# Why Quantum Computing?

## Hackathons as a way to foster ecosystems


**Dr. Taha Selim**

**General Manager, MolKet SAS**

**Founder iQafé**


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مكتبة الإسكندرية

gesda Geneva Science and Diplomacy Anticipator

OQI Open Quantum Institute

iQafé

International Year of Quantum Science and Technology

qBraid

QWORLD

IBM

# 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**

# PhD publications >

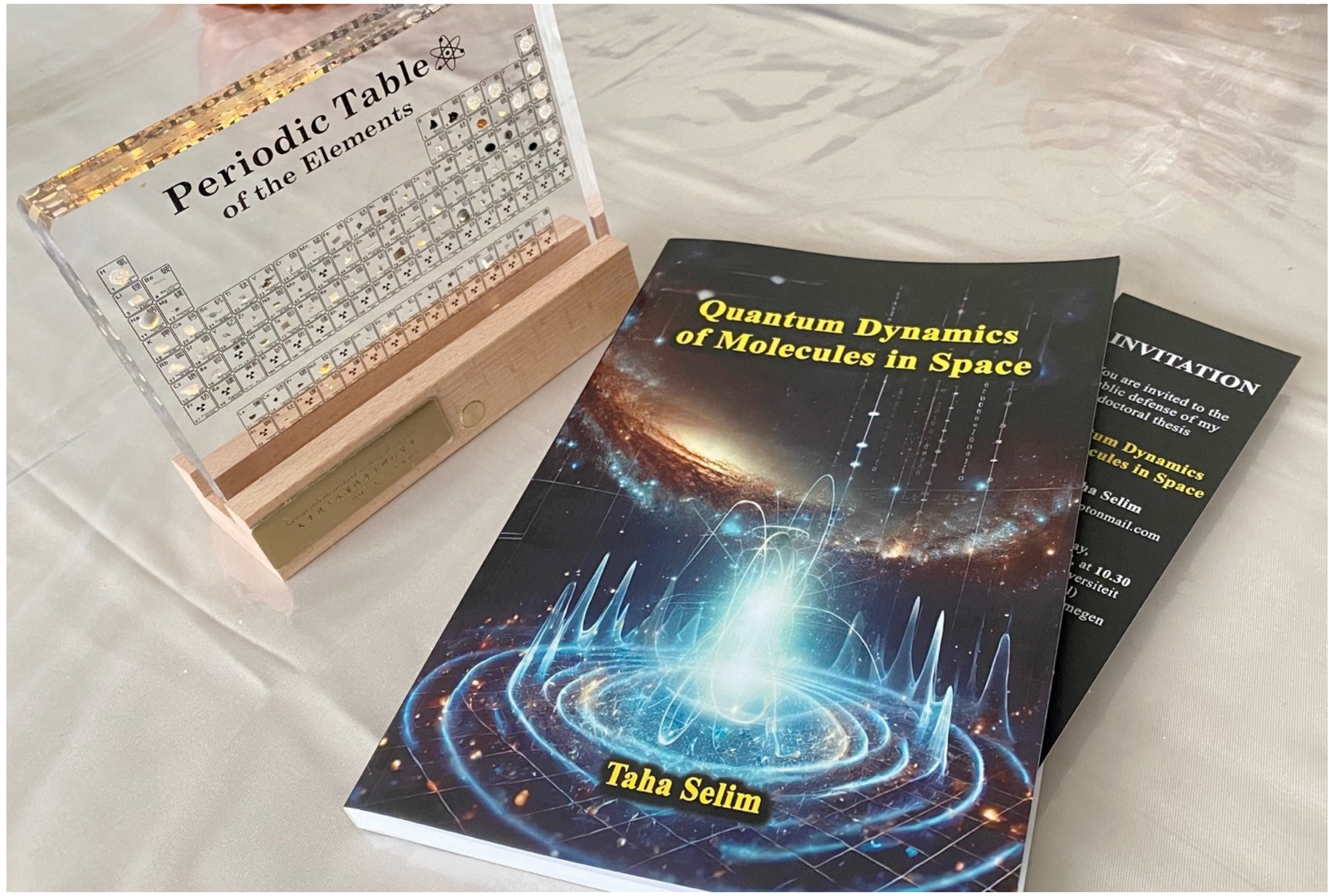
**This presentation is based on my PhD research, which is detailed in the following publications:**

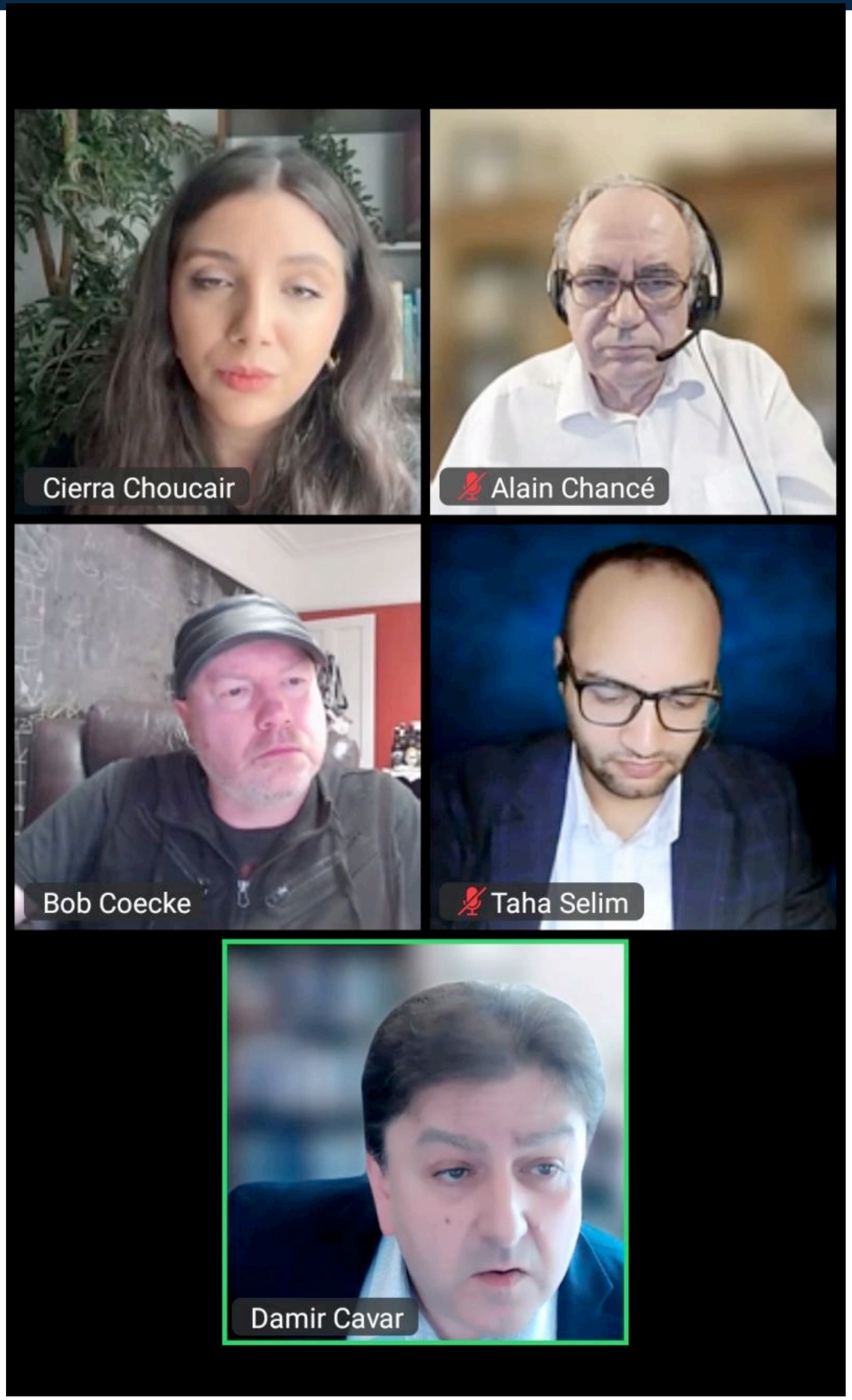
- Taha Selim. (2024). Quantum dynamics of molecules in space: Theoretical studies and efficient computational methods for collision-induced rovibrational transition rates in molecules. [Doctoral dissertation, Radboud University]. https://repository.ubn.ru.nl/handle/2066/311101

