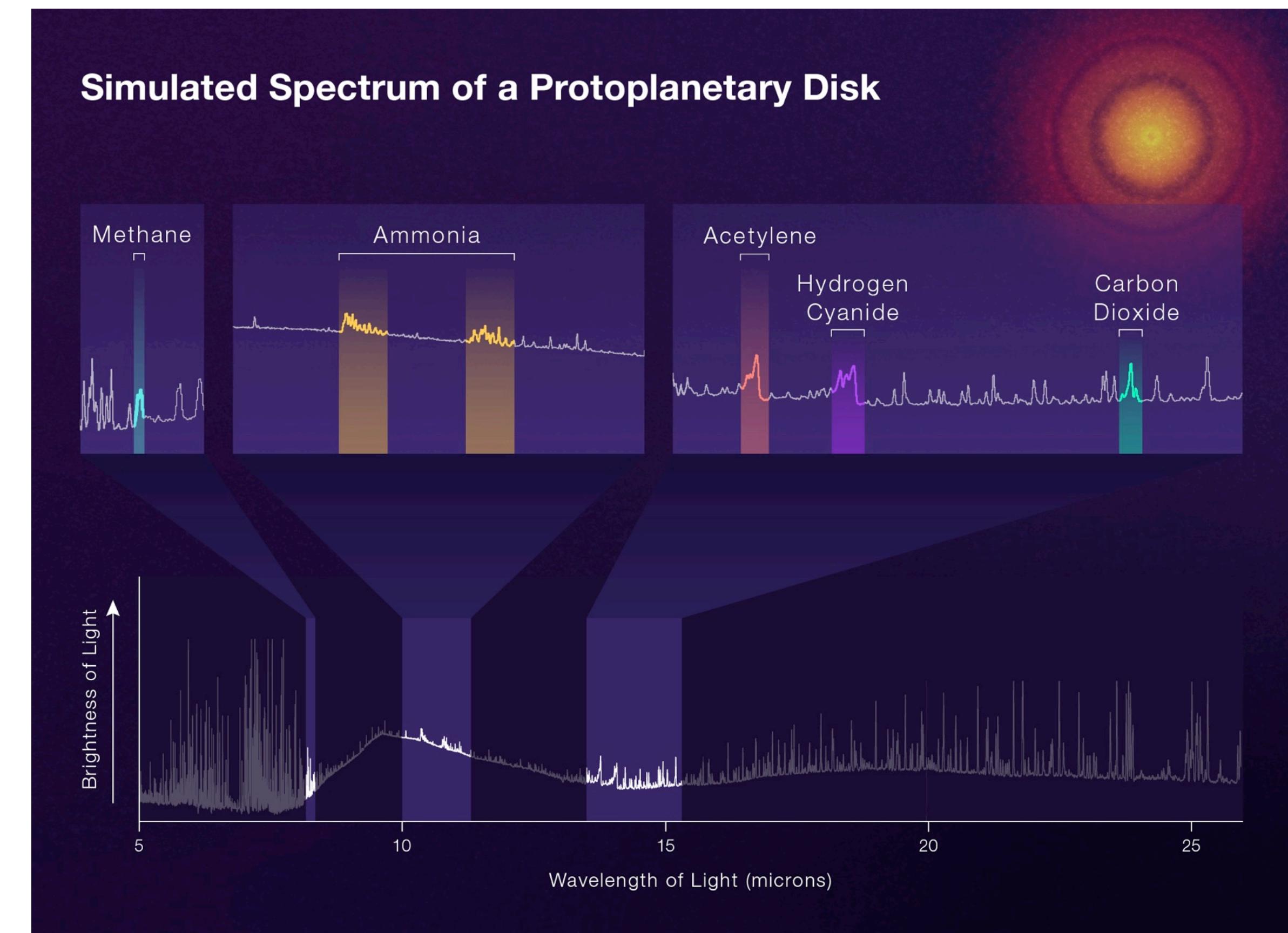
**Powerful near and mid-infrared observational capabilities**

# | CO<sub>2</sub> as a molecular quantum sensor >

The spectra reports the **chemistry** in these **interstellar media**:

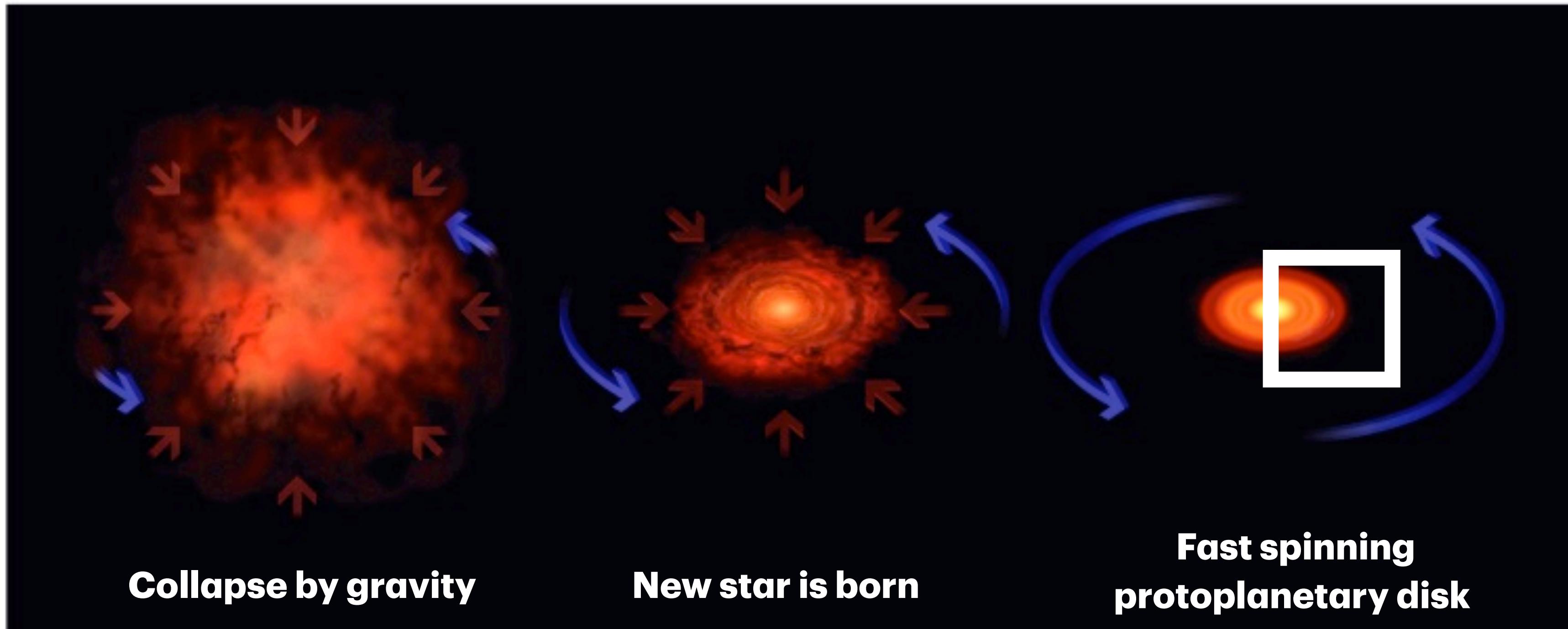
- Local temperature.
- Molecular abundances.
- More information.

**Goal:** to decipher the spectra and extract the **useful data**



Credit: NASA, ESA, CSA, Leah Hustak (STScI)

# | CO<sub>2</sub> as a molecular quantum sensor >



© Addison-Wesley Longman



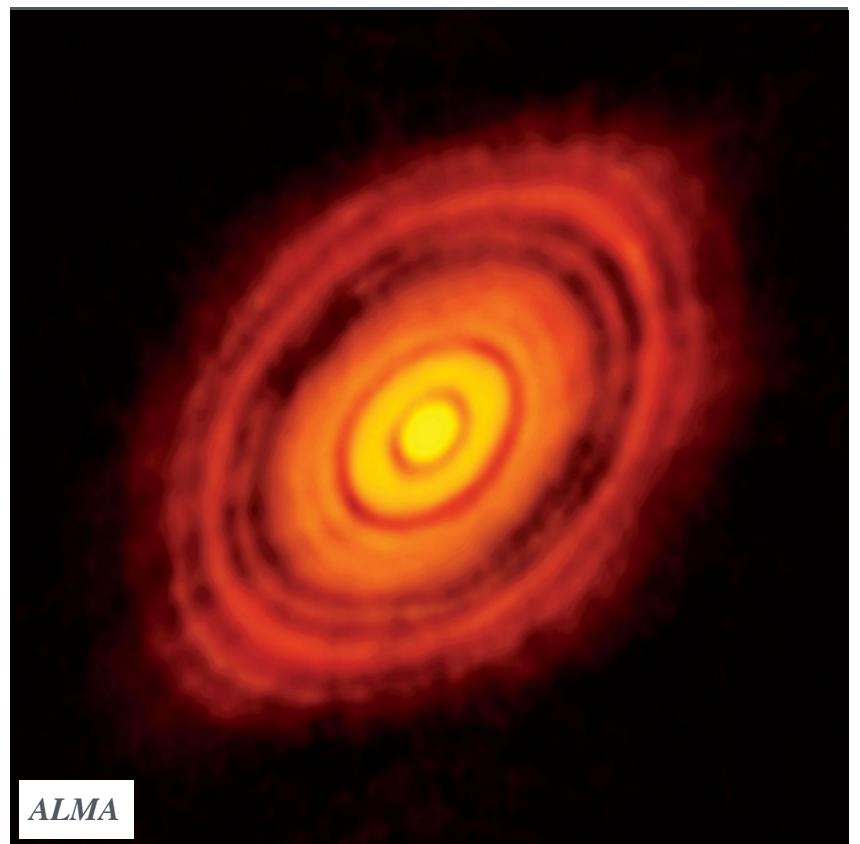
Conceptual illustration

## Key molecules

CO   CO<sub>2</sub>   HCN   H<sub>2</sub>O   C<sub>2</sub>H<sub>2</sub>   CH<sub>4</sub>

# | CO<sub>2</sub> is a key molecule in interstellar media >

**CO<sub>2</sub> was found in interstellar media and (exo-)planets**



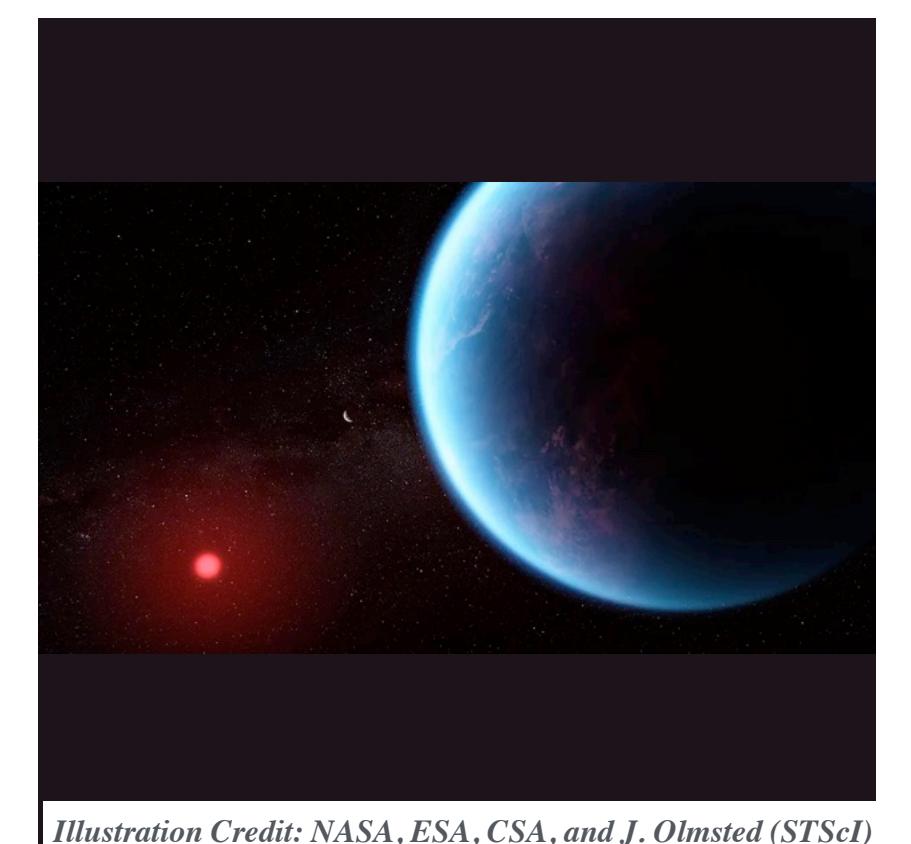
Protoplanetary disk T Tauri Star



Venus



Jupiter's moon Europa



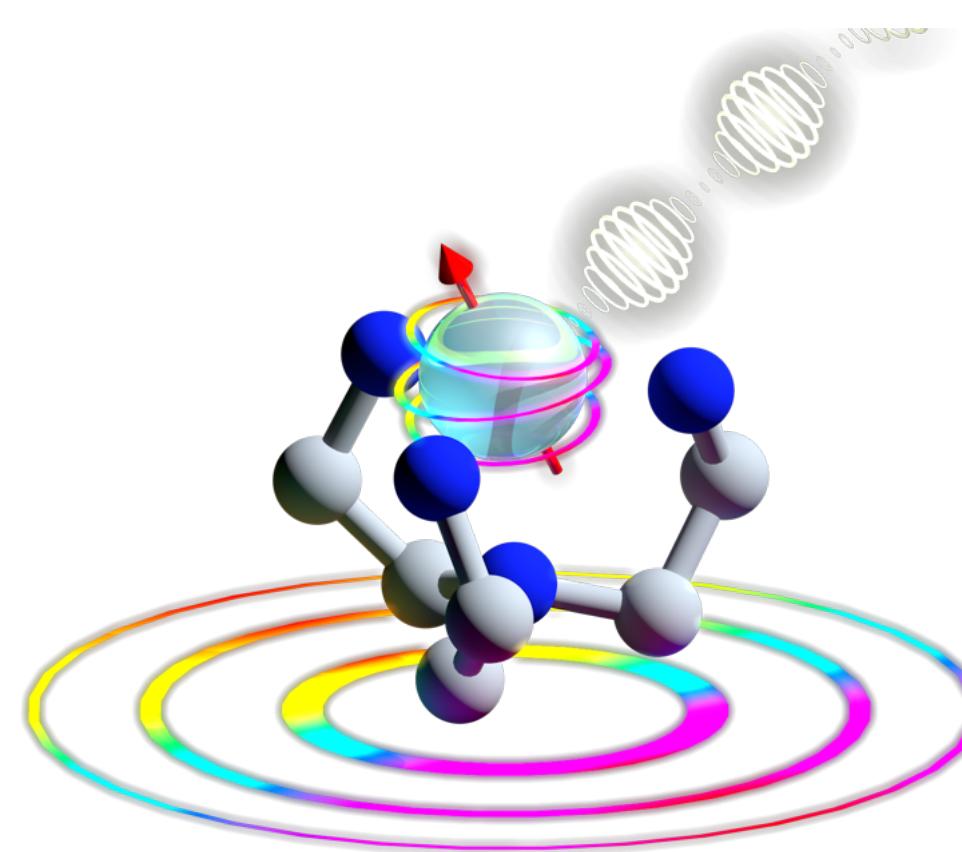
Exoplanet K2-18 b

*Illustration Credit: NASA, ESA, CSA, and J. Olmsted (STScI)*

# | What is quantum molecular dynamics? >

## Quantum Chemistry

Quantum mechanical treatments of **electrons**



## Quantum Molecular Dynamics

Quantum mechanical treatments of both electrons & nuclei

## Molecular Dynamics

Classical mechanical treatments of **nuclei**

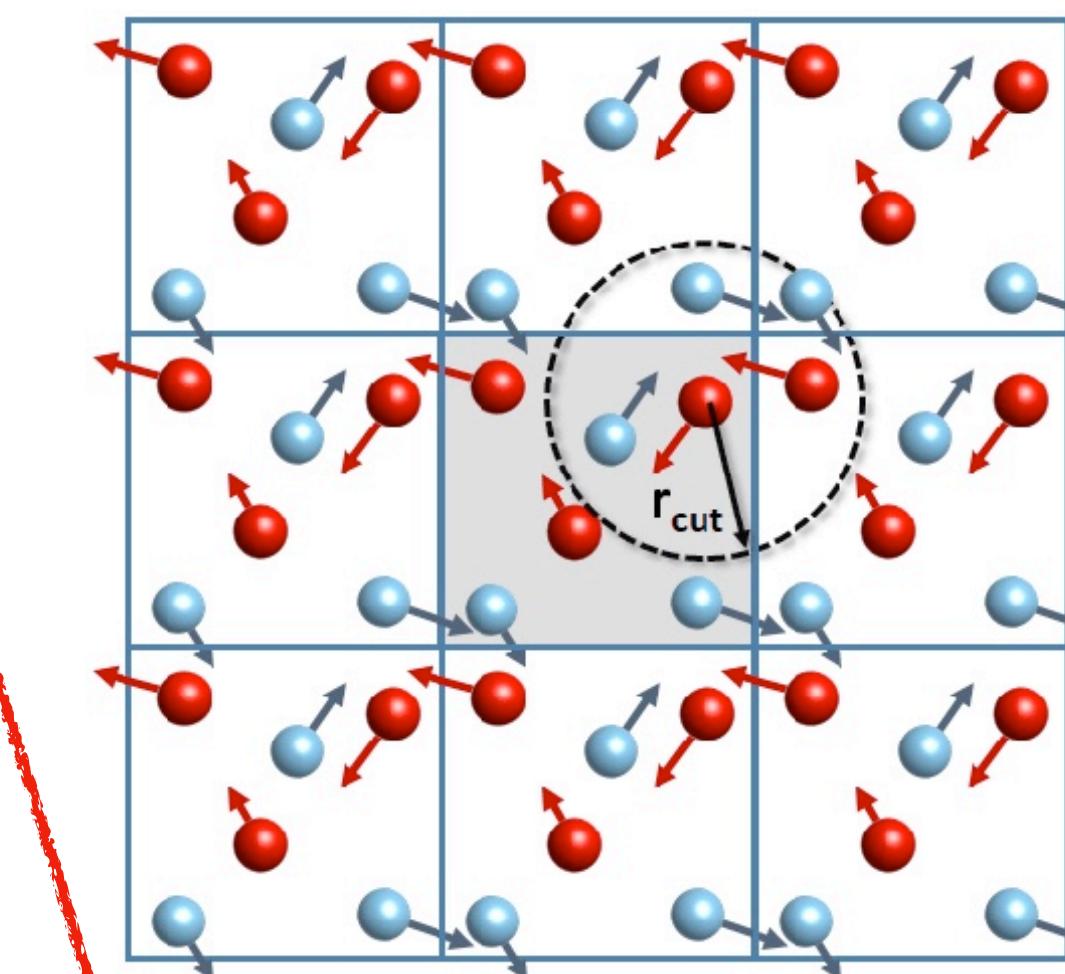


Image: [Jacob Chapman](#)

Credit: Rachael Tremlett/Macmillan Publishers Limited

# | CO<sub>2</sub> : Rotational-vibrational states >

CO<sub>2</sub> three vibrational modes - two modes are infrared active

Labeling the rovibrational quantum state: 5 quantum numbers

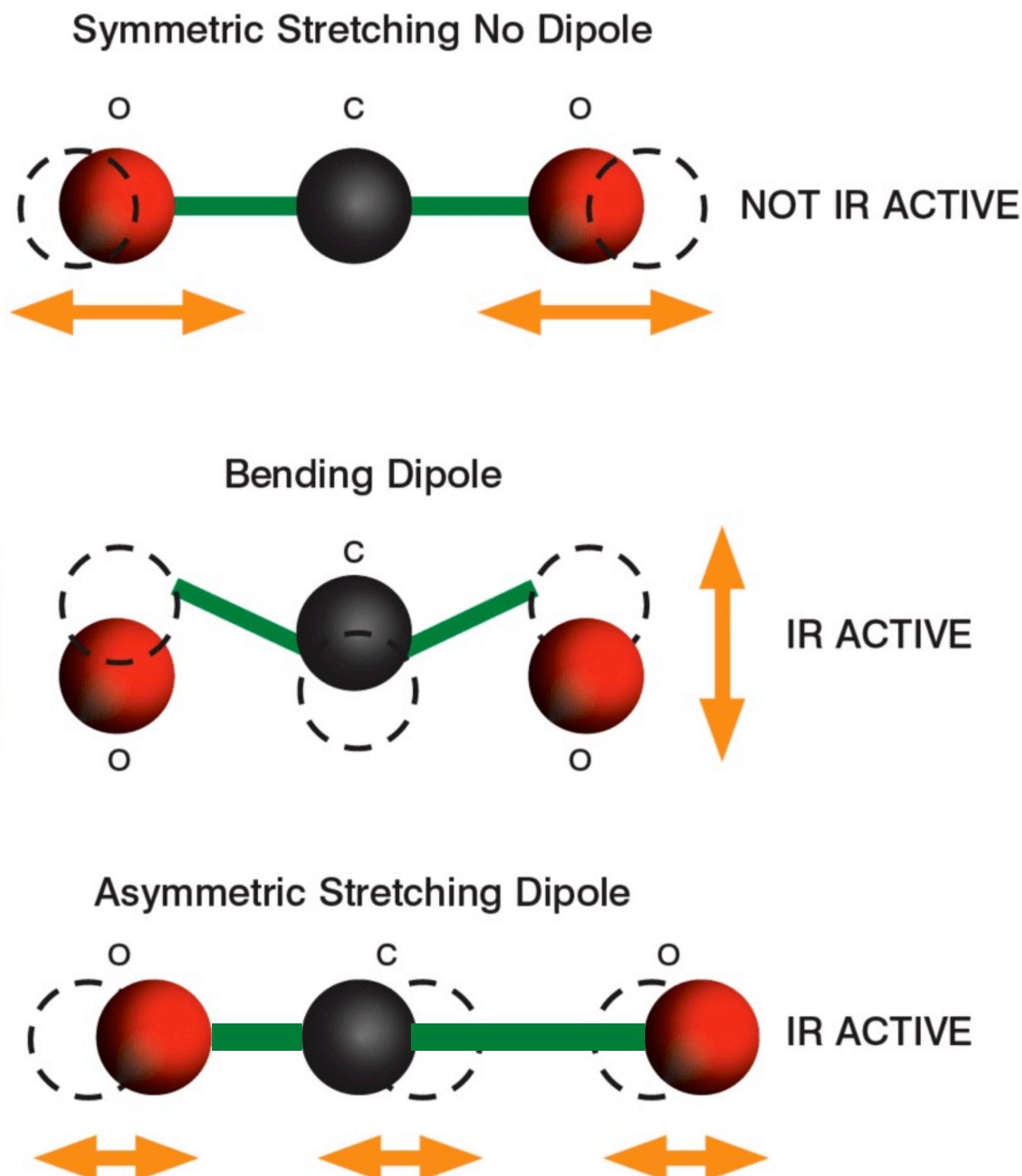
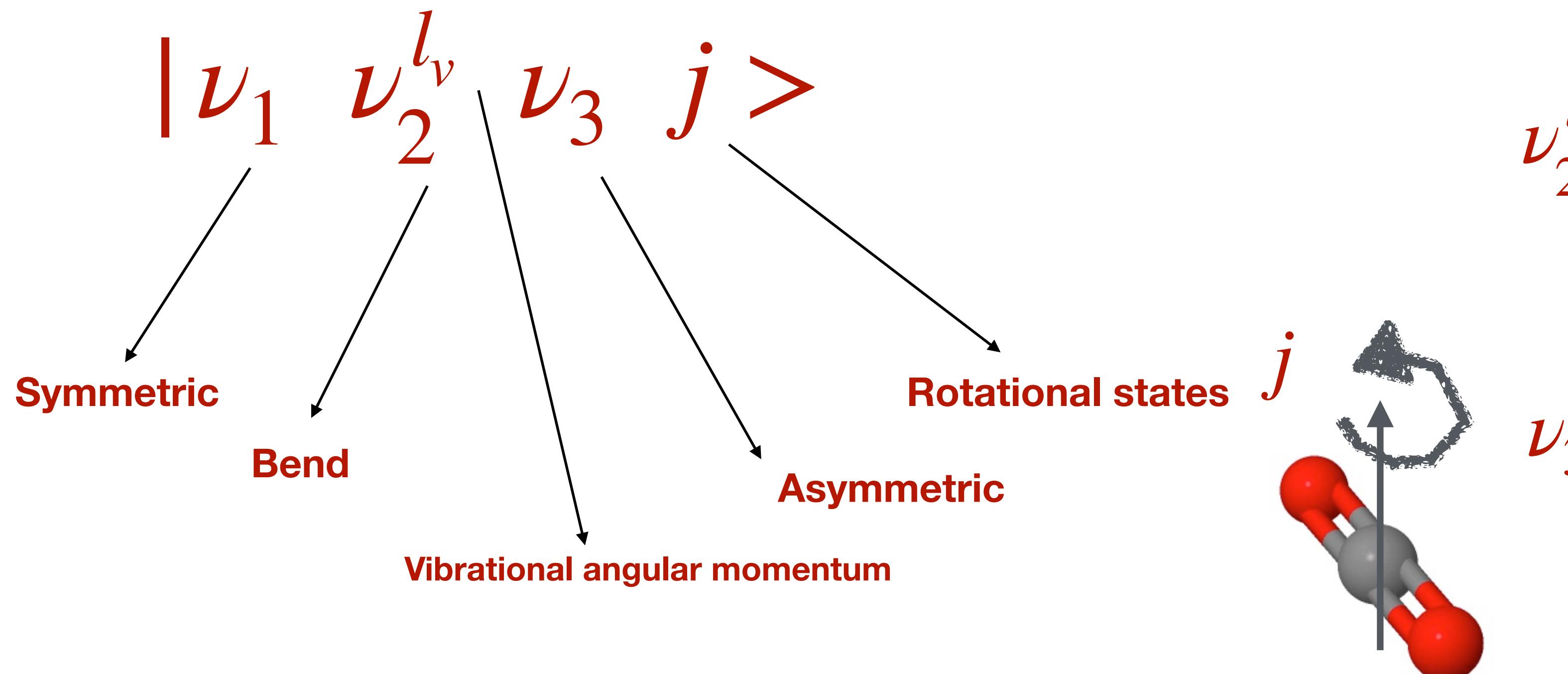


Image credit: lifford Jones

| Simulating molecular collisions of CO<sub>2</sub>-He >

# | Recipe for simulating CO<sub>2</sub> + He inelastic collisions >

First, we construct the 1D Hamiltonian  $\hat{H}_{CO_2}$  to obtain the rotational-vibrational wavefunctions and energy eigenvalues of CO<sub>2</sub> ( $v\ 0^0\ 0\ j$ ):

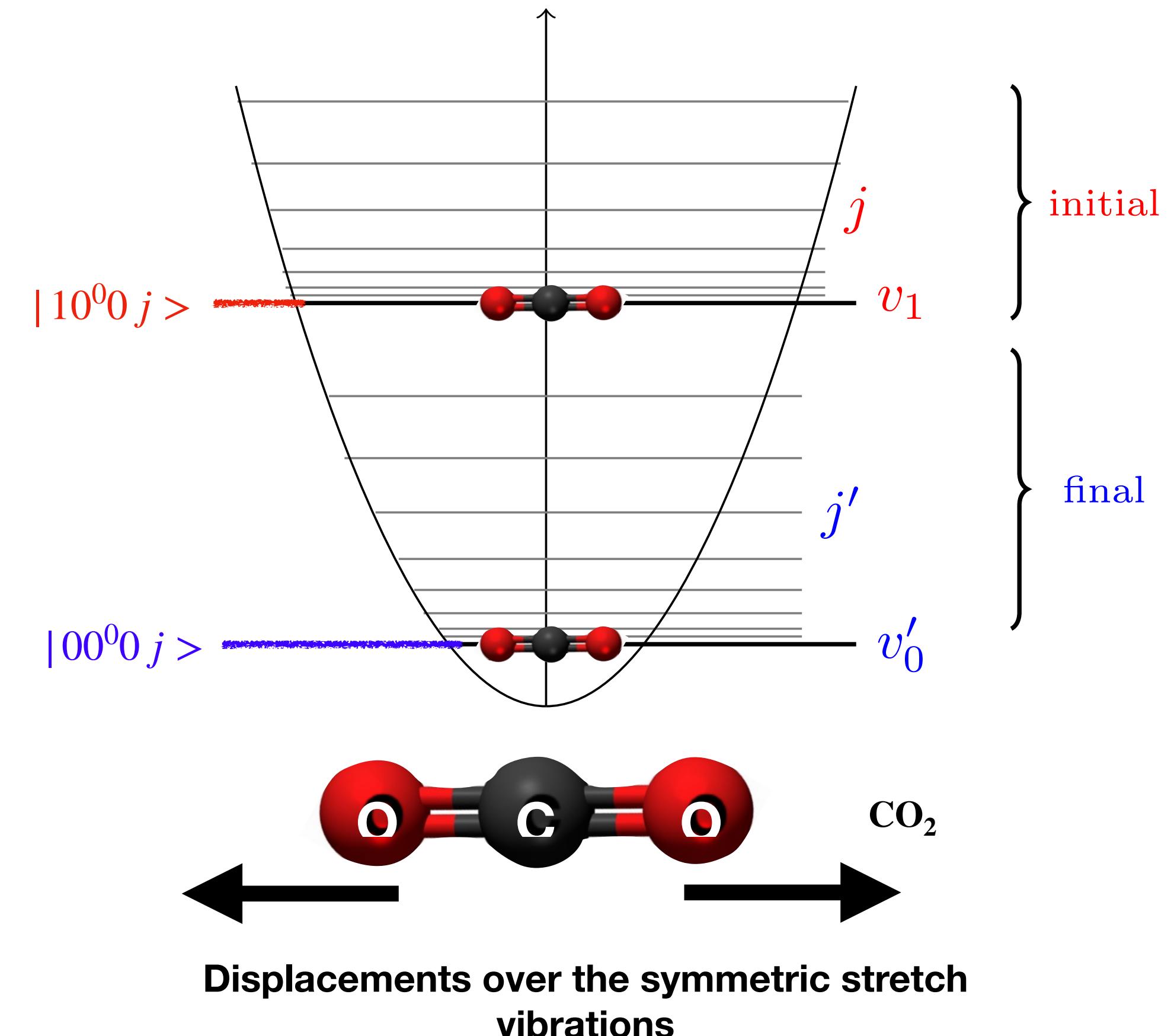
$$\hat{H}_{CO_2}(Q) = - \underbrace{\frac{\hbar^2}{2\mu_{CO_2}(Q)} \frac{\partial^2}{\partial Q^2}}_{\text{Nuclear motion}} + \underbrace{\frac{\hat{j}^2}{2I(Q)}}_{CO_2 \text{ angular Momentum}} + \underbrace{V_{CO_2}(Q)}_{\text{1D potential}}$$

CO<sub>2</sub> computational basis/space:

$$| v\ 0^0\ 0\ j \rangle$$

CO<sub>2</sub> rotational vibrational wave functions:

$$| v\ j \rangle = \chi_{vj}(Q) Y_{j0}(\theta, 0)$$



# | Simulating CO<sub>2</sub> + He inelastic collisions >

Second, we construct the 3D Hamiltonian of the dimer  $\hat{H}_{HeCO_2}$  to obtain the scattering wavefunctions and channel basis:

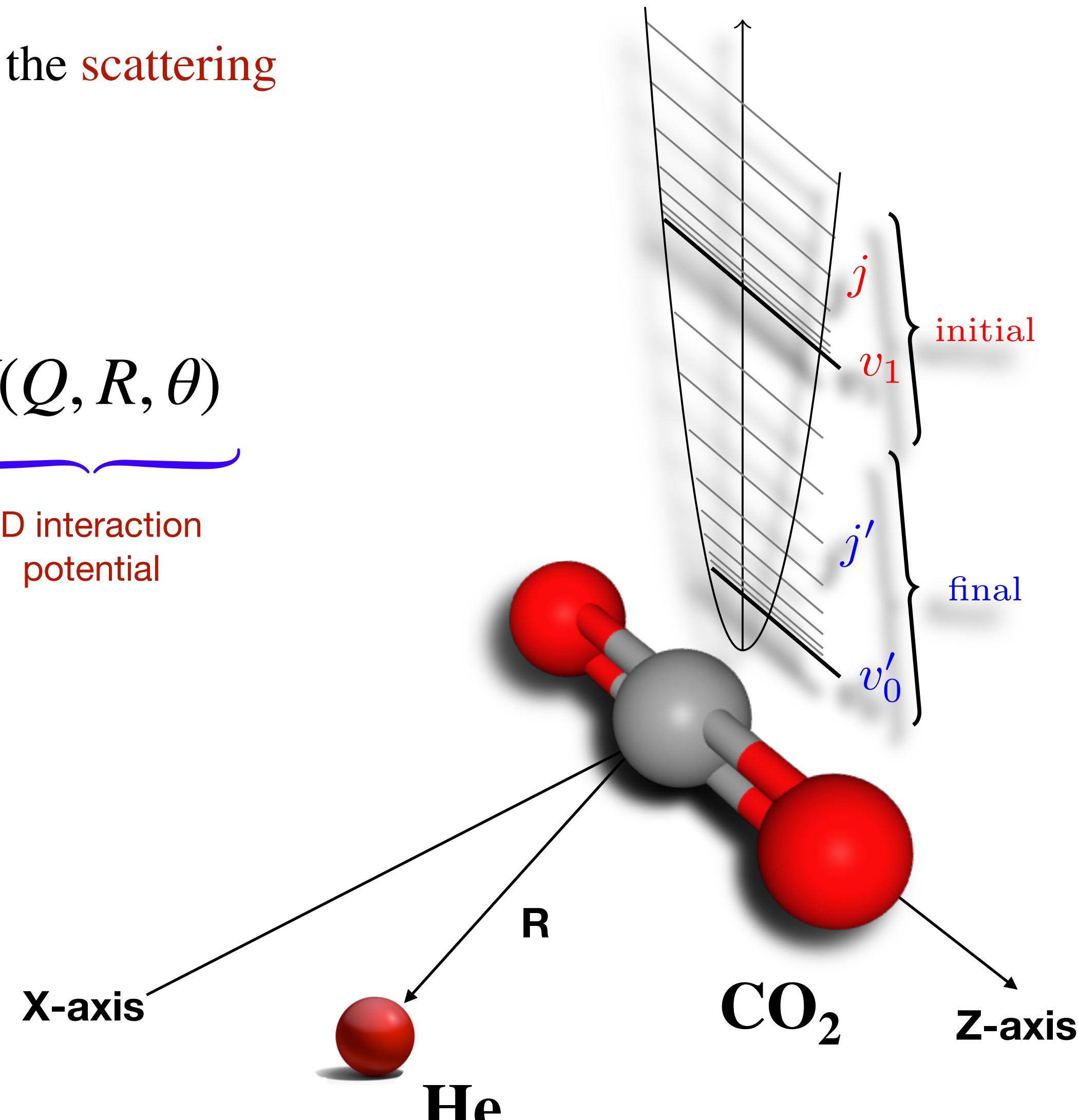
$$\hat{H}_{HeCO_2} = \underbrace{-\frac{1}{2\mu R} \frac{\partial^2}{\partial R^2} R}_{\text{Kinetic energy of the dimer}} + \underbrace{\hat{H}_{CO_2}}_{CO_2 \text{ Hamiltonian}} + \underbrace{\frac{\hat{L}^2}{2\mu R^2}}_{\text{Angular kinetic energy of the dimer}} + \underbrace{V(Q, R, \theta)}_{\text{3D interaction potential}}$$

dimer: refers to both He+CO<sub>2</sub>

**HeCO<sub>2</sub> computational basis/space, used for solution:**

**Space-fixed (SF):**  $|v j L | JM_J >$

**Body-fixed (BF):**  $|v j \Omega | JM_J >$

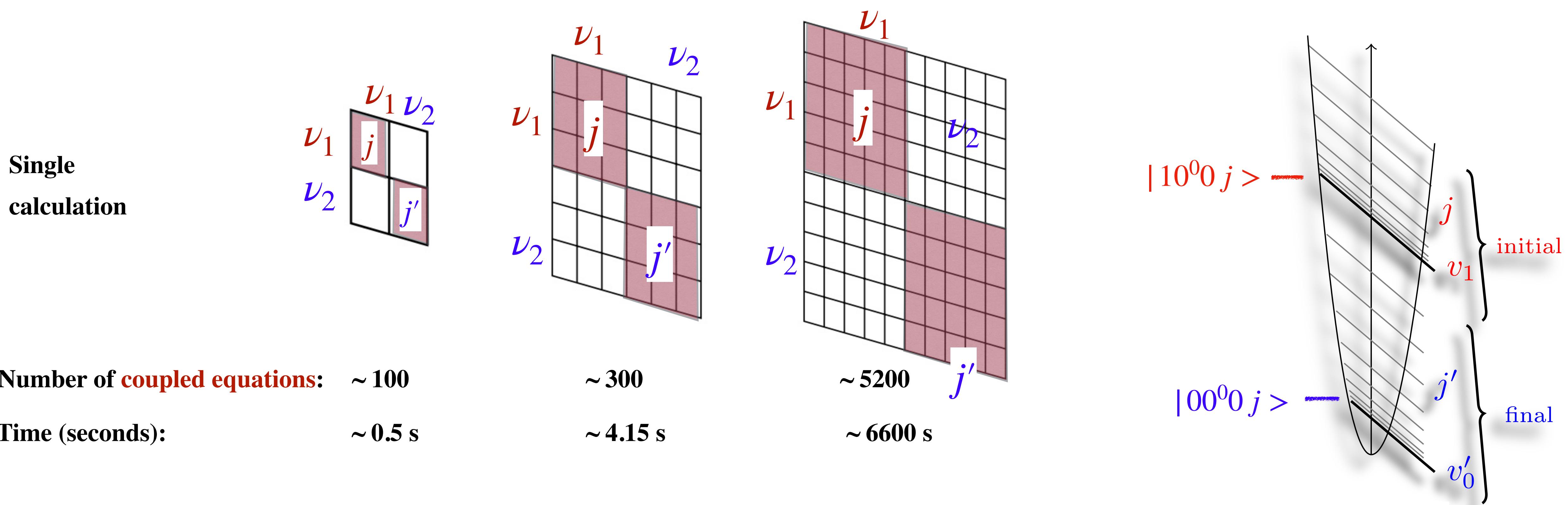


© Taha Selim

# | Computational complexity of molecular simulations >

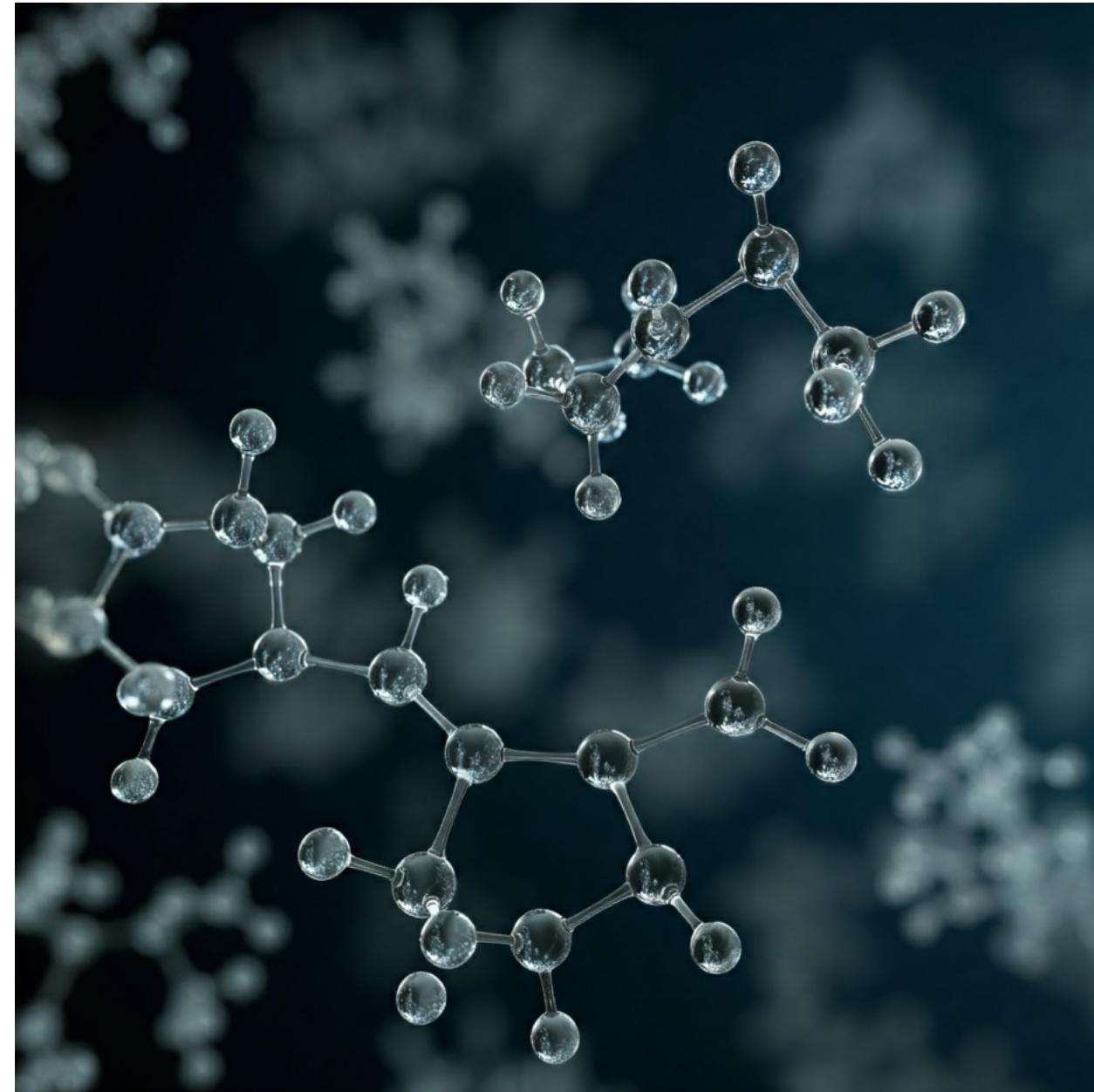
## Example: Rovibrational transitions in CO<sub>2</sub> induced by collisions with He

Time  $\propto$  (Number of coupled equations)<sup>3</sup>

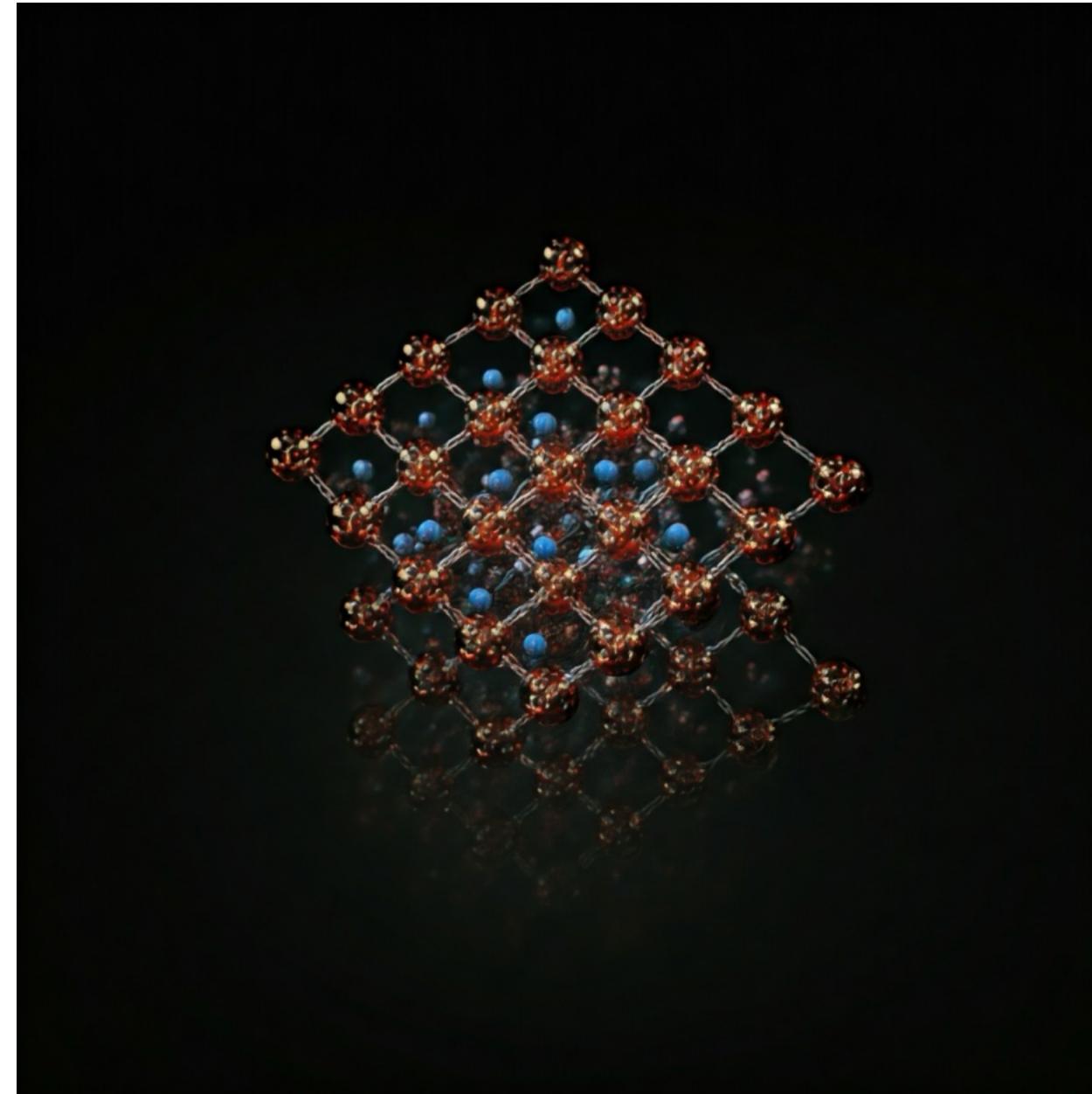


# | Overcoming computational challenges with Quantum Computing >

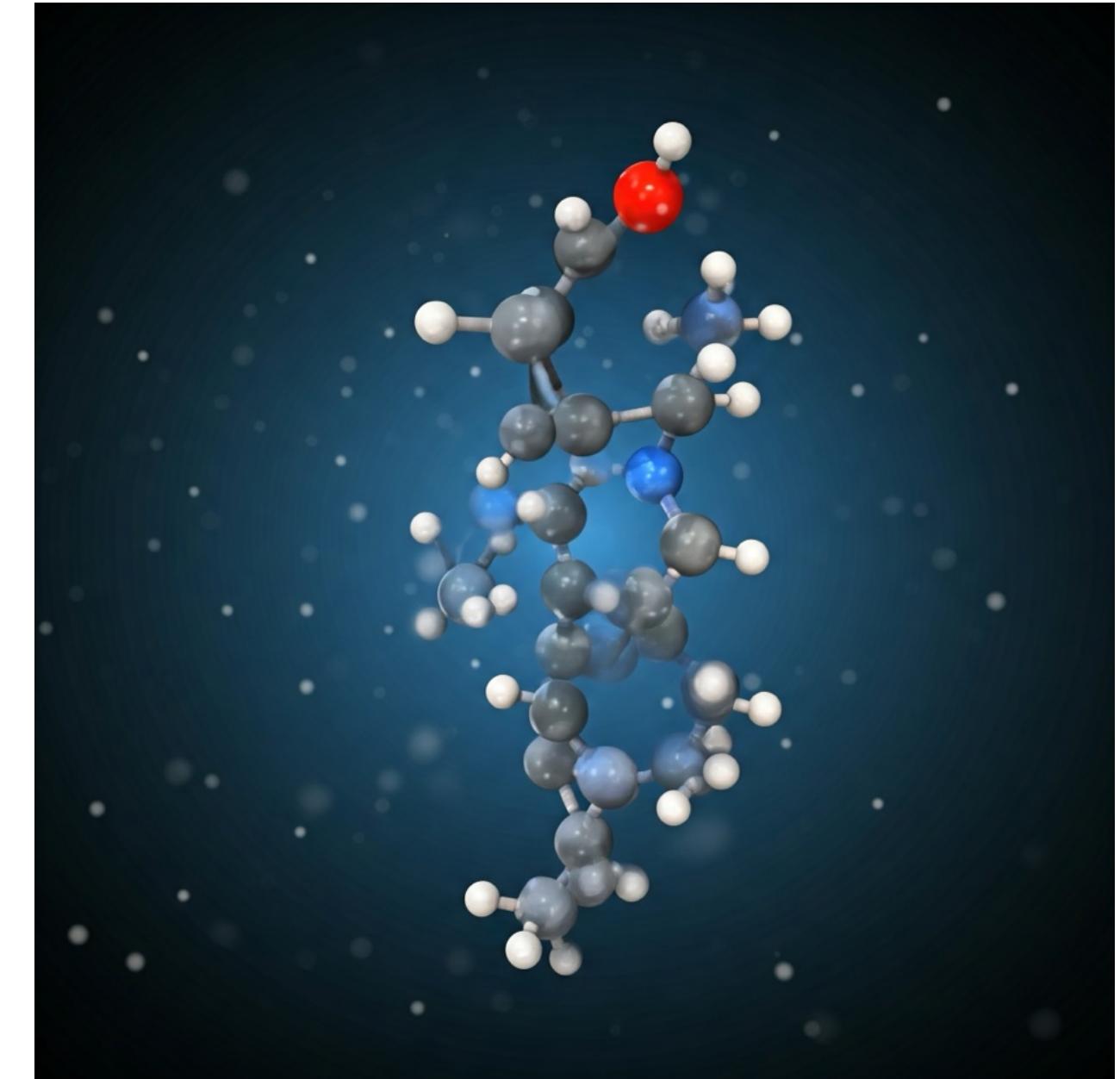
# | Computational complexity of molecular simulations >