- 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

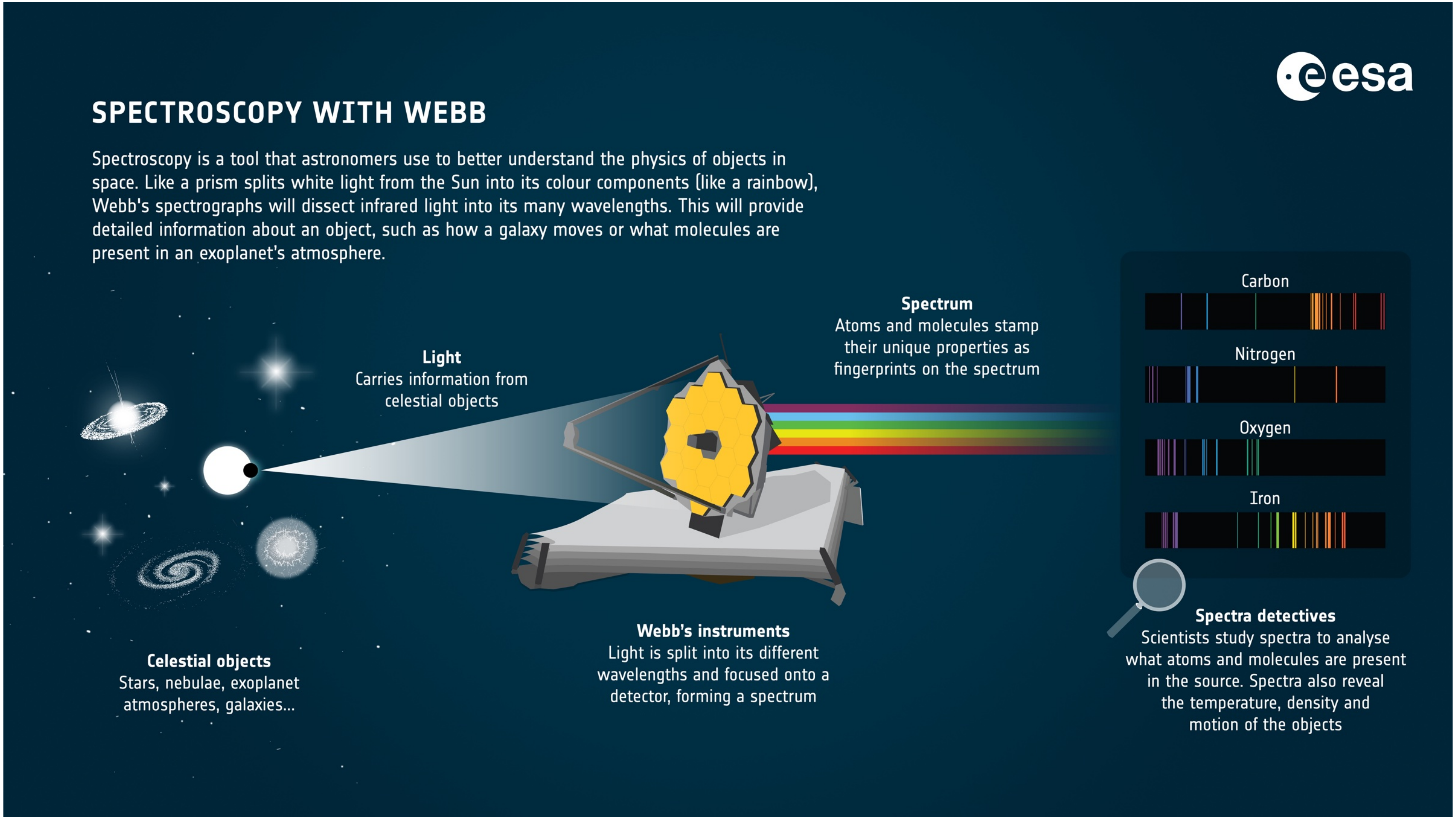
- Taha Selim, Ad van der Avoird, & Gerrit C. Groenenboom. (2022). Efficient computational methods for rovibrational transition rates in molecular collisions. The Journal of Chemical Physics, 157(6), 064105. https://pubs.aip.org/aip/jcp/article/157/6/064105/2841671/Efficient-computational-methods-for-rovibrational