Molecular Design



Material Design



Drug Design

**Require quantum chemistry calculations:**

**Examples:**

- Molecular dynamics simulations
- Molecular properties
- Electronic structure calculations

# | Classical computing vs. quantum computing >

Classical bits:

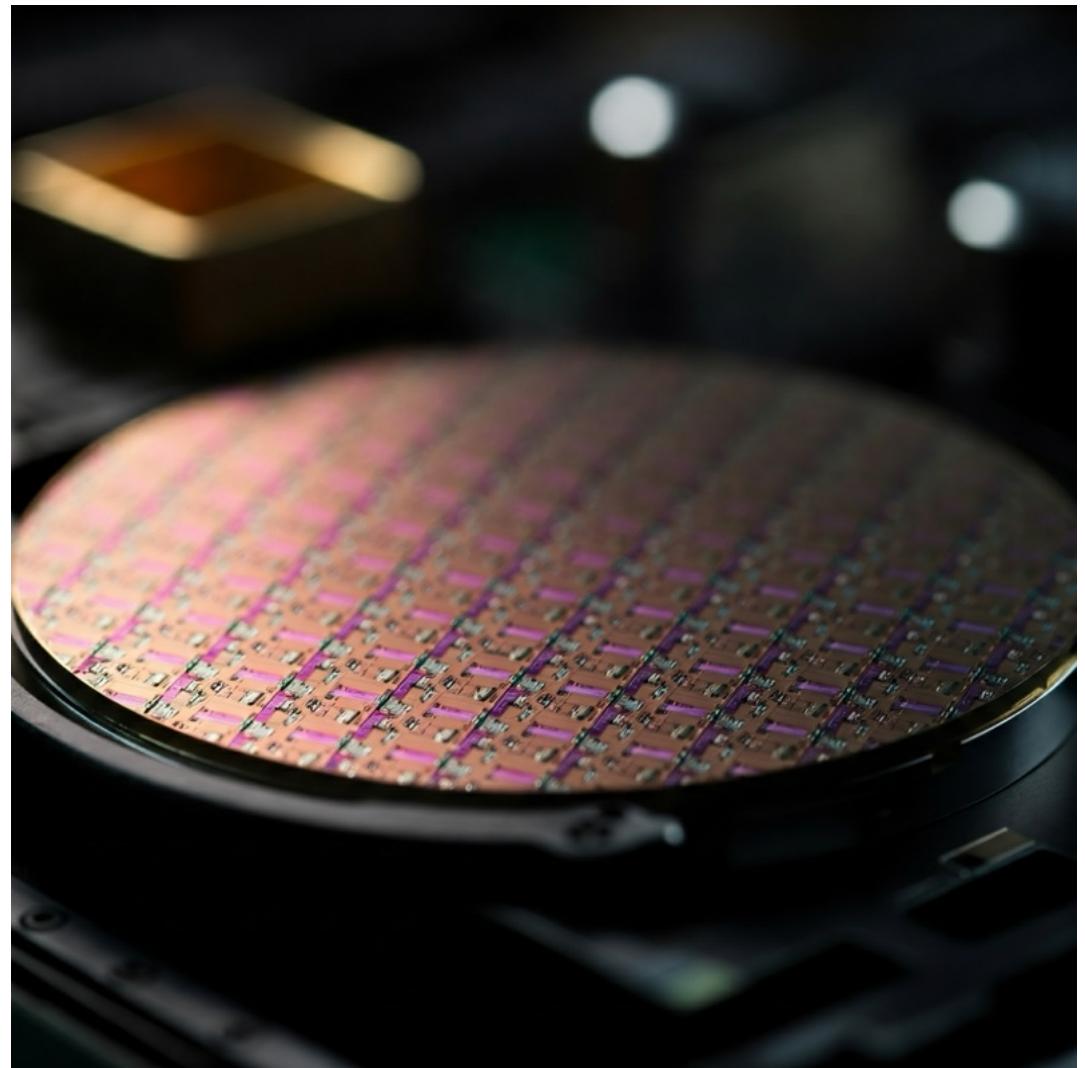
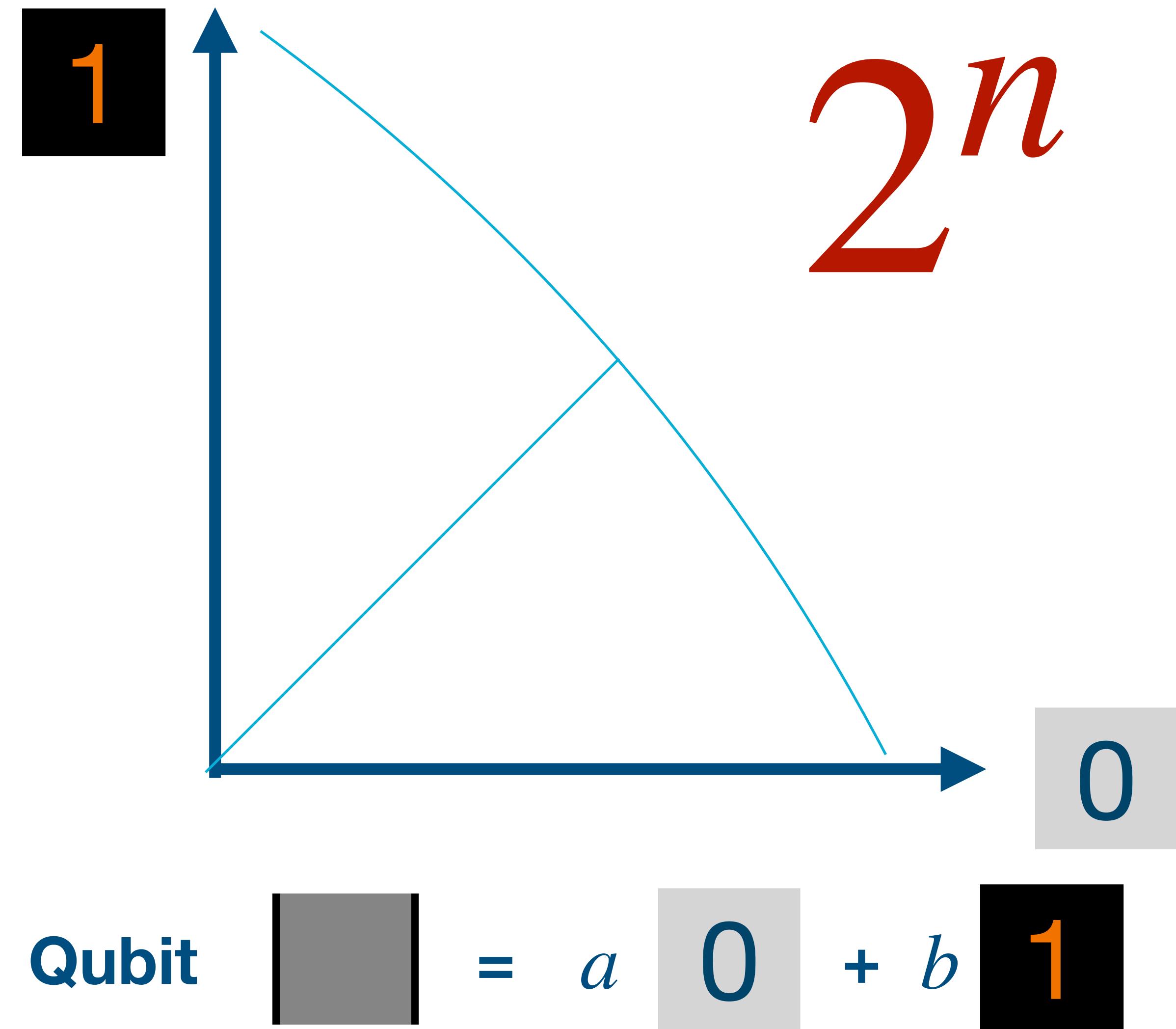


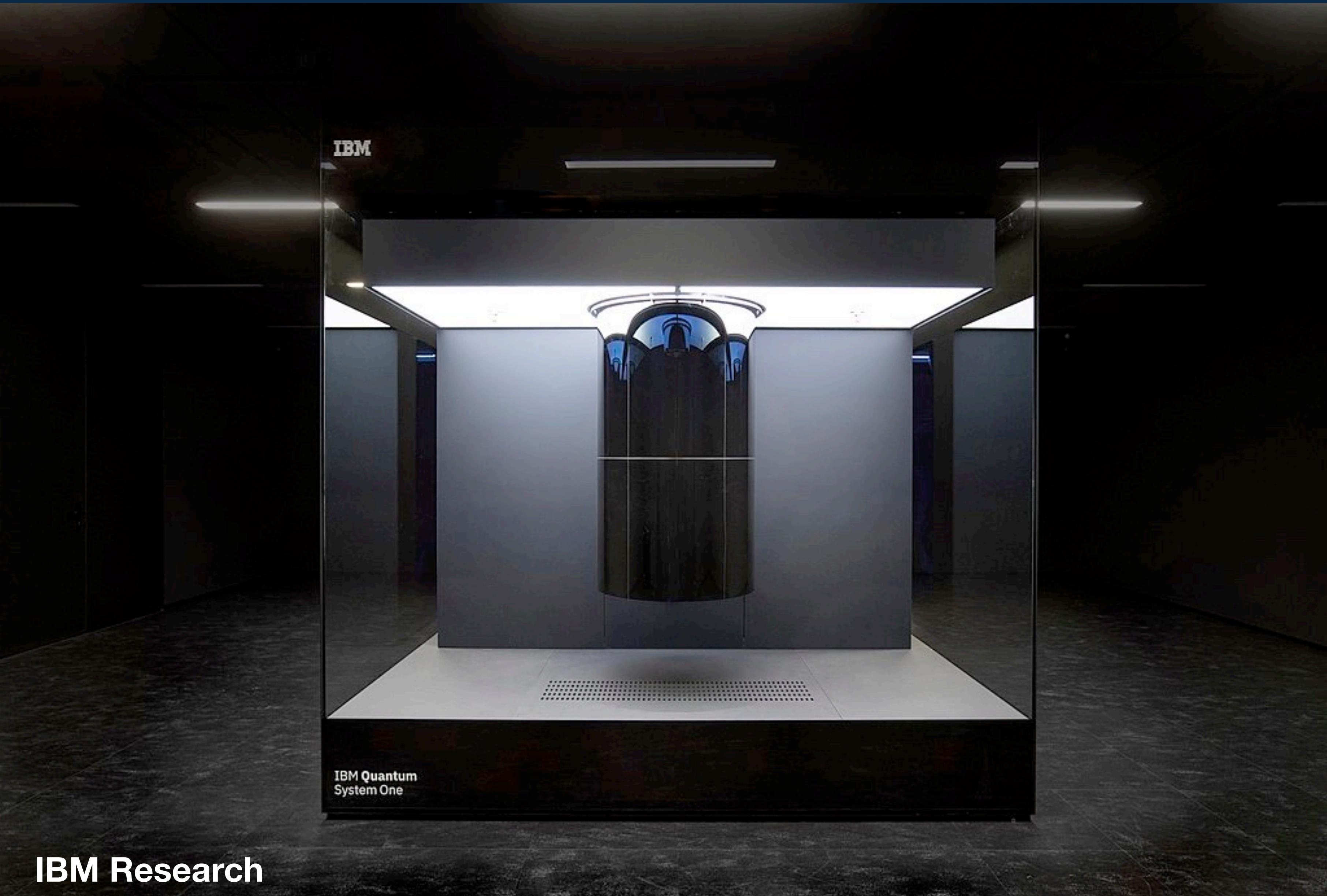
Illustration of a wafer

**Bit**      0      1

Quantum bits (qubits):



# | IBM quantum computer >



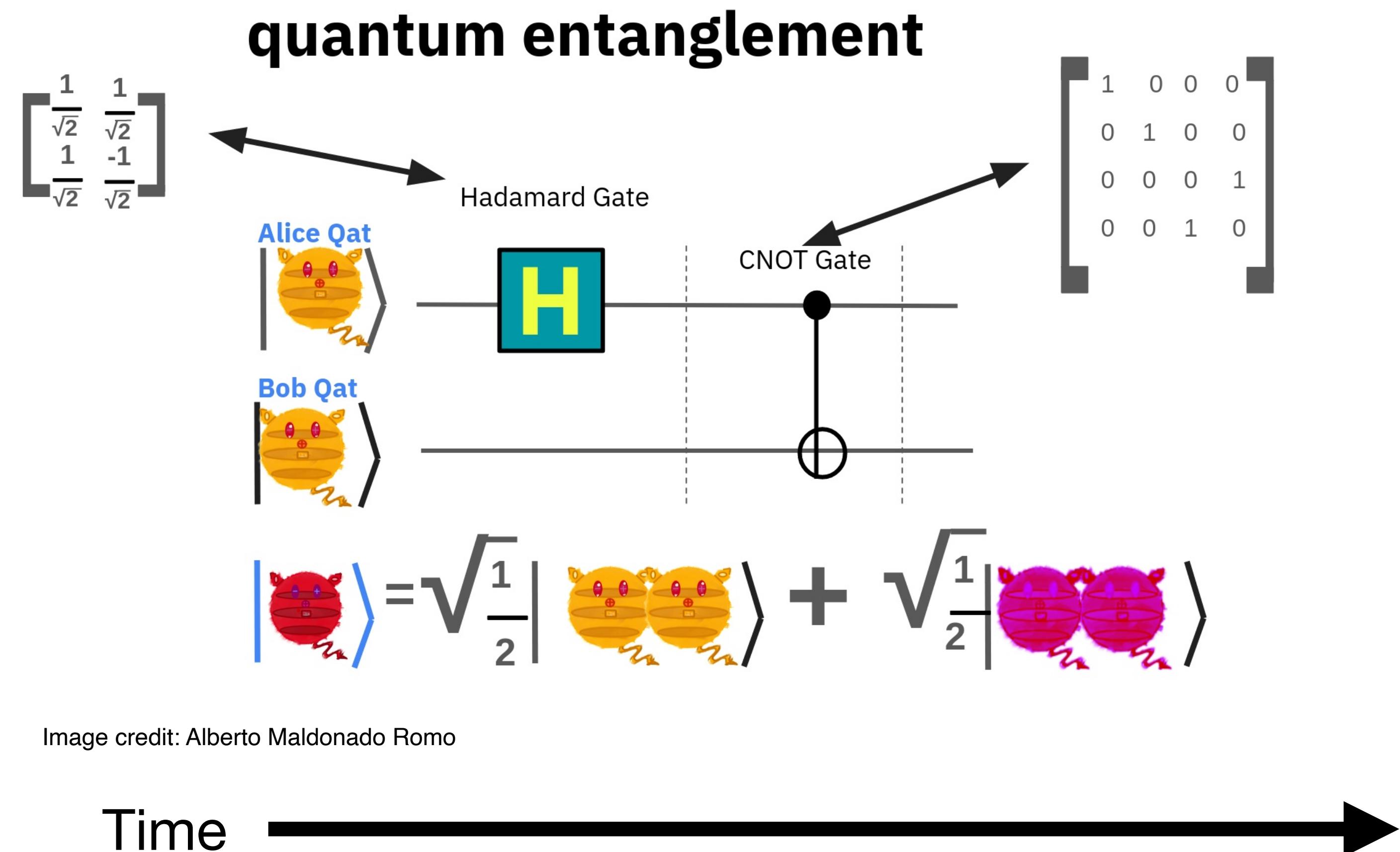
**IBM Research**

# | Quantum circuits >

A sequence of gates applied to a given quantum register of qubits:

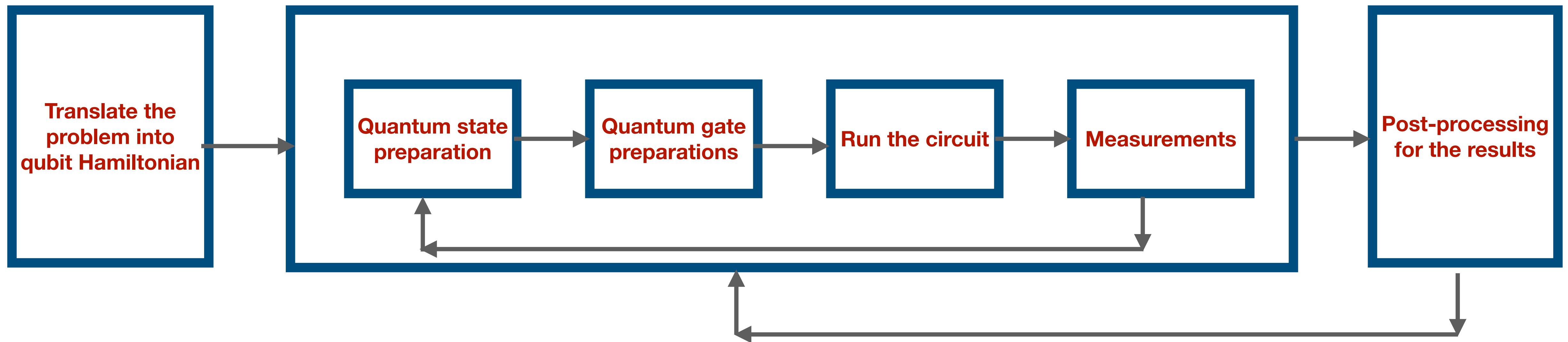


IBM Q



# | Quantum computing algorithm workflow >

**Software layer: adapt the problem by mapping it to quantum mechanical spin qubit Hamiltonian.**



**Hardware layer: translate the problem into qubits and quantum gates.**

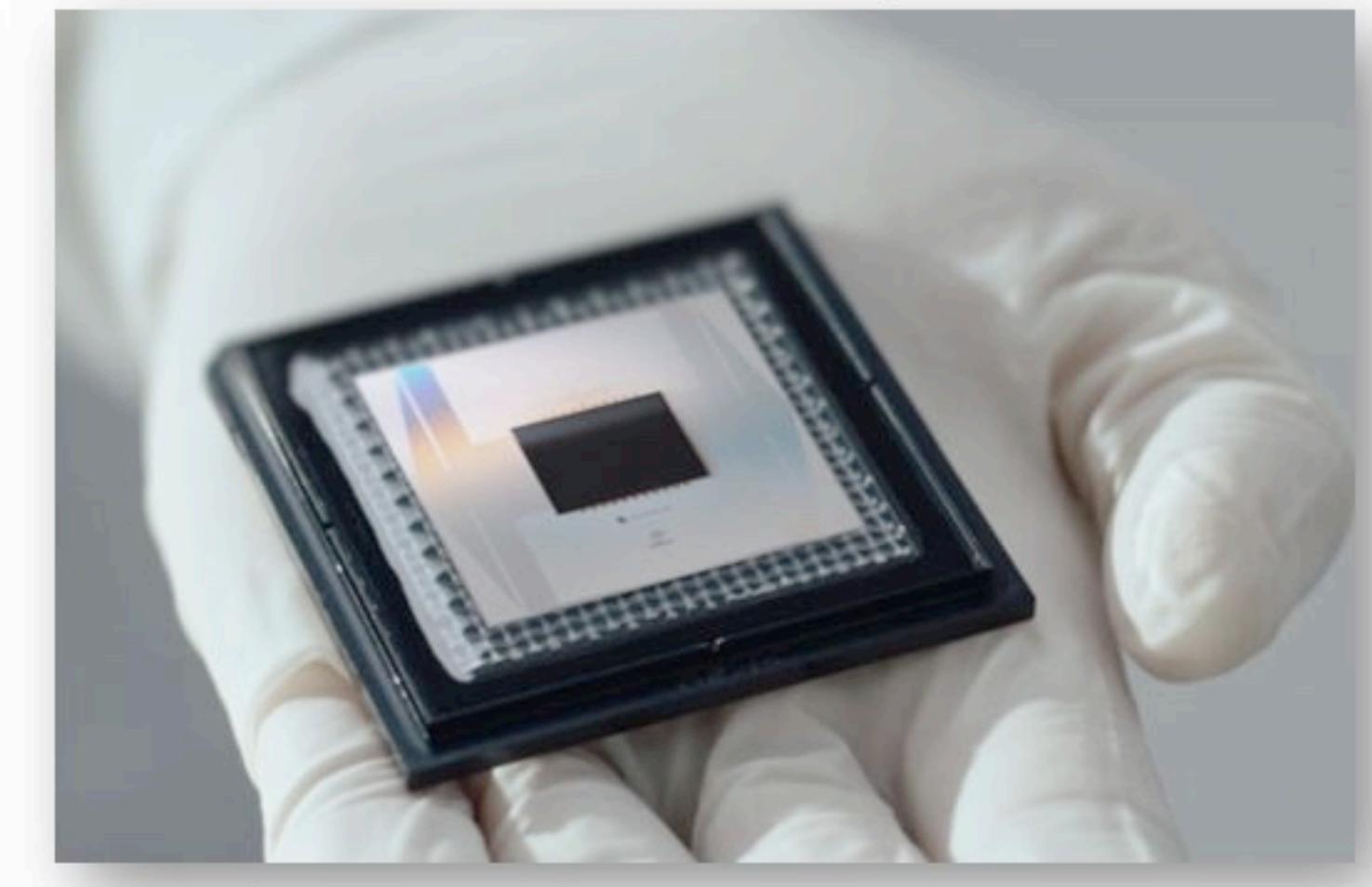
# | Available quantum computers, accessed via the cloud >

Different types of quantum computing, each has its own mechanism.



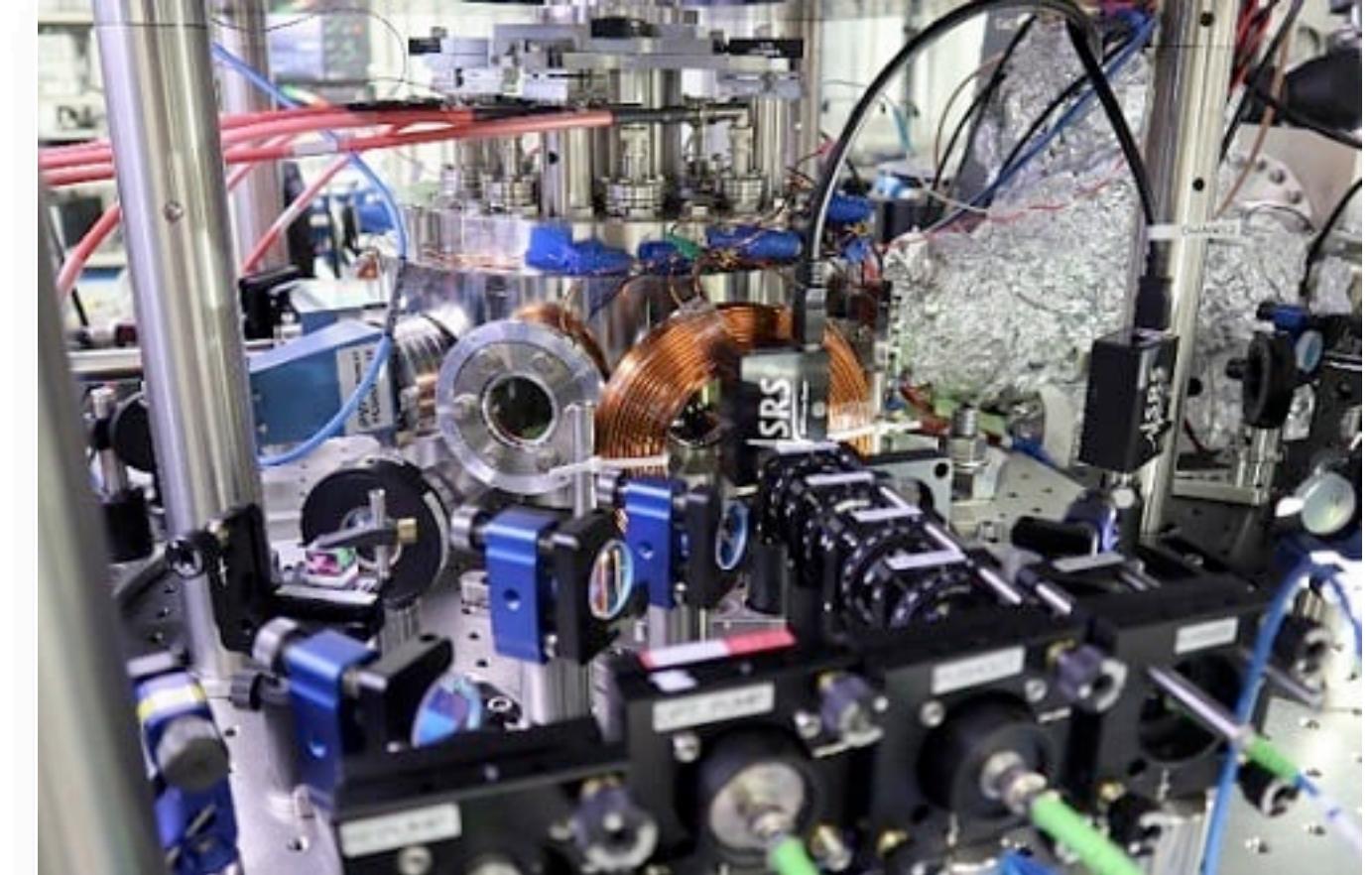
QuiX - <https://www.quixquantum.com/>

**Photonic quantum processor**



Google, new Willow chip

**Superconducting quantum processor**



*Kenji Ohmori group at the Institute for Molecular Science.  
Courtesy of Takafumi Tomita.*

**Ultracold neutral atoms  
quantum processor**

**Manufacturers of the same type have their own technologies as well.**

# | Available quantum computers, portable technologies >

# Different types of quantum computing, each has its own mechanism.



# SpinQ

# Nuclear Magnetic Resonance (MRI)

$\sim$  2 qubits

## - hard to scale



# Raspberry pi

# Quantum circuit emulator

~ 100 euros



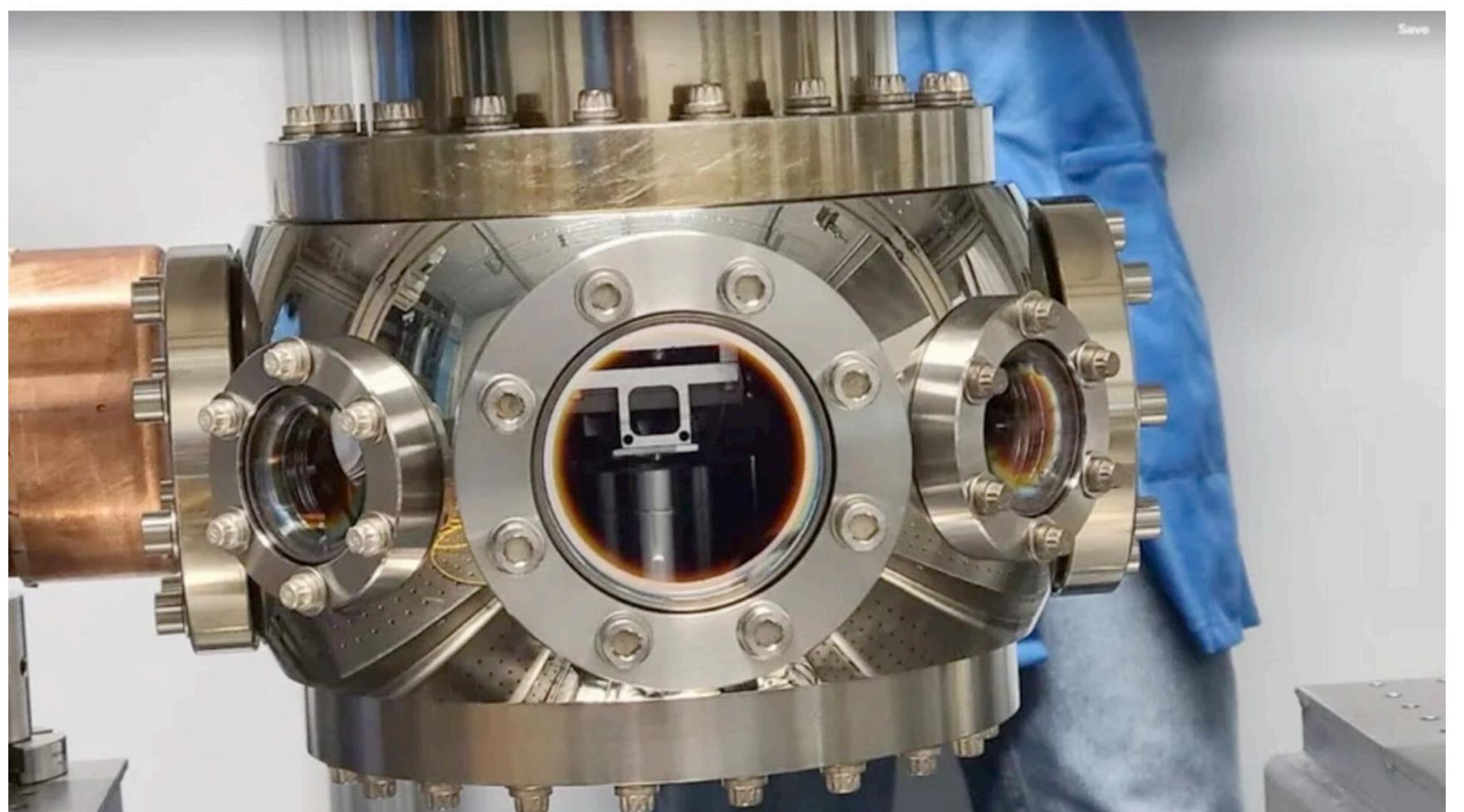
# NVIDIA Jetson Orin Nano Super Developer Kit

# Quantum circuit emulator + AI applications

~ 250 euros

# | Available quantum computers, portable technologies >

**Open Quantum Design (OQD), a non-profit based in Waterloo, is breaking down barriers to quantum computing with the release of the world's first open-source, full-stack trapped-ion quantum computer. This initiative grants free access to both hardware and software, empowering researchers, developers, and institutions globally to explore and contribute to the field.**



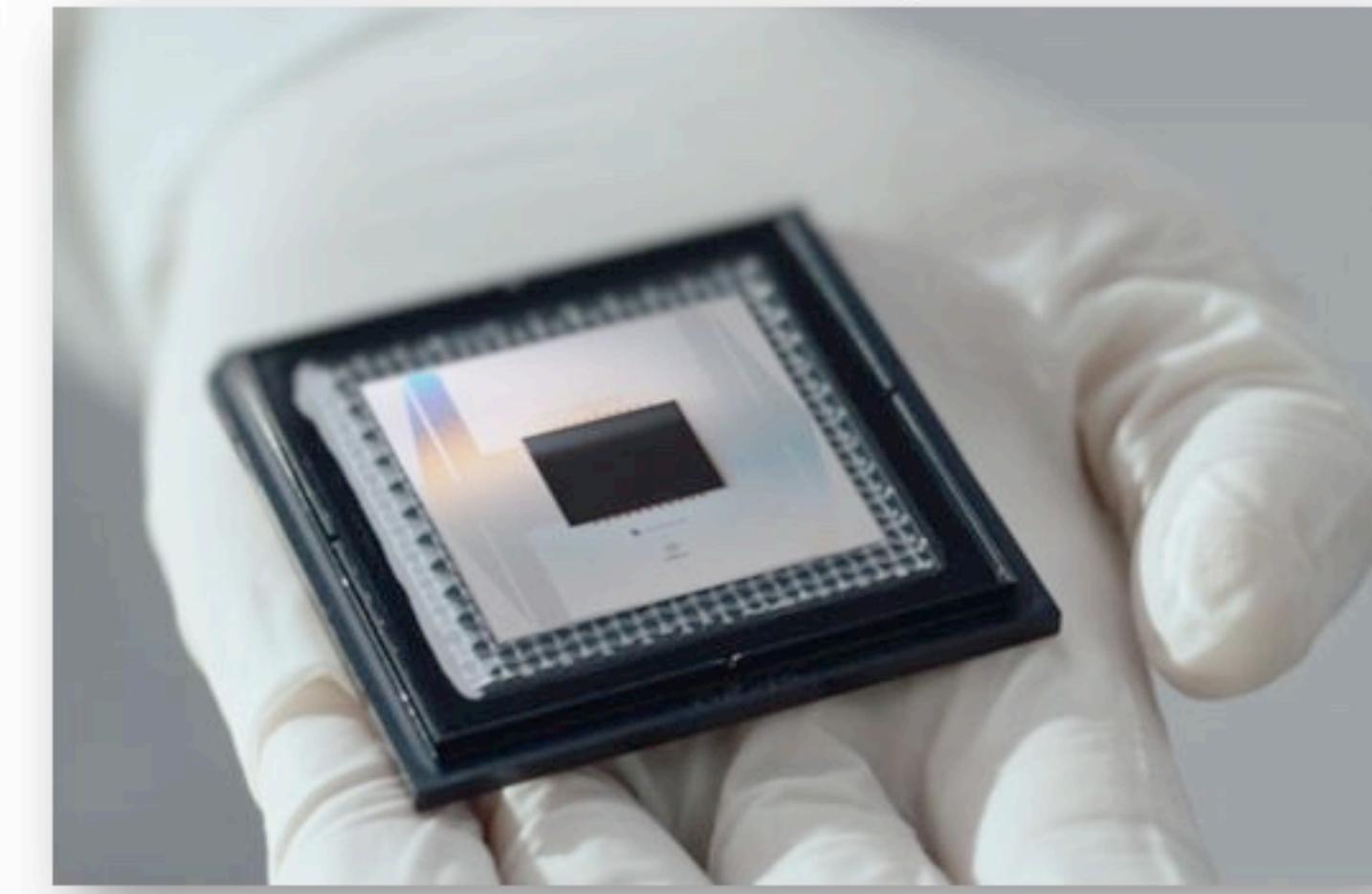
**World's first open-source trapped-ion quantum computer unveiled**

By Aman Tripathi

Jan 17, 2025 | 12:59 PM

## Sources of error in quantum computing:

- Environmental effect
- Unwanted interactions between qubits
- Imperfections in control mechanisms (electronics, readouts, ...etc)
- Fragilely of quantum states, decoherence



## Solution, error correction codes

- Example: surface code.
- Differs per technology.

## Google, new Willow chip

- Number of qubits: 105

### Chip 1

- Single-qubit gate error<sup>1</sup> (mean, simultaneous):  $0.035\% \pm 0.029\%$
- Two-qubit gate error<sup>1</sup> (mean, simultaneous):  $0.33\% \pm 0.18\%$  (CZ)

### Chip 2

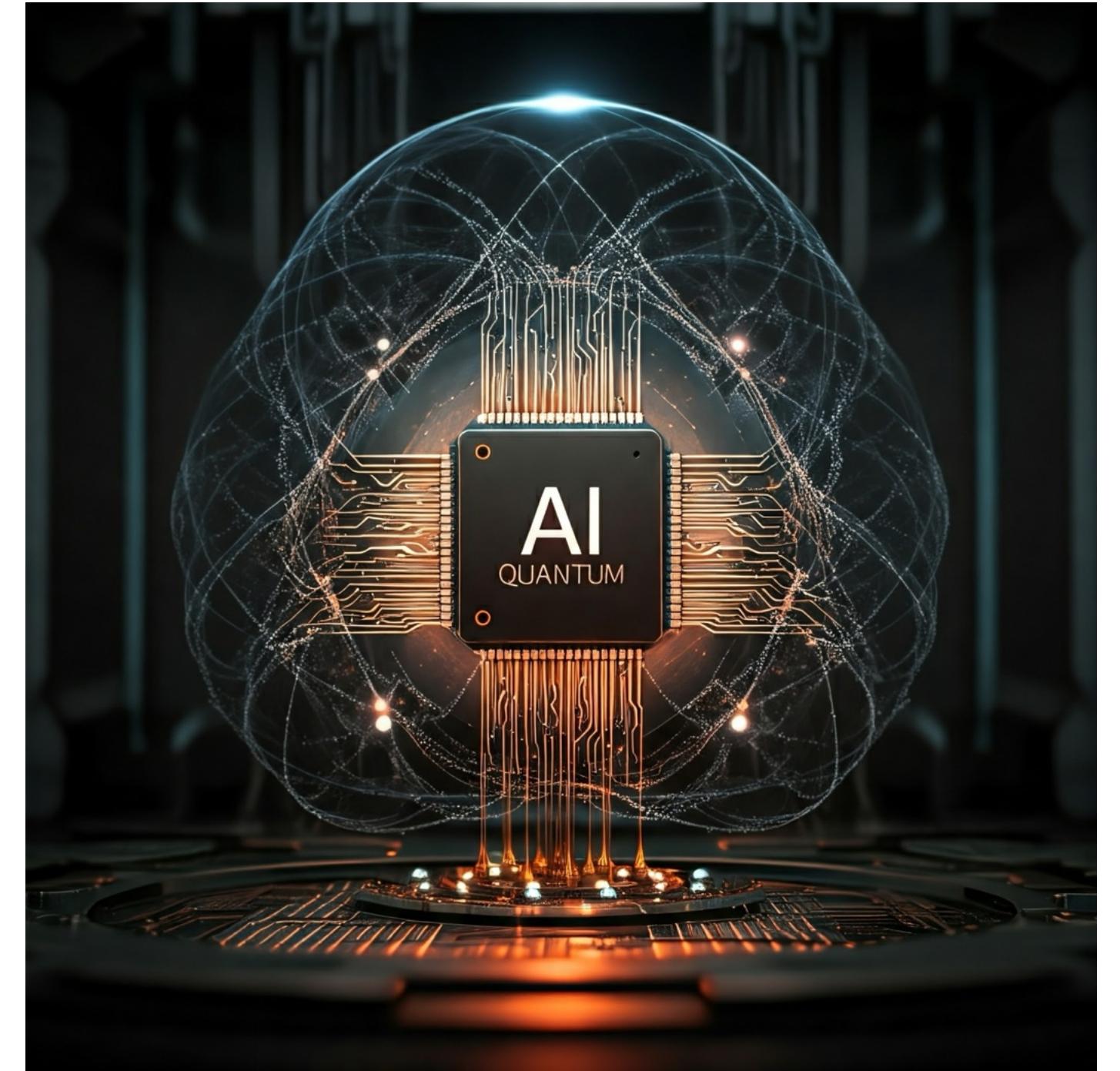
- Single-qubit gate error<sup>1</sup> (mean, simultaneous):  $0.036\% \pm 0.013\%$
- Two-qubit gate error<sup>1</sup> (mean, simultaneous):  $0.14\% \pm 0.052\%$  (iswap-like)
- Measurement error (mean, simultaneous):  $0.67\% \pm 0.51\%$  (terminal, all qubits)

Computing power:  $1.05 \times 10^{30}$

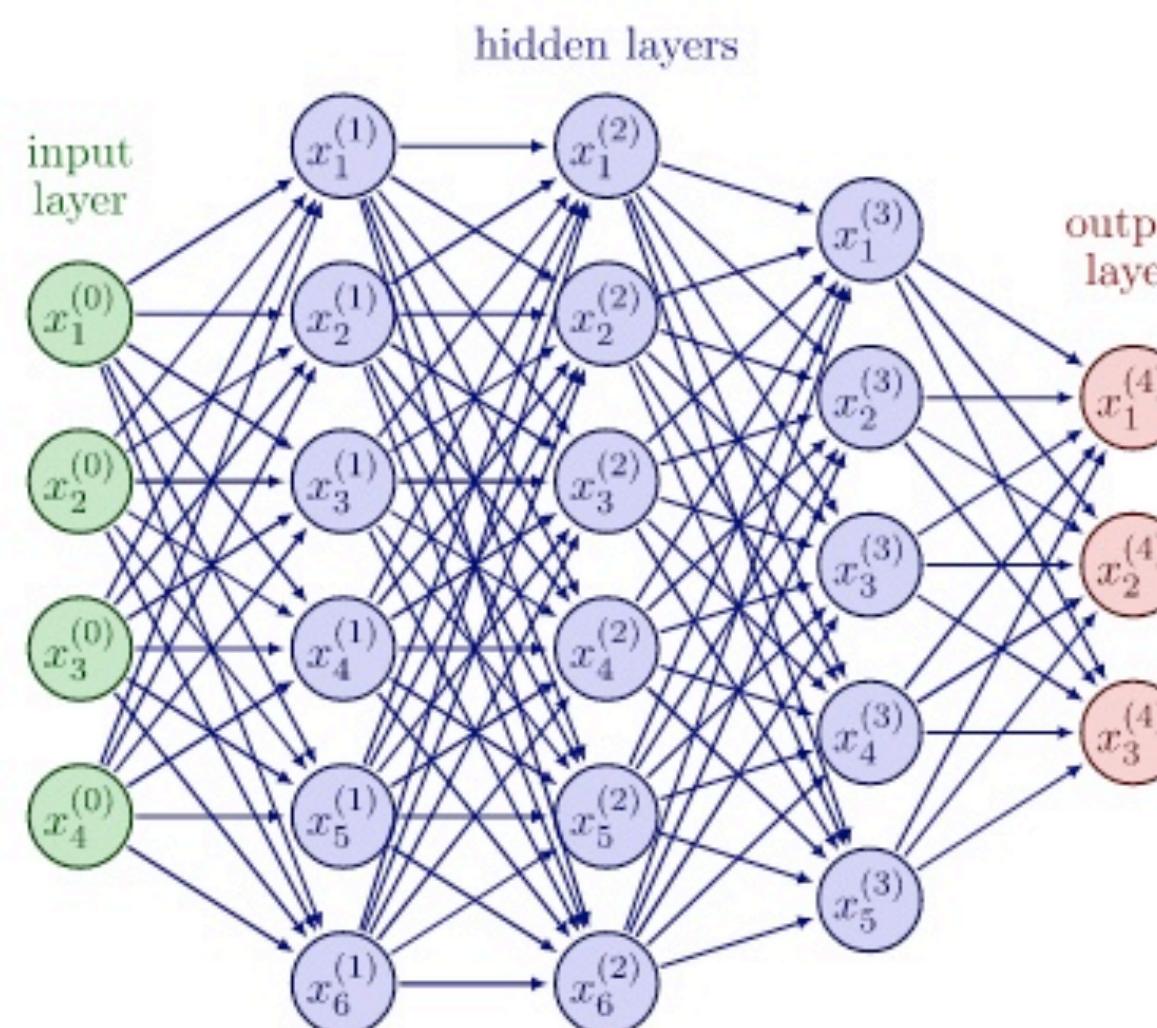
| Overcoming computational challenges with Physics-inspired (quantum)AI >

AI helps in translating the quantum algorithm into hardware efficiently:

- **Improved Quantum Algorithm Design:** replace parts of the algorithm with physics-informed AI agents, (function approximators).
- **Efficient Quantum Circuit Optimization:** optimize the mapping to qubits; reduce the number of gates leading to substantially improve the efficiency of the quantum circuits.
- **Accelerated Quantum Simulations:** accelerate the simulation of quantum systems, enabling researchers to study complex phenomena and design new materials.
- **Enhanced Quantum Error Correction:** assist developing more robust error correction techniques.



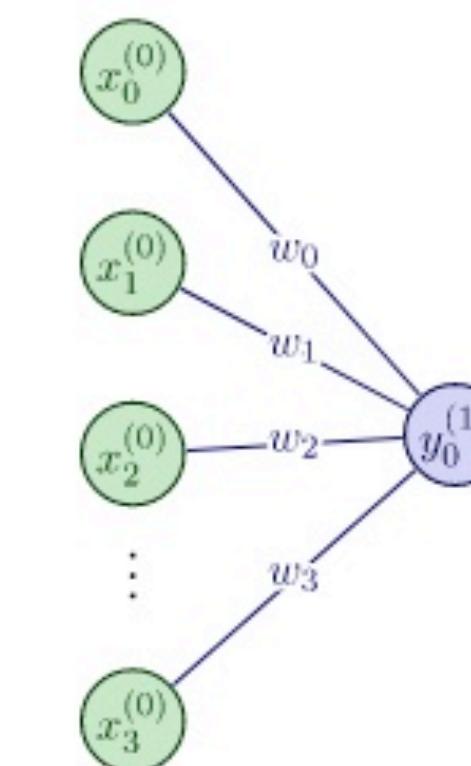
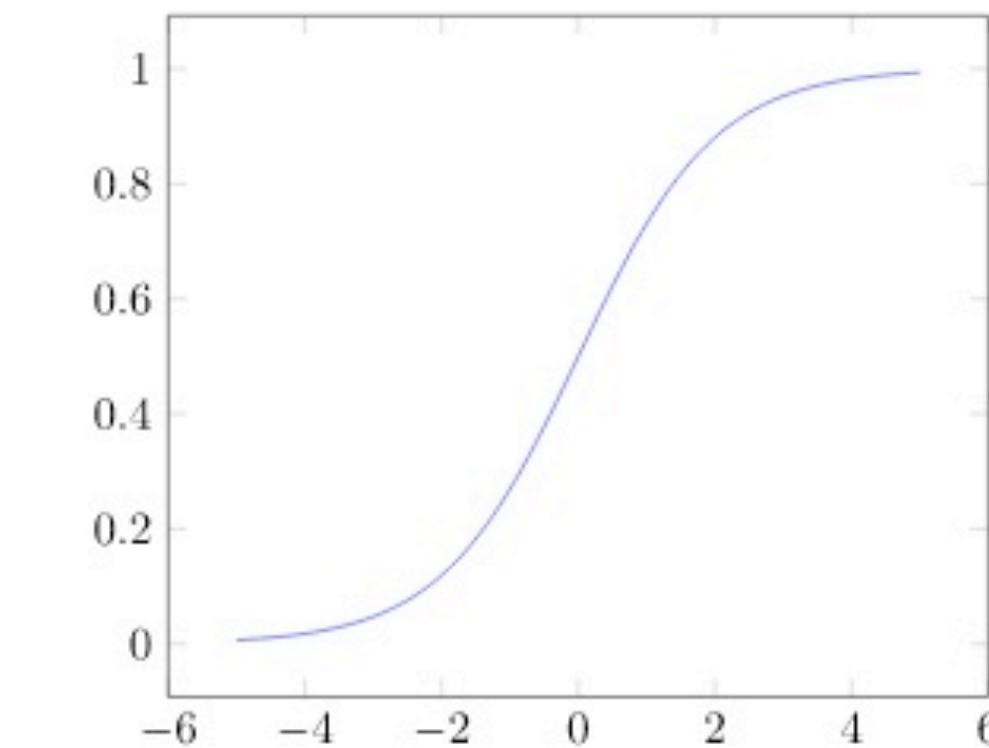
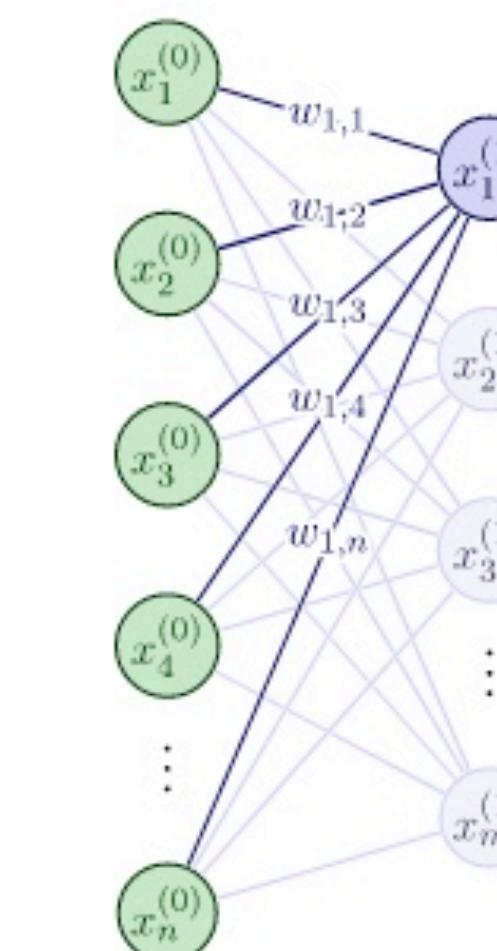
# The Universal Approximation Theorem