- 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

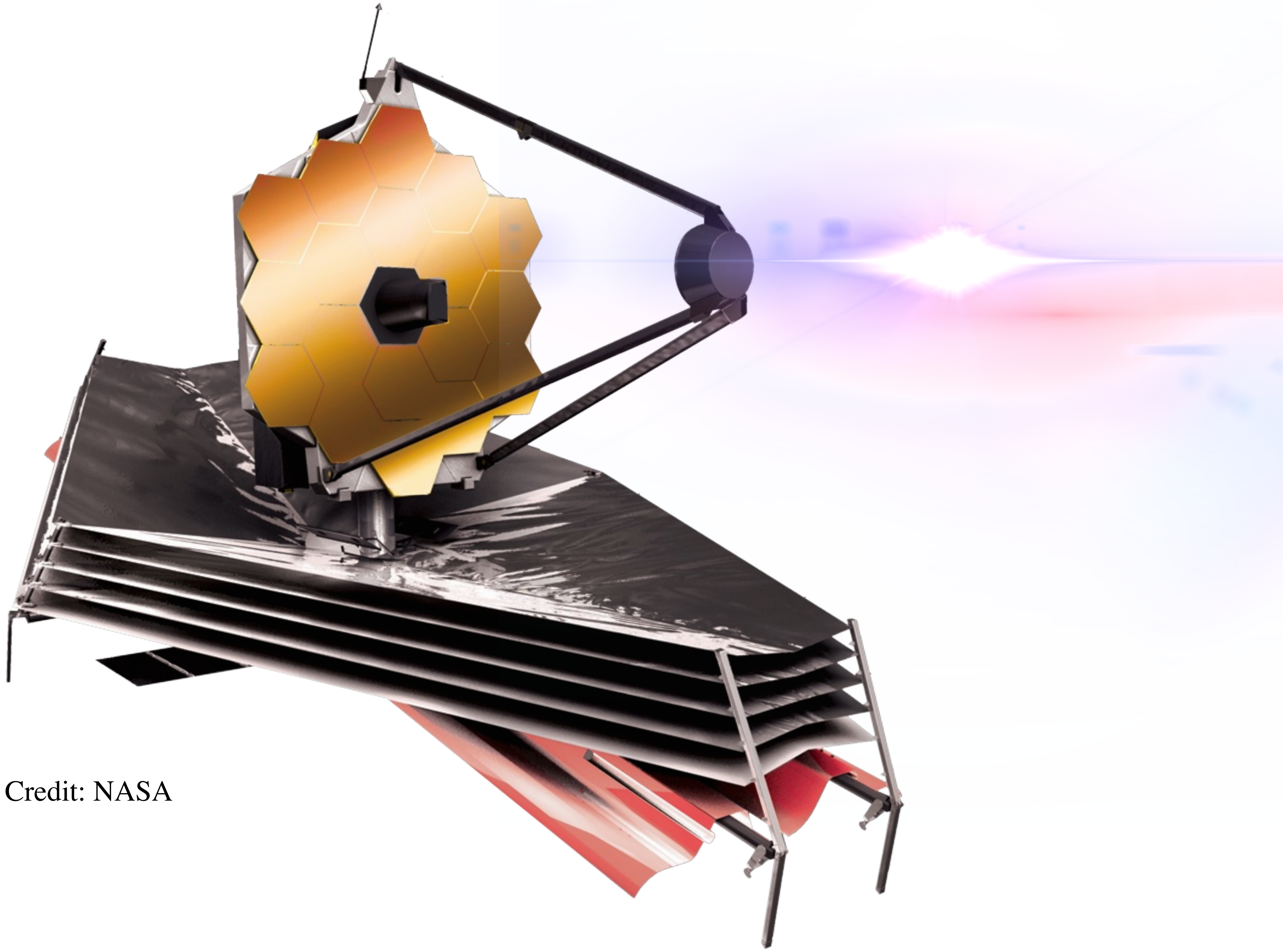



Cierra Choucair
Alain Chancé
Bob Coecke
Taha Selim
Damir Cavar

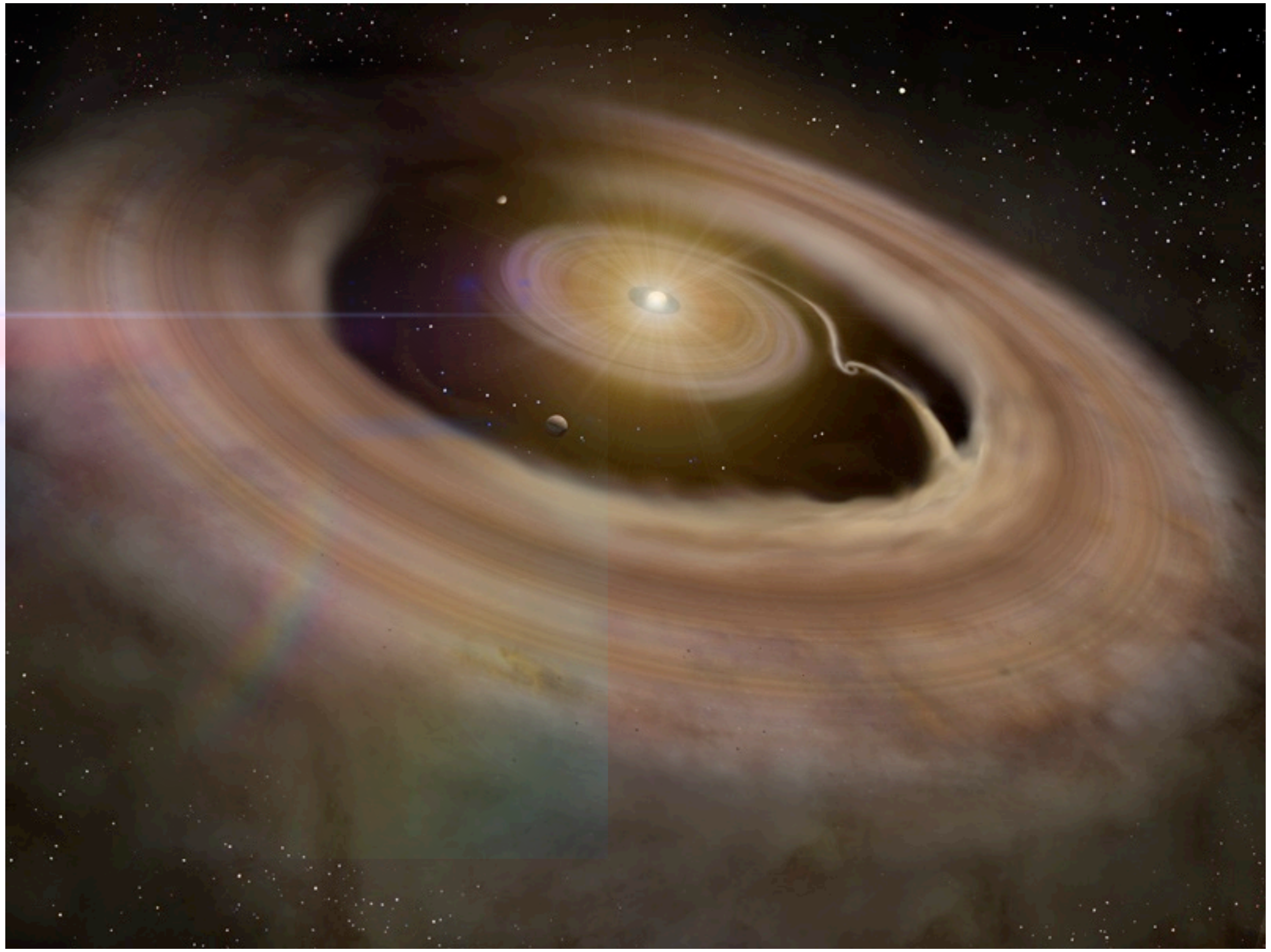
# Quantum molecular dynamics & the JWST >



# James Webb Space Telescope (JWST) >



Credit: NASA



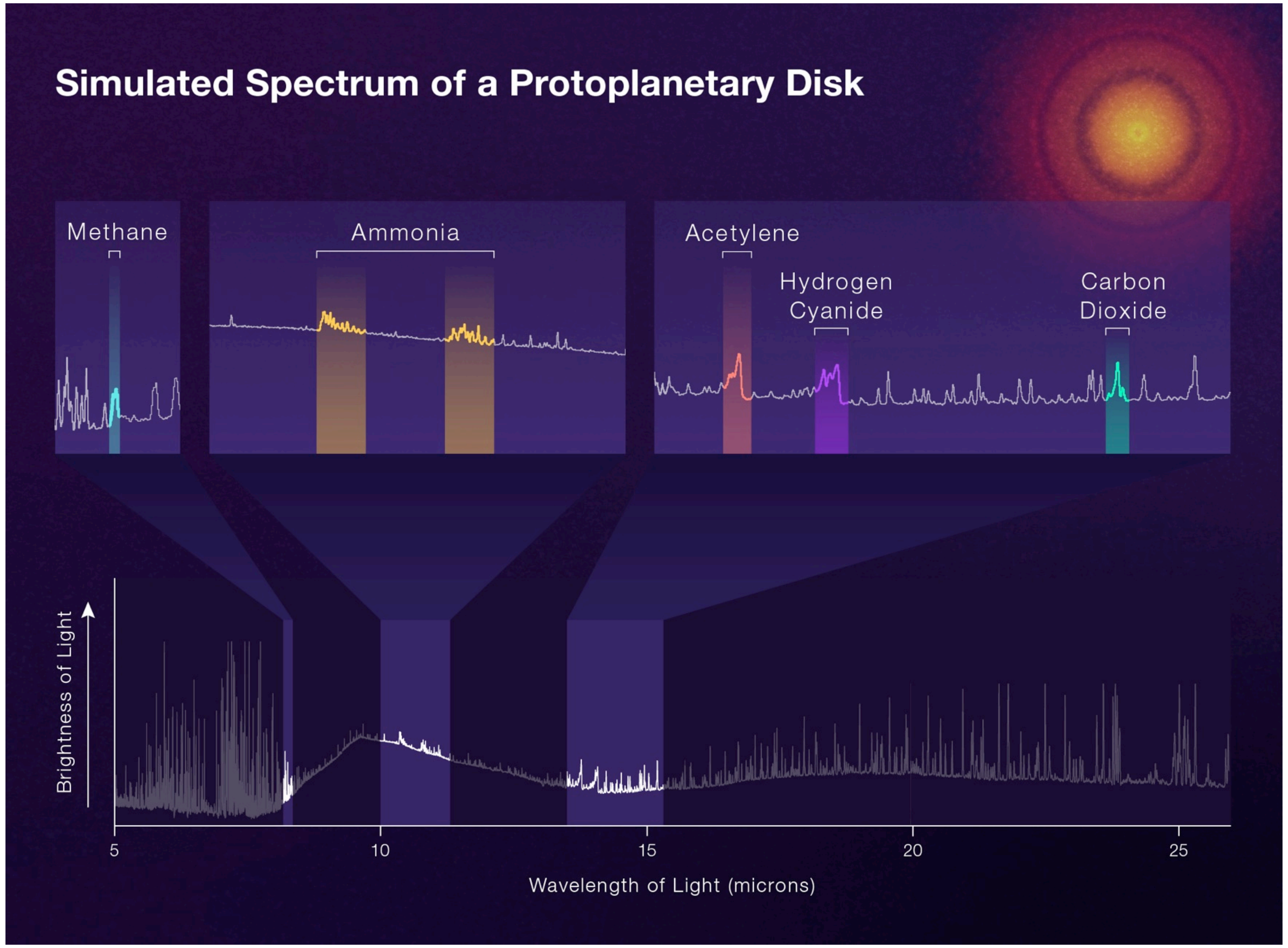
**Powerful near and mid-infrared observational capabilities**

# | $CO_2$ as a molecular quantum sensor >

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

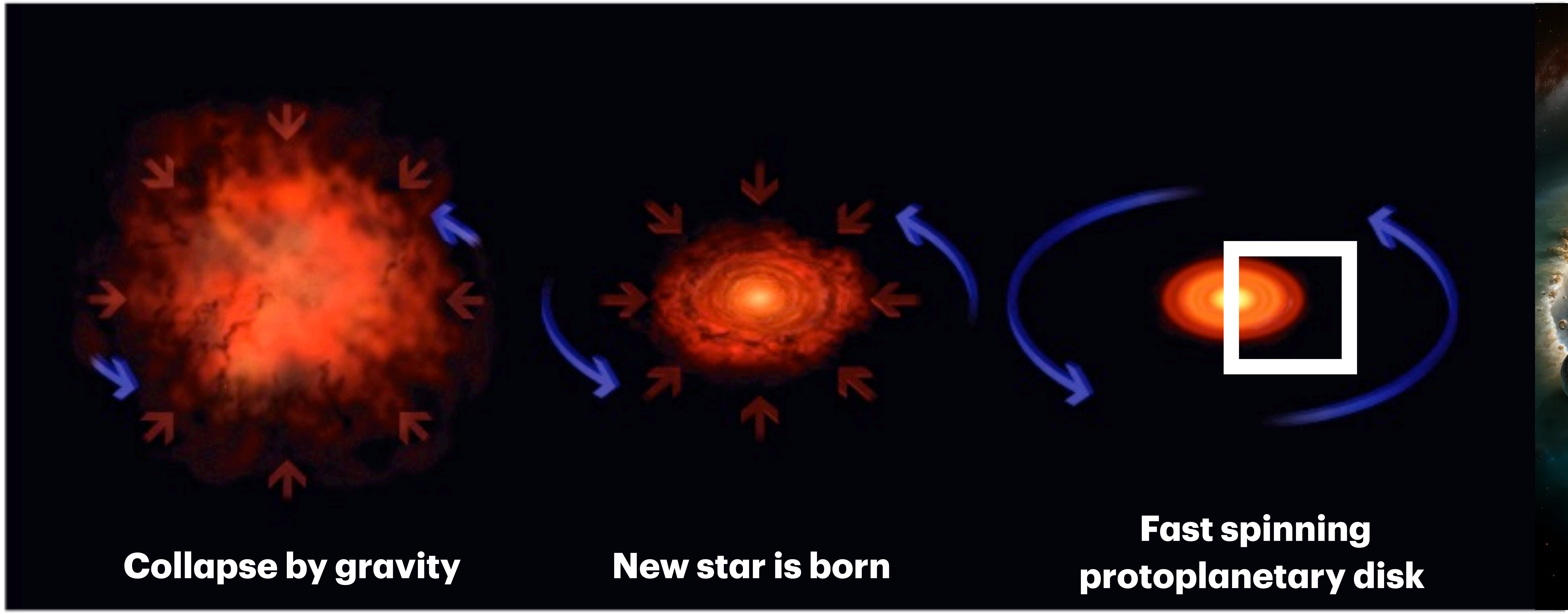
- Local temperature.
- Molecular abundances.
- More information.

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

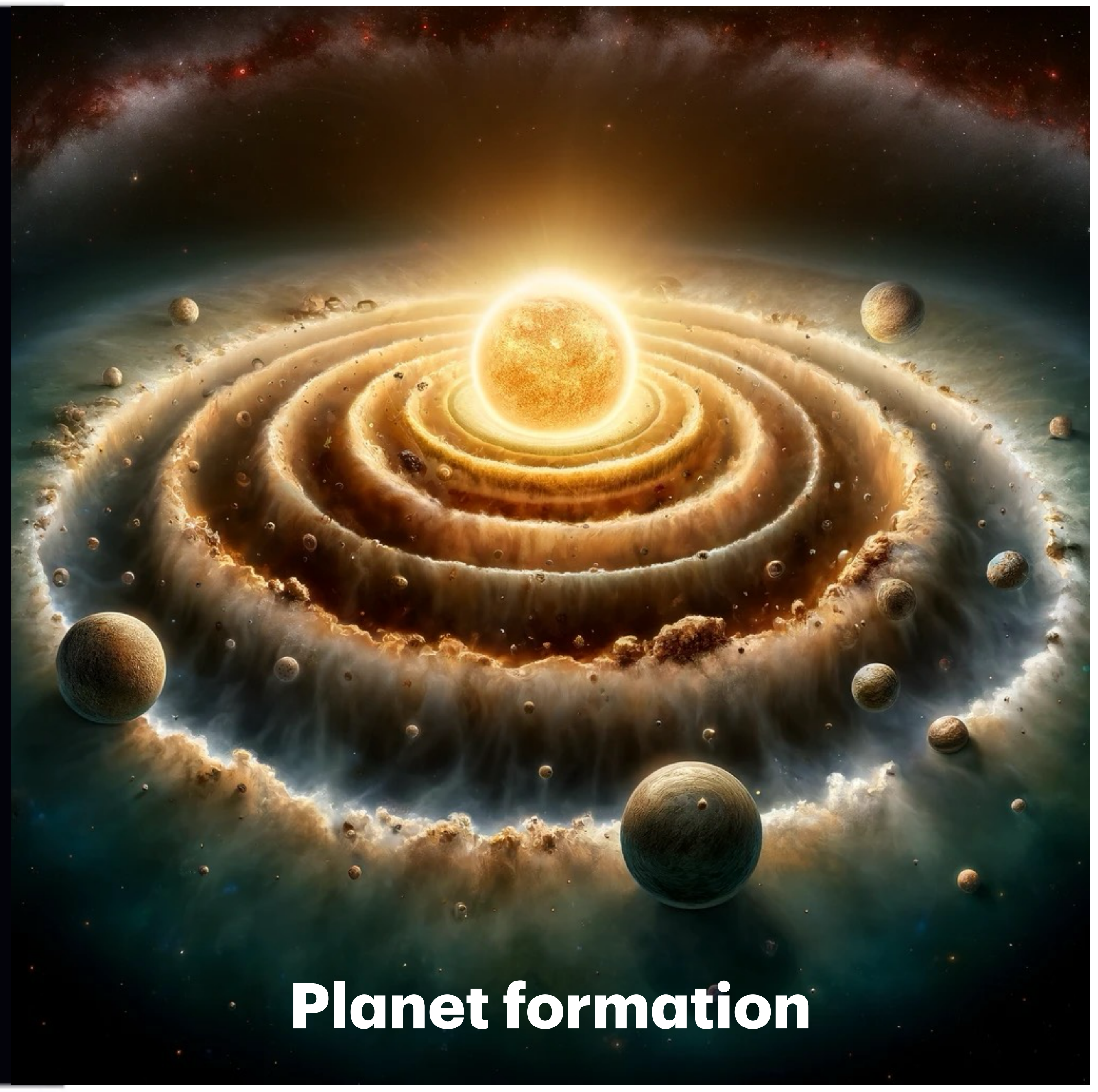



Credit: NASA, ESA, CSA, Leah Hustak (STScI)

# | $CO_2$ as a molecular quantum sensor >




© Addison-Wesley Longman




Conceptual illustration

**Key molecules** $CO$ $CO_2$ $HCN$ $H_2O$ $C_2H_2$ $CH_4$

# Simulating $CO_2$ + He inelastic collisions >

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

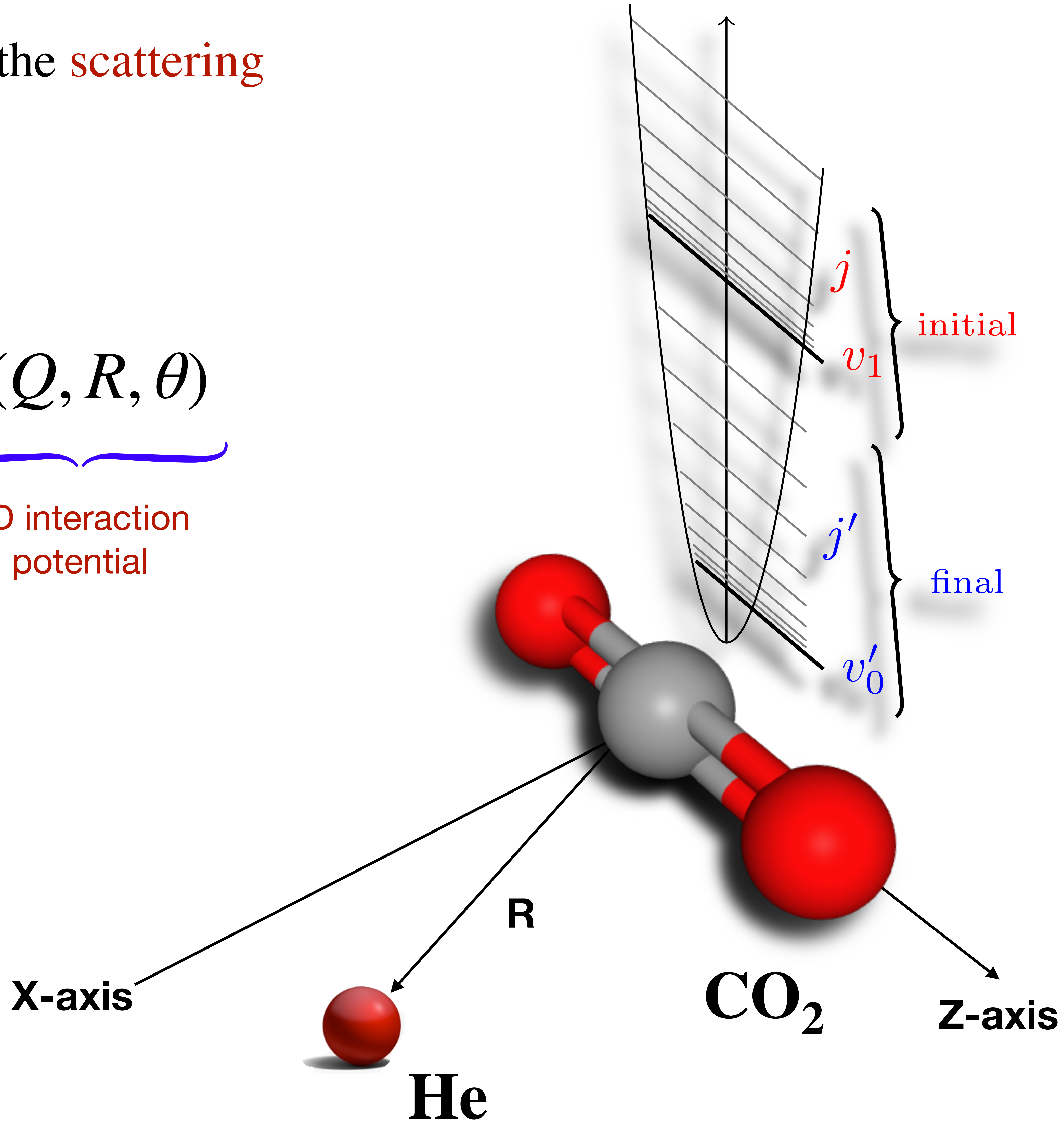
$$\hat{H}_{HeCO_2} = \underbrace{-\frac{1}{2\mu R}\frac{\partial^2}{\partial R^2}R}_{\text{Kinetic energy of the dimer}} + \underbrace{\hat{H}_{CO_2}}_{CO_2\text{ Hamiltonian}} + \underbrace{\frac{\hat{L}^2}{2\mu R^2}}_{\text{Angular kinetic energy of the dimer}} + \underbrace{V(Q,R,\theta)}_{\text{3D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