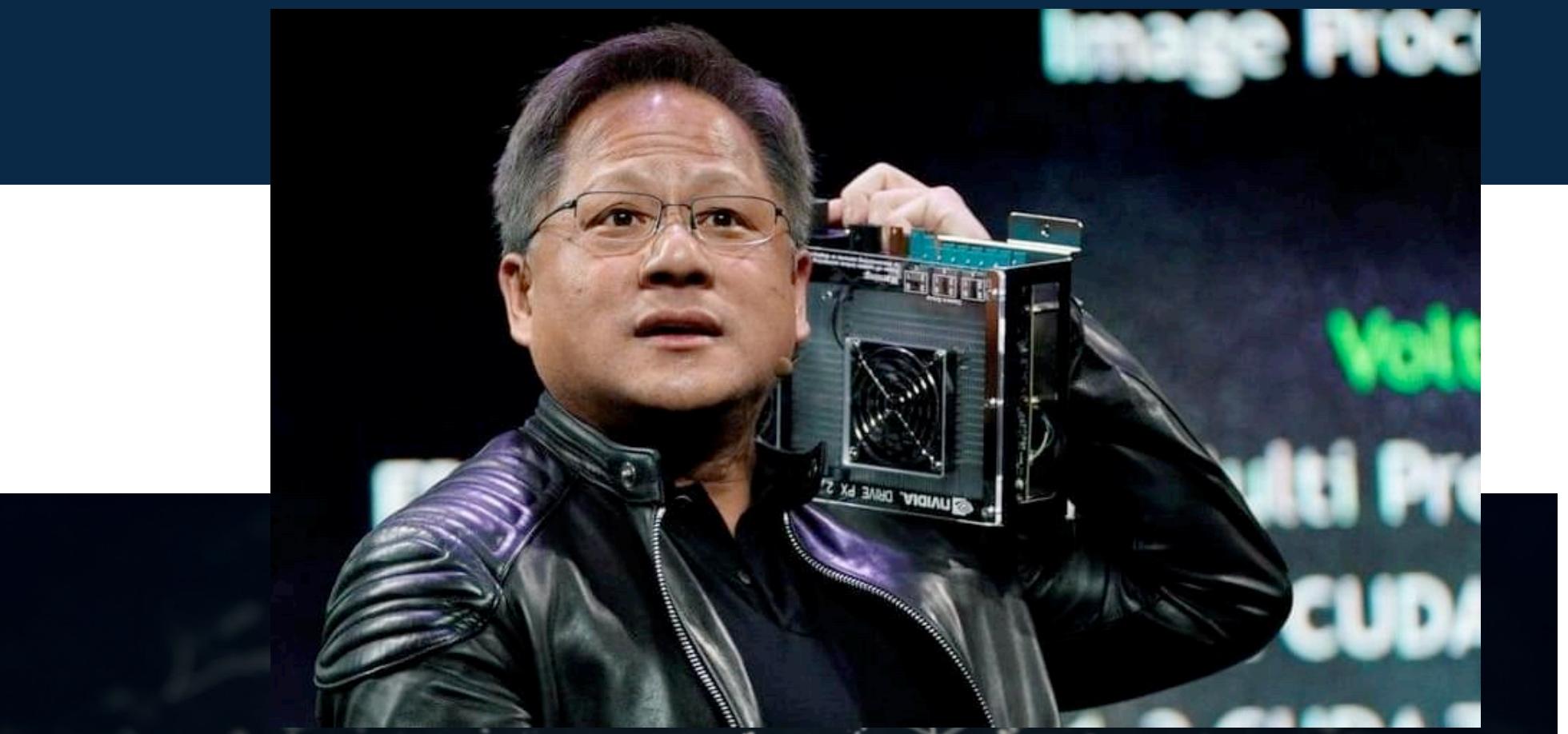
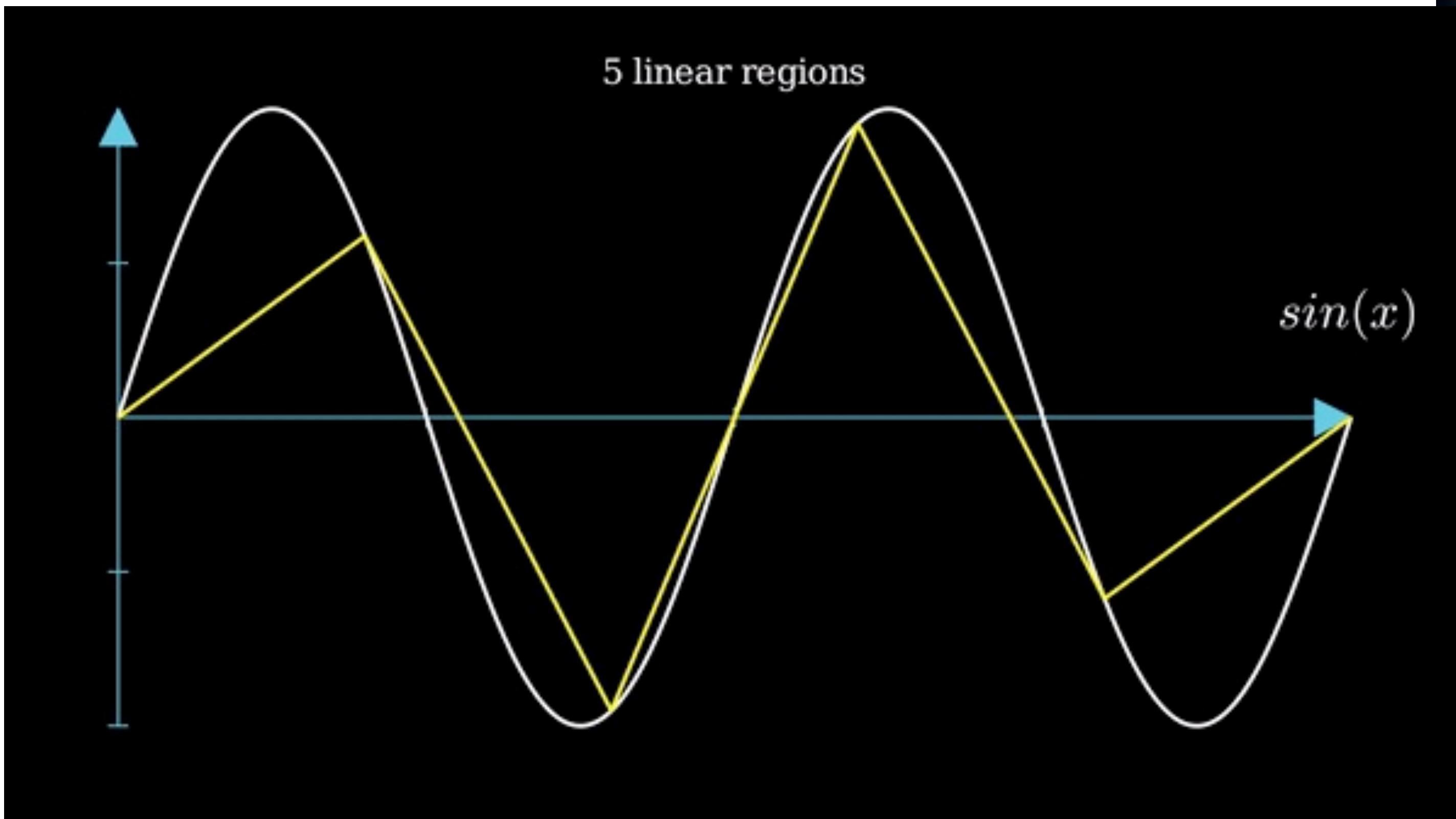
$$W^{(l)} = \begin{pmatrix} w_{1,1}^{(l)} & w_{1,2}^{(l)} & \dots & w_{1,n}^{(l)} \\ w_{2,1}^{(l)} & w_{2,2}^{(l)} & \dots & w_{2,n}^{(l)} \\ \dots & \dots & \ddots & \dots \\ w_{m,1}^{(l)} & w_{m,2}^{(l)} & \dots & w_{m,n}^{(l)} \end{pmatrix}$$

$$\begin{aligned} \psi(x) &:= \sigma \left( \sum_{i=1}^n x_i w_i - b \right) \\ &= \sigma(\underbrace{w^\top \bullet x - b}_{\in \mathbb{R}}), \end{aligned}$$

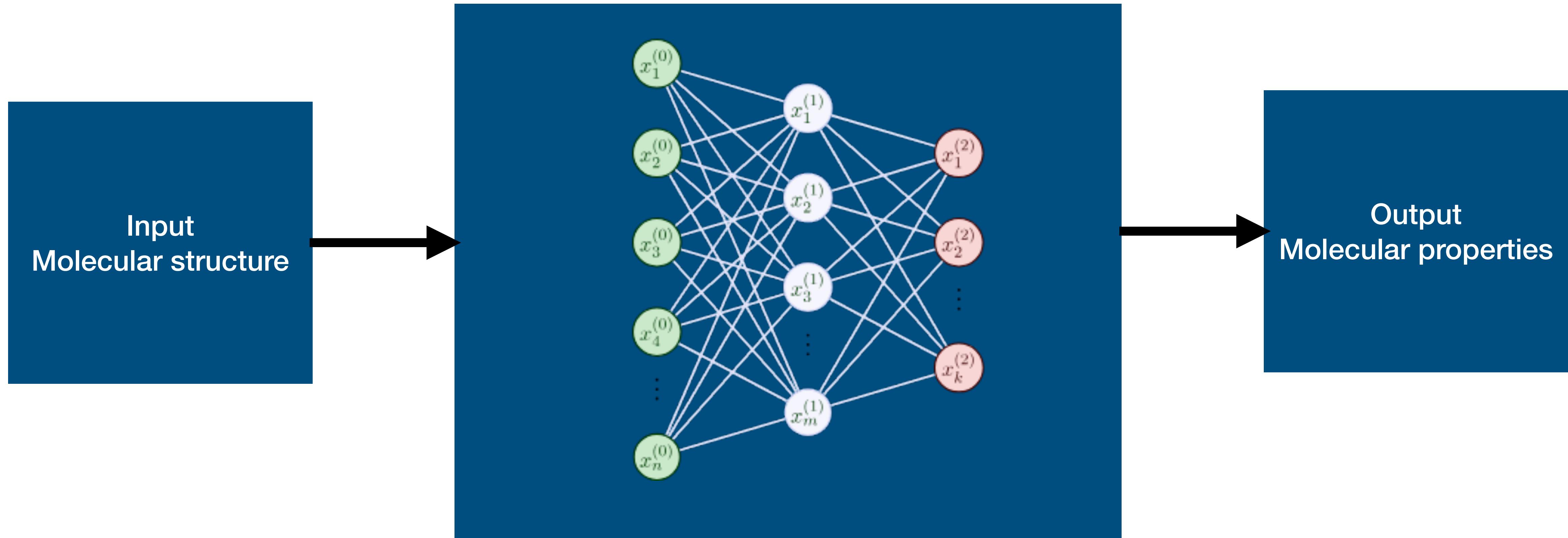
$$\int_{x \in \mathbb{R}^n} \sigma(w^\top x - b) d\mu(x) = 0 \quad \forall w \in \mathbb{R}^n, b \in \mathbb{R}$$



# Universal function approximator >



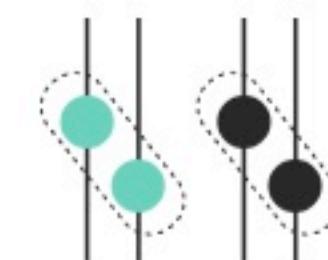
# | Universal function approximator >



- Examples: approximating physical laws, physical structure!

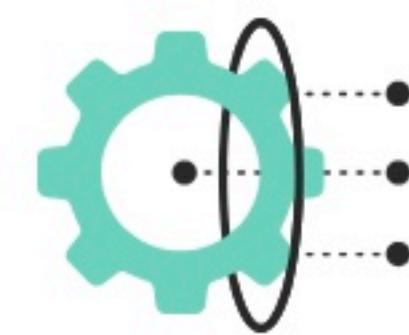
# Quantinuum Announces Generative Quantum AI Breakthrough with Massive Commercial Potential

Quantinuum Unveils Generative Quantum AI Framework that Harnesses Unique Quantum-Generated Data to Tackle Complex Problems Impossible for Classical Computing



## Compositional Intelligence

We are developing a new kind of AI—compositional intelligence—that promises to tackle some of the biggest outstanding problems in the field, such as interpretability.

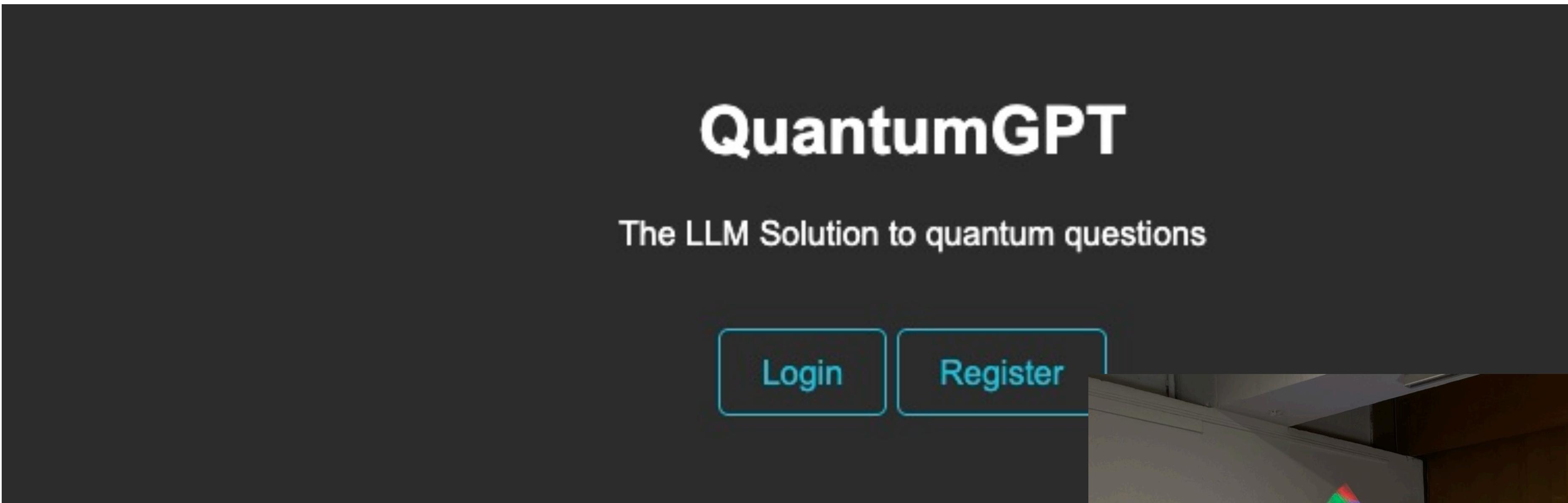


## AI/Machine Learning

Quantum AI and machine learning will look a lot different from the classical AI we're used to. Our team remains on the cutting-edge of this emerging field.

<https://www.quantinuum.com/press-releases/quantinuum-announces-generative-quantum-ai-breakthrough-with-massive-commercial-potential>

# | QuantumGPT: LLM-based solutions for quantum problems >



[/https://www.quantumgpt.science](https://www.quantumgpt.science)



# Advanced machine-learning algorithms for protein structure >

ARTICLE · Volume 9, Issue 7, P1828-1849, July 13, 2023 · [Open Archive](#)

[Download Full Issue](#)

## Generative design of *de novo* proteins based on secondary-structure constraints using an attention-based diffusion model

Bo Ni<sup>1</sup> · David L. Kaplan<sup>2</sup> · Markus J. Buehler<sup>1,3,4</sup>

Affiliations & Notes ▾ Article Info ▾

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### » The bigger picture

The design of *de novo* protein sequences has great potential in achieving superior combinations of novel functions and mechanical properties beyond known, natural proteins. However, the tremendous number of possible sequences and the cost of experimental testing make the effective search and validation of superior *de novo* protein candidates extremely challenging. Here, we leverage a diffusion-model-based deep-learning framework to efficiently generate novel protein sequences that meet a desired overall secondary-structure fractional content or per-residue type of secondary structure. The generated sequences show novelty beyond existing, natural ones. By robustly generating various novel sequences with the desired structural features, our model provides rapid strategies for a target-guided *de novo* protein design that leads to novel discoveries of superior protein materials for various biological and engineering applications and can be extended for other design objectives in future work.