dimer: refers to both He+$CO_2$

**$HeCO_2$ computational basis/space, used for solution:**

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

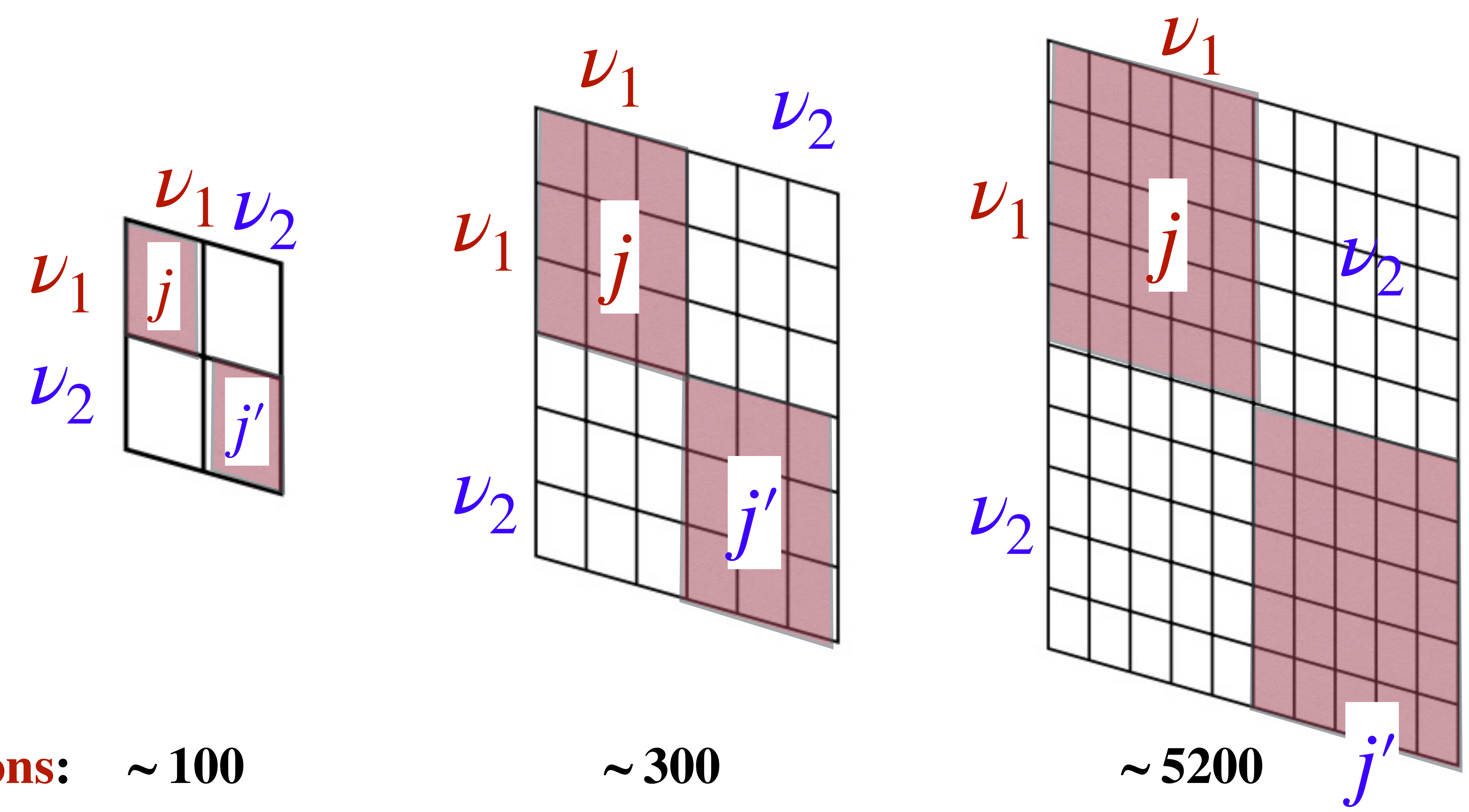
**Body-fixed (BF):** $|v\ j\ \Omega\,|\,JM_J>$



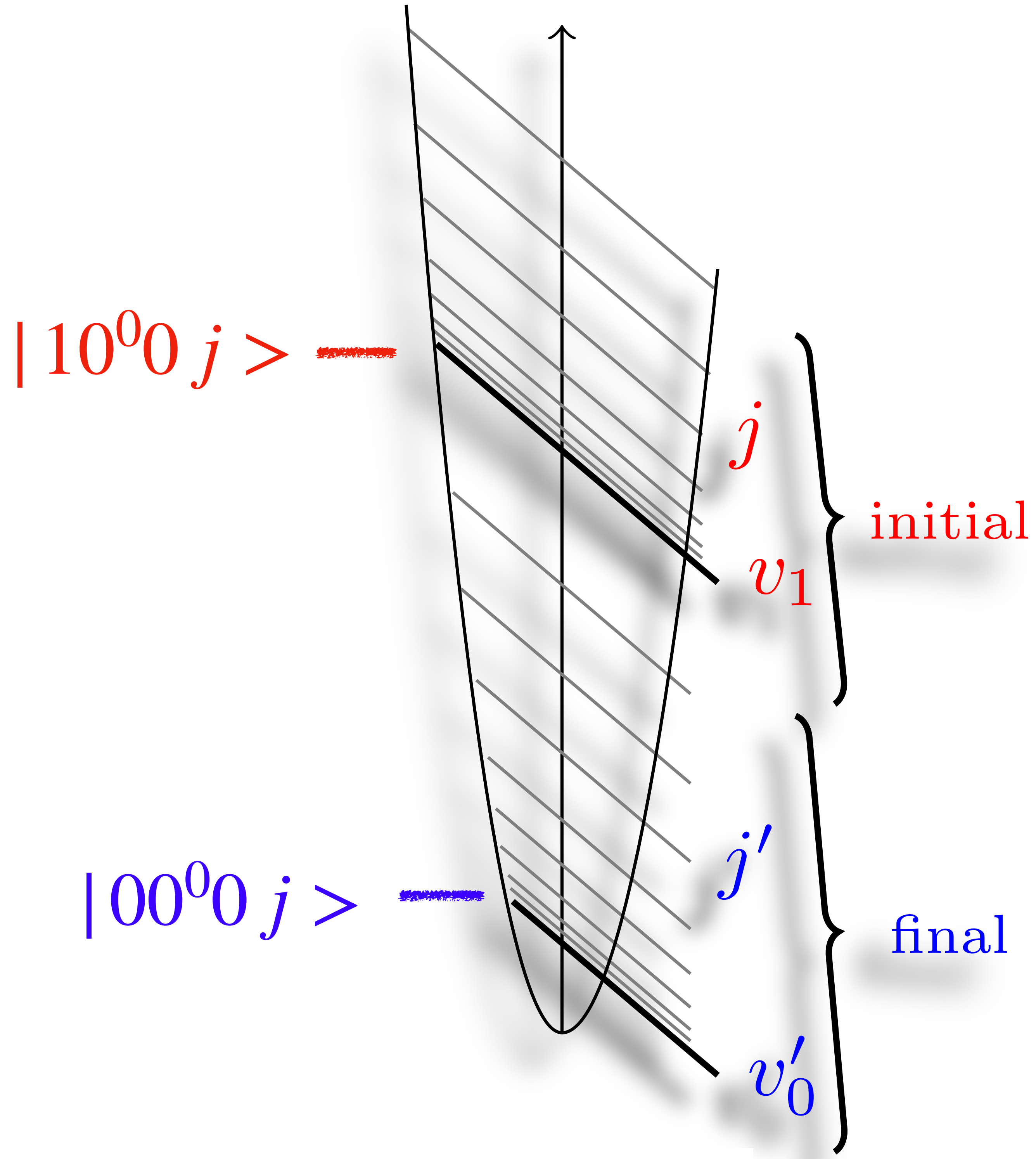
## Example: Rovibrational transitions in $CO_2$ induced by collisions with $He$

**Time $\propto$ (Number of coupled equations)$^3$**

**Single calculation**



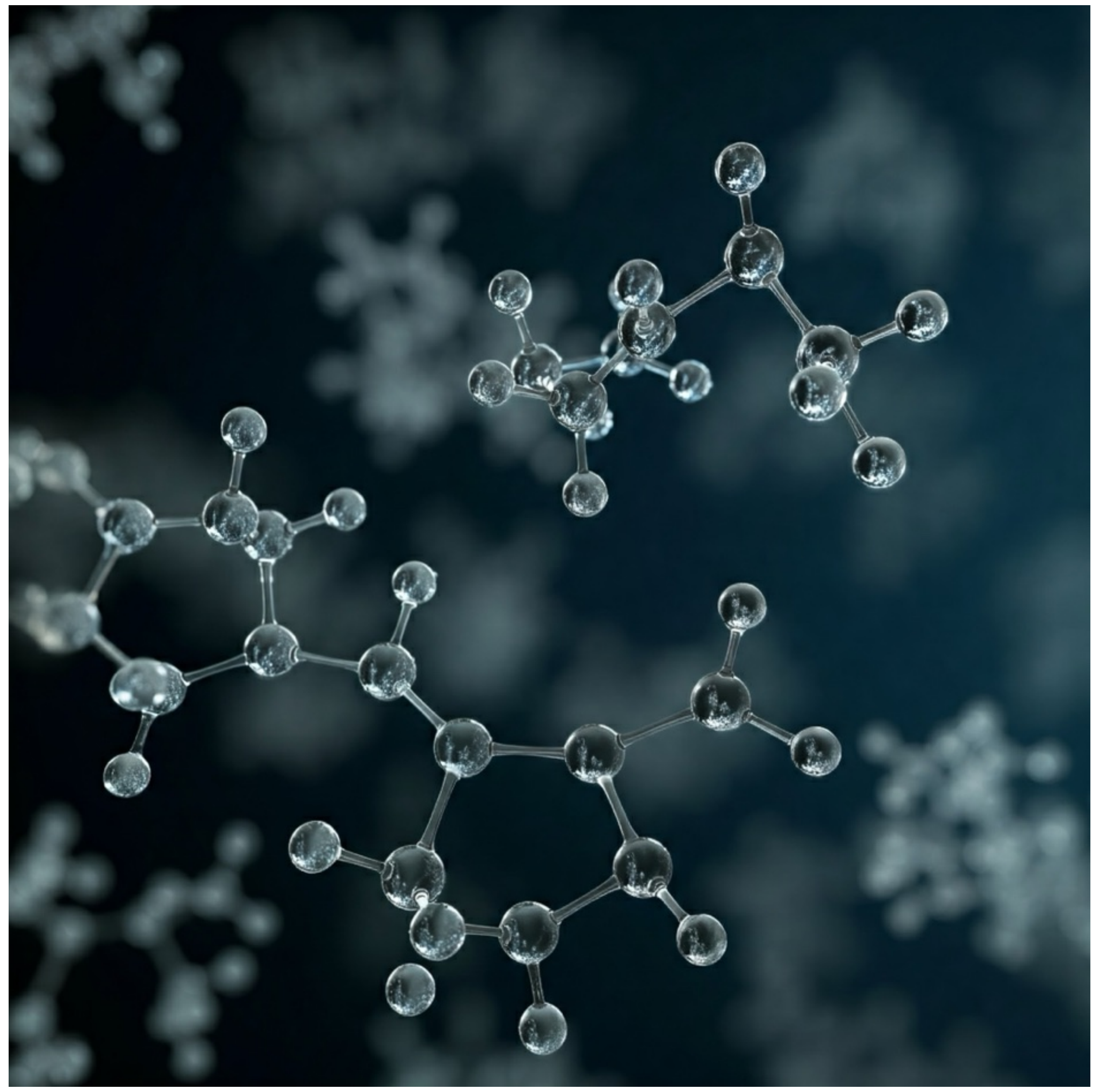

| | | | |
|---|---|---|---|
| **Number of coupled equations:** | **~100** | **~300** | **~5200** |
| **Time (seconds):** | **~0.5 s** | **~4.15 s** | **~6600 s** |



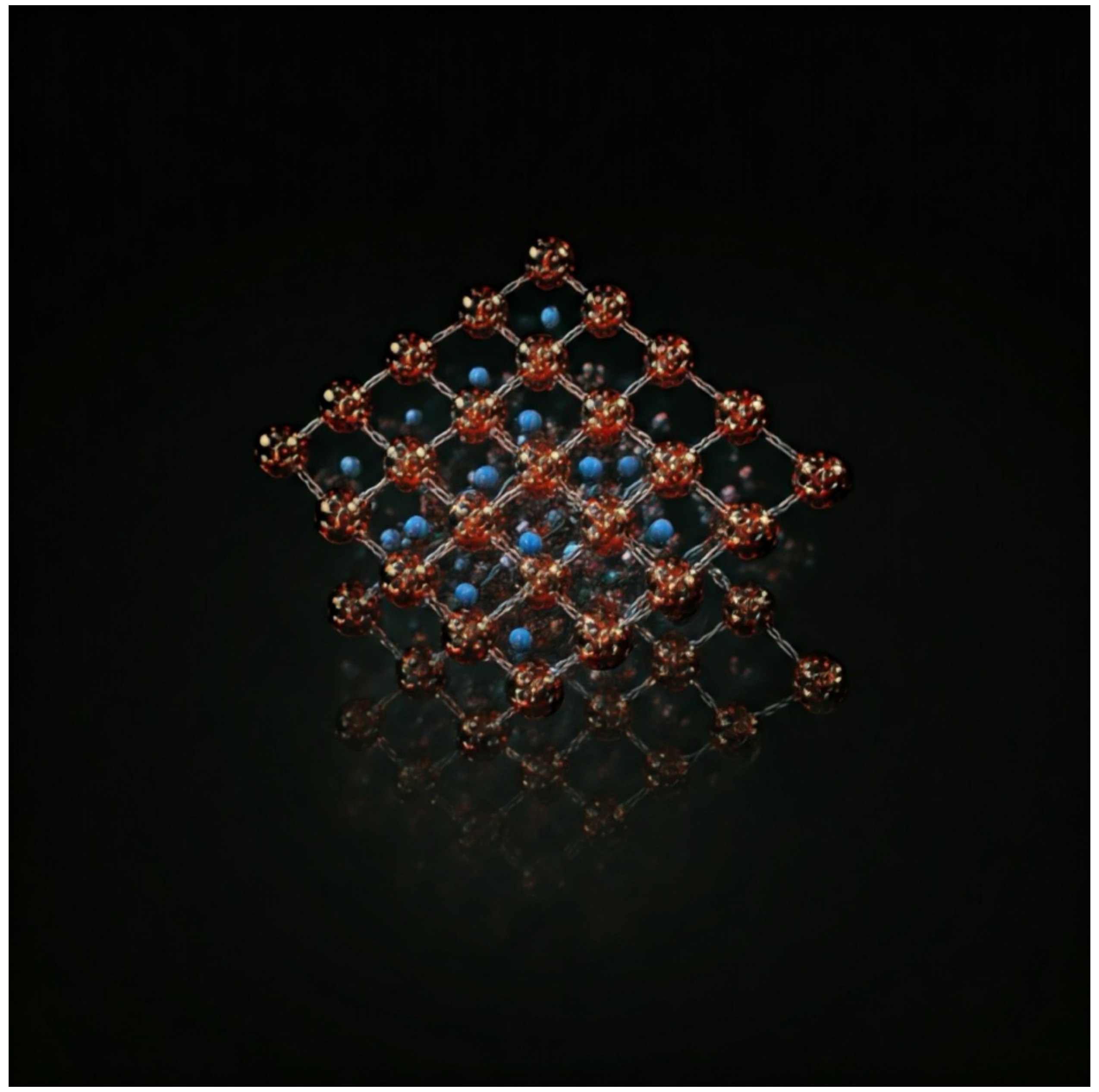

**Example: symmetric stretch**

Taha Selim et al. J. Chem. Phys., 157, 064105 (2022)

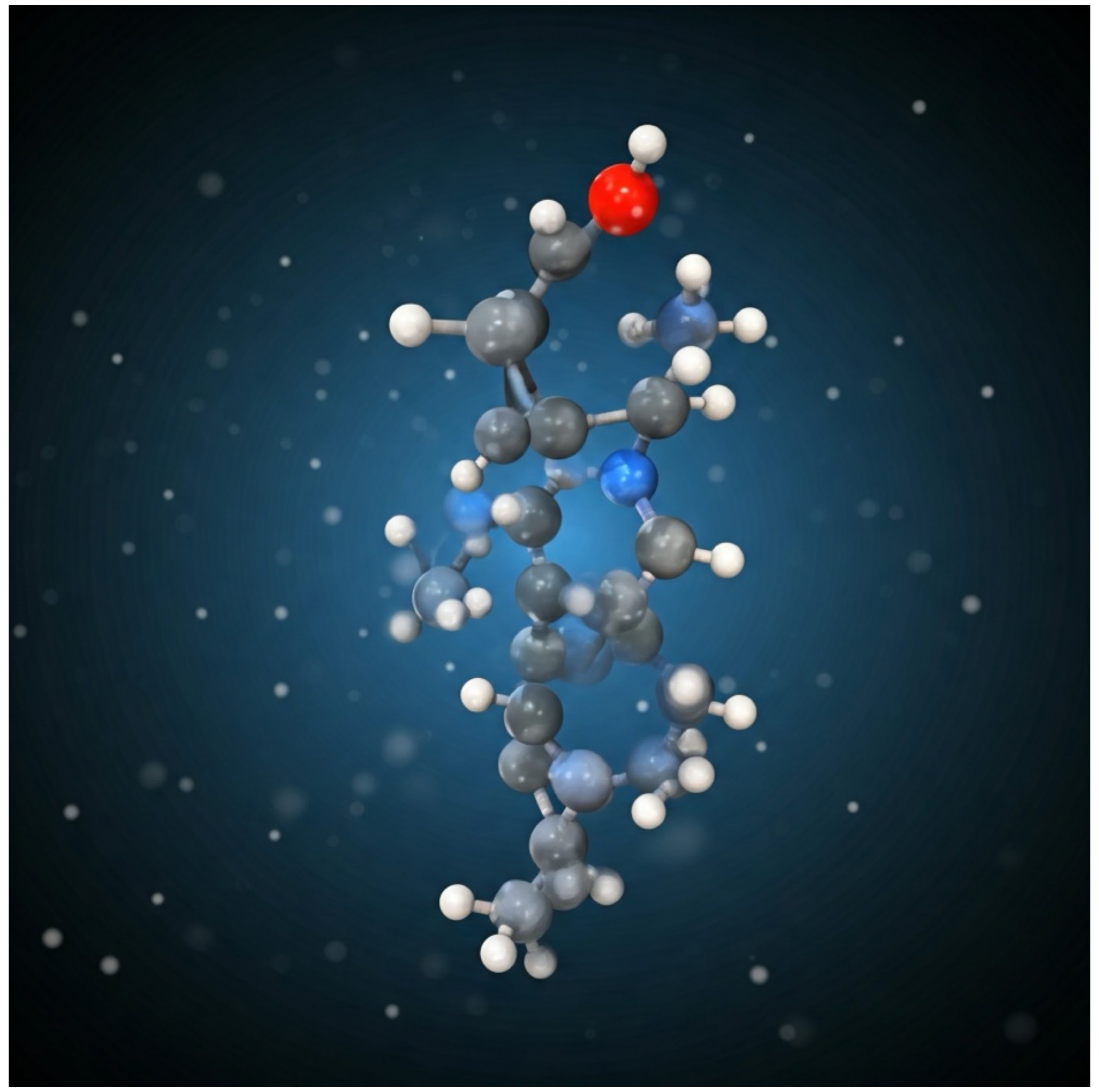
# Computational complexity of molecular simulations >



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:

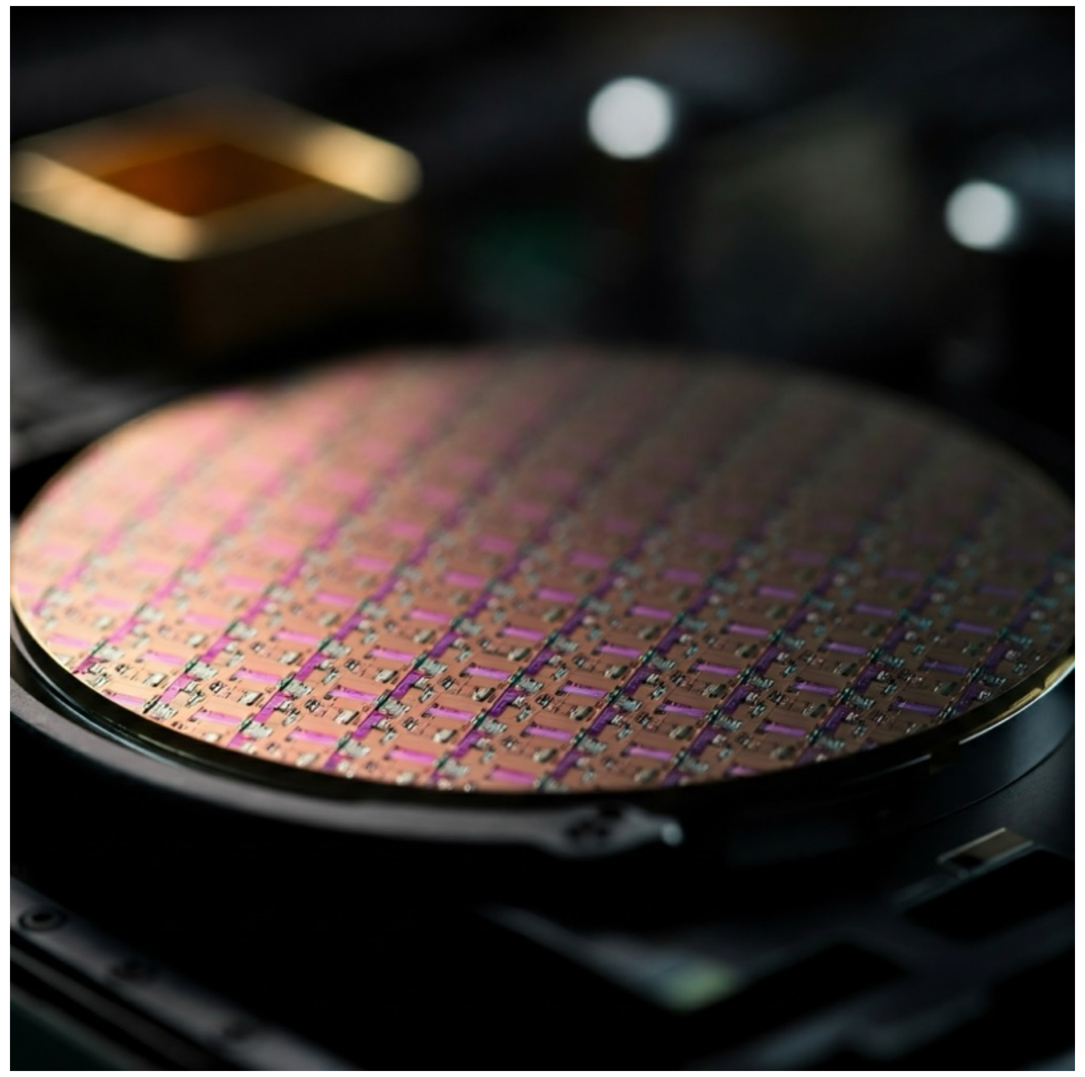
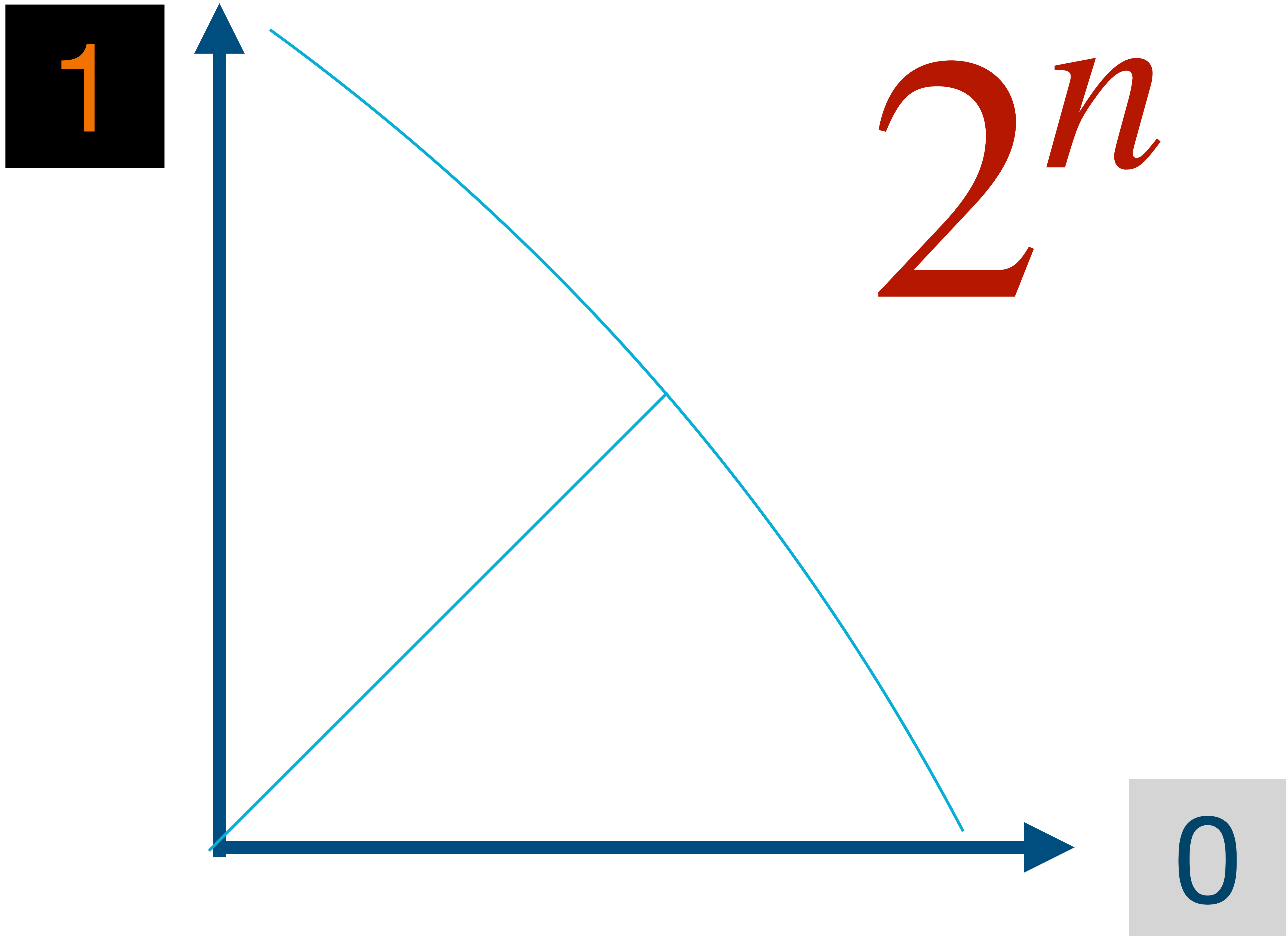


Illustration of a wafer

**Bit** 0 1

## Quantum bits (qubits):



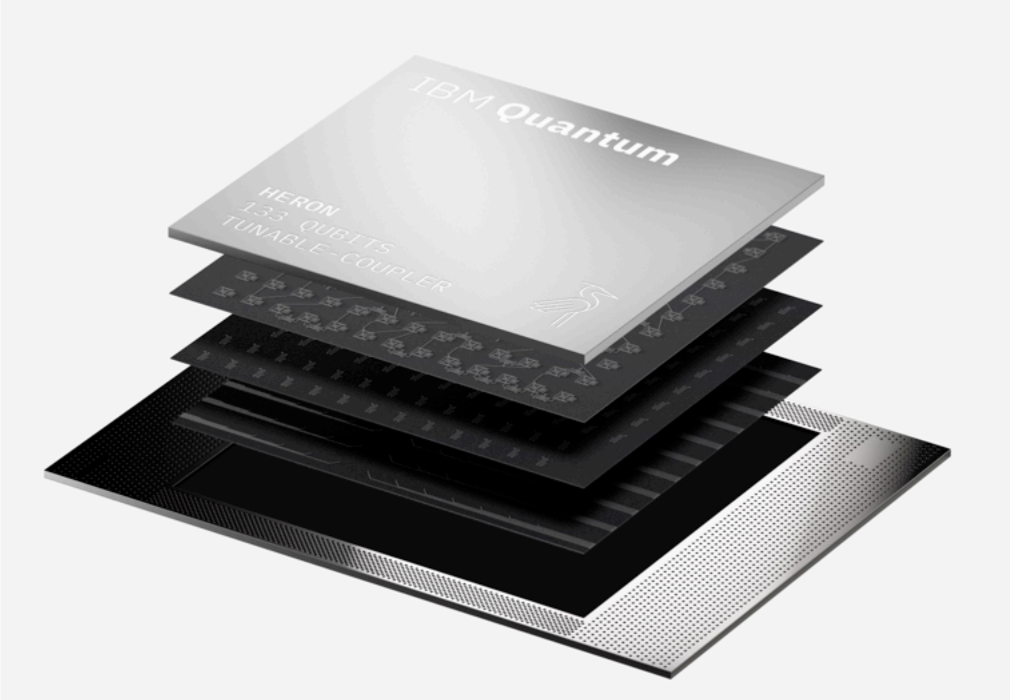

$$2^n$$

**Qubit** $= a$ 0 $+ b$ 1

# IBM quantum computer >

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

IBM Q



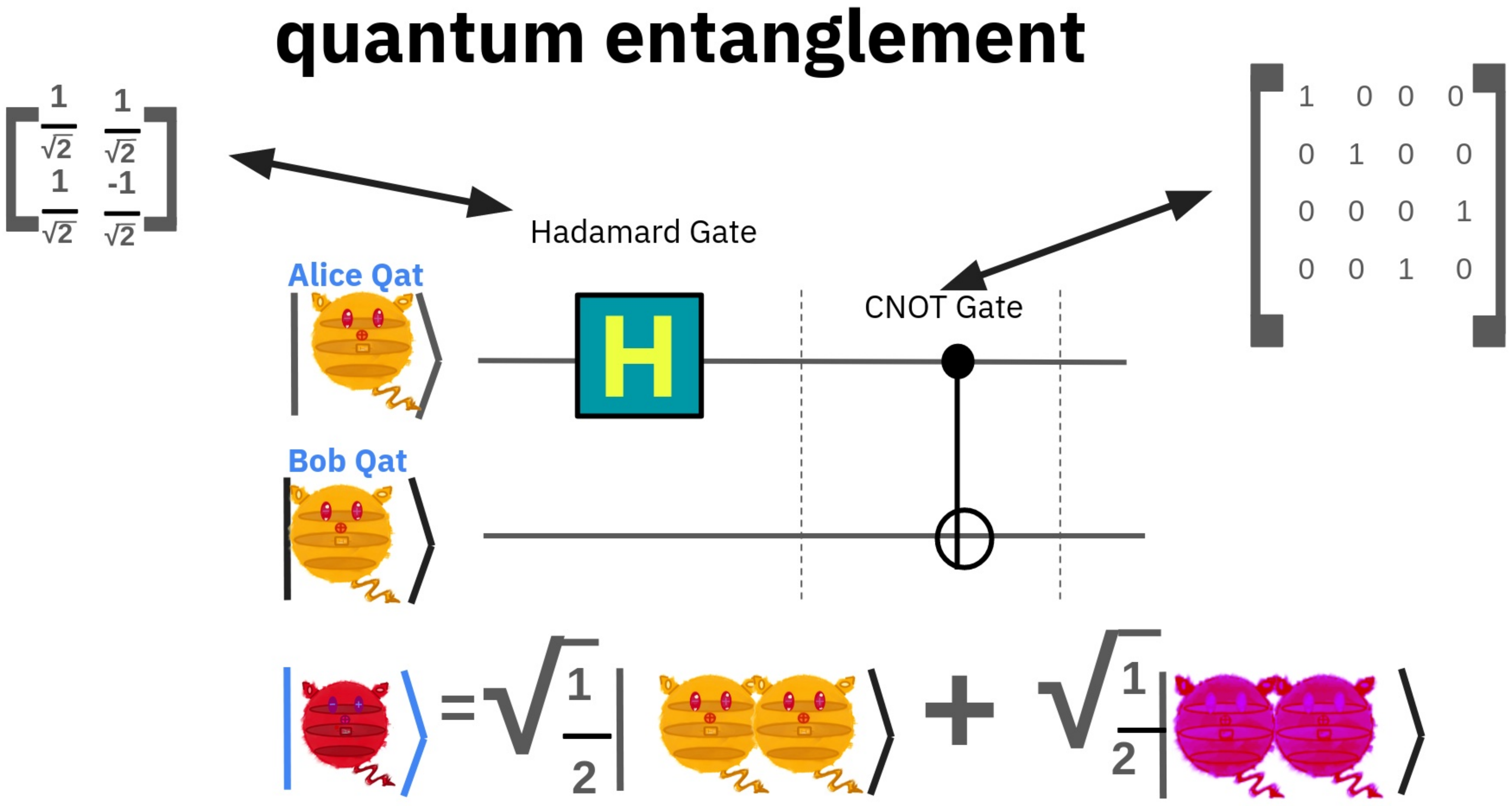