### AI system can generate novel proteins that meet structural design targets

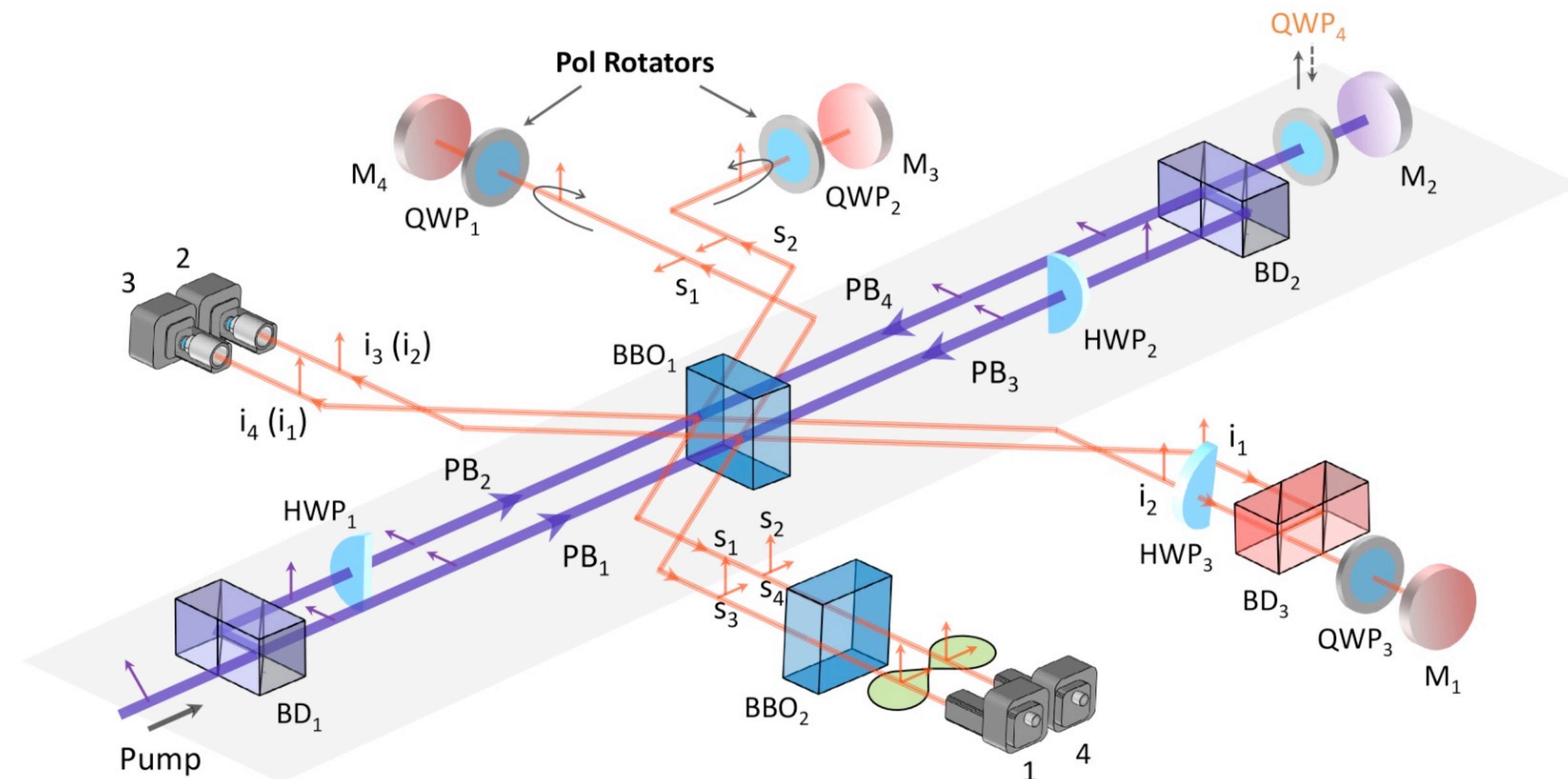
These tunable proteins could be used to create new materials with specific mechanical properties, like toughness or flexibility.

Adam Zewe | MIT News Office  
April 20, 2023



<https://linkinghub.elsevier.com/retrieve/pii/S2451929423001390>

# | Re-design quantum entanglement experimental protocol >



[PyTheus](#)

<https://journals.aps.org/prl/abstract/10.1103/PhysRevLett.133.233601>

<https://www.newscientist.com/article/2459102-ai-found-a-new-way-to-create-quantum-entanglement/>

NewScientist

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Enter search keywords

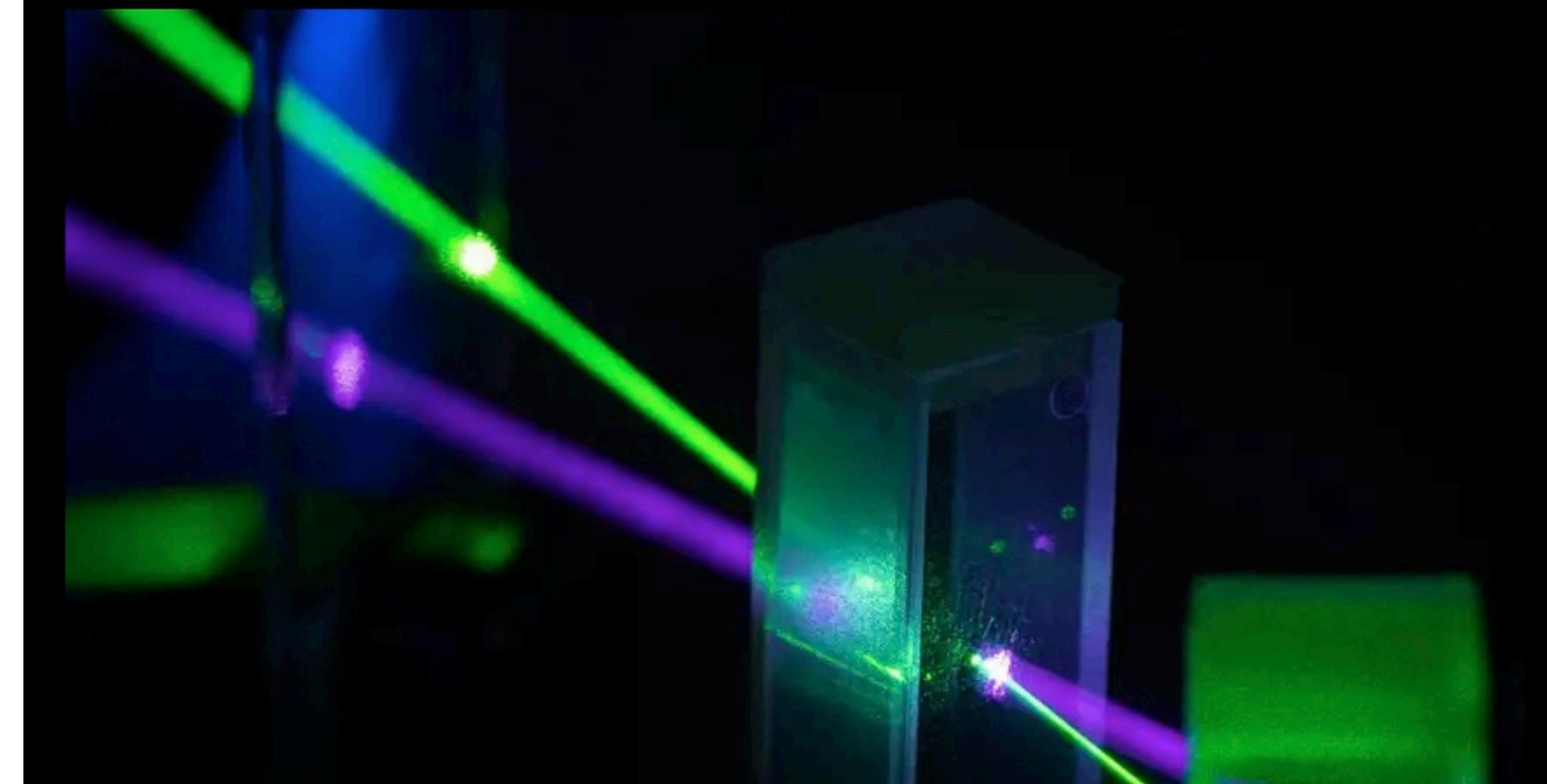
Physics

## AI found a new way to create quantum entanglement

In a surprise discovery, researchers found a new way to generate quantum entanglement for particles of light, which could make building quantum information networks easier

By Karmela Padavic-Callaghan

6 December 2024



## | Quantum AI community building >

# QUANTUM COMPUTING & AI

The banner features a dark blue background with a wavy teal line at the top. The title 'QUANTUM COMPUTING & AI' is in large, bold, teal letters. Below the title are five circular portraits of speakers, each with their name and title below it. To the right, there's a QR code, the date and time 'DEC 19<sup>TH</sup>, 2024 19:00-22:00 EET', and a 'REGISTER NOW' button. Logos for Bibliotheca Alexandrina and iQafé are at the bottom.

**Youssef Eldakar**  
Head, International School of Information Science  
Bibliotheca Alexandrina

**Dr. Taha Selim**  
Directeur Général, MolKit SAS

**Prof. Dr. Ahmed Younes**  
Professor of Quantum Computing  
Alexandria University

**Alain Chancé**  
Président, MolKit SAS

**Jan Blommaart**  
Managing Partner, BioDAC

**Prof. Dr. Ahmed Shawky Moussa**  
Professor of Computing and Computational Science  
Cairo University

DEC 19<sup>TH</sup>, 2024  
19:00-22:00 EET

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iQafé

## **Outreach:**

- Public lectures and demonstrations to raise awareness.
- School visits and workshops to engage students.
- Online resources and tutorials for self-learning.

## **Hackathons:**

- Quantum coding challenges to foster innovation.
- Collaborative projects to solve real-world problems.
- Mentorship and networking opportunities.

## **Summer Schools:**

- Intensive courses on quantum computing fundamentals.
- Hands-on experience with quantum hardware and software.
- Interaction with leading researchers in the field.

## **Virtual Labs:**

- Online platforms for simulating quantum computers.
- Access to real quantum devices remotely.
- Experimentation and algorithm development tools.

## **Community Building:**

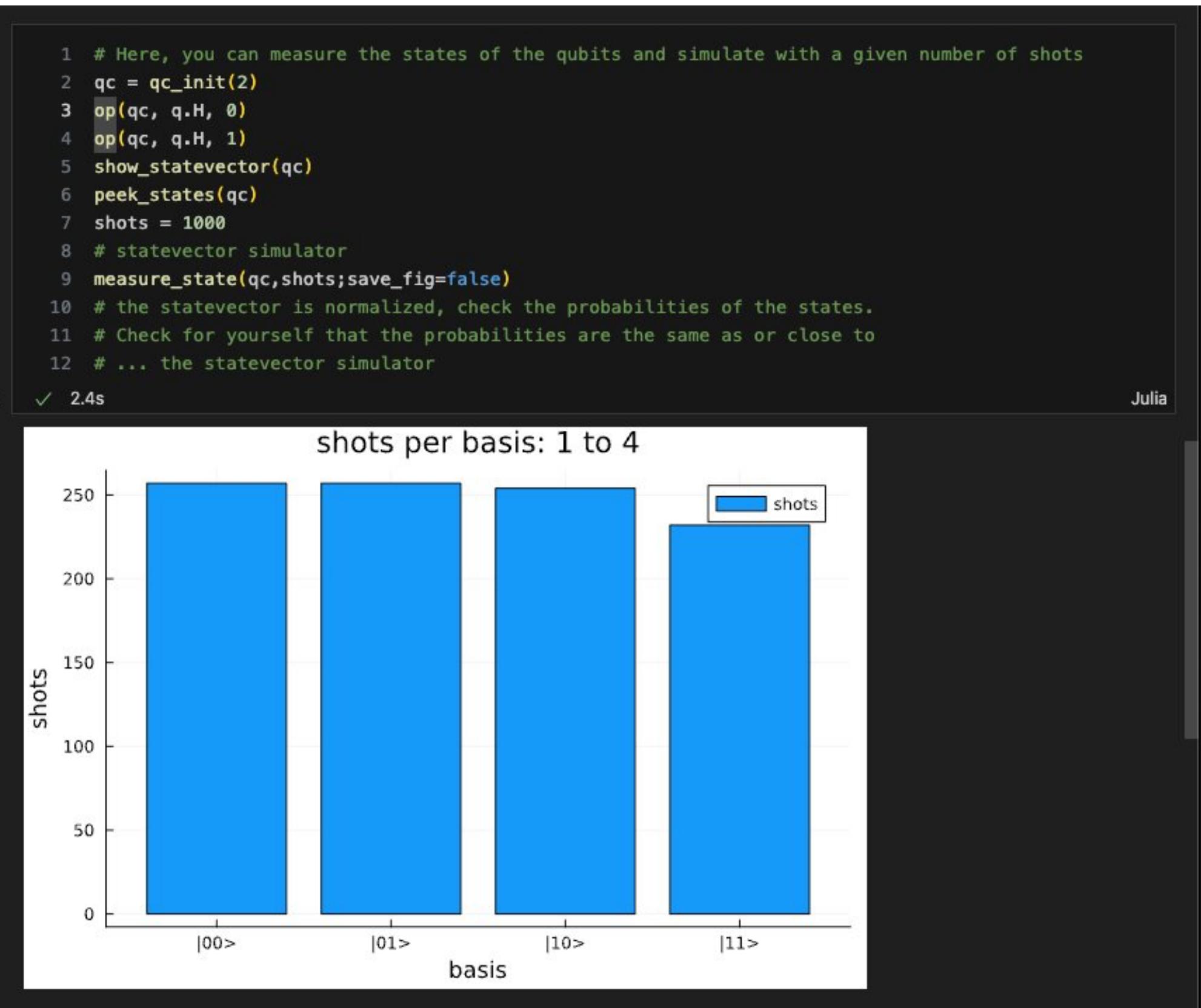
- Online forums and discussion groups.
- Conferences and meetups for knowledge sharing.
- Support for local quantum computing initiatives.

## Our own optimized Julia-based quantum simulator for chemistry and quantum molecular sensing simulations.

```

1 # create a quantum circuit with 3 qubits
2 qc = qc_init(3)
3 # create a given state on q_0
4 op(qc, q.X, 0)
5 op(qc, q.H, 0)
6 # create bell pair
7 op(qc, q.H, 1)
8 op(qc, q.X, 2, q1_control = 1)
9 # reverse the operation of the bell pair
10 op(qc, q.X, 1, q1_control = 0)
11 op(qc, q.H, 0)
12 # qubits 0 and 1 are measured
13 qubits = [0,1] # qubits to measure
14 bas = "Zbas" # basis to measure
15

```



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MolKet's cloud:  
[www.molket.io](http://www.molket.io)

GitHub:  
[molket-io/molket.jl](https://github.com/molket-io/molket.jl)

**mol|ket**>

## | References >

Bernardini, F., Huerta Alderete, C., & Korenkevych, D. (2023). Quantum computing with trapped ions: A beginner's guide. *arXiv preprint arXiv:2303.16358*.  
<https://arxiv.org/abs/2303.16358>

"Trapped ion quantum computers" from the PennyLane website provides a comprehensive overview of trapped ion technology, including qubit manipulation, gate implementation, and the strengths and challenges of this quantum computing platform. [https://pennylane.ai/qml/demos/tutorial\\_trapped\\_ions](https://pennylane.ai/qml/demos/tutorial_trapped_ions)

Google's Willow quantum processor, featuring improved qubit connectivity and reduced error rates, represents a significant advancement in quantum computing technology, as detailed in their 2023 blog post (Google, 2023).

<https://blog.google/technology/research/google-willow-quantum-chip/>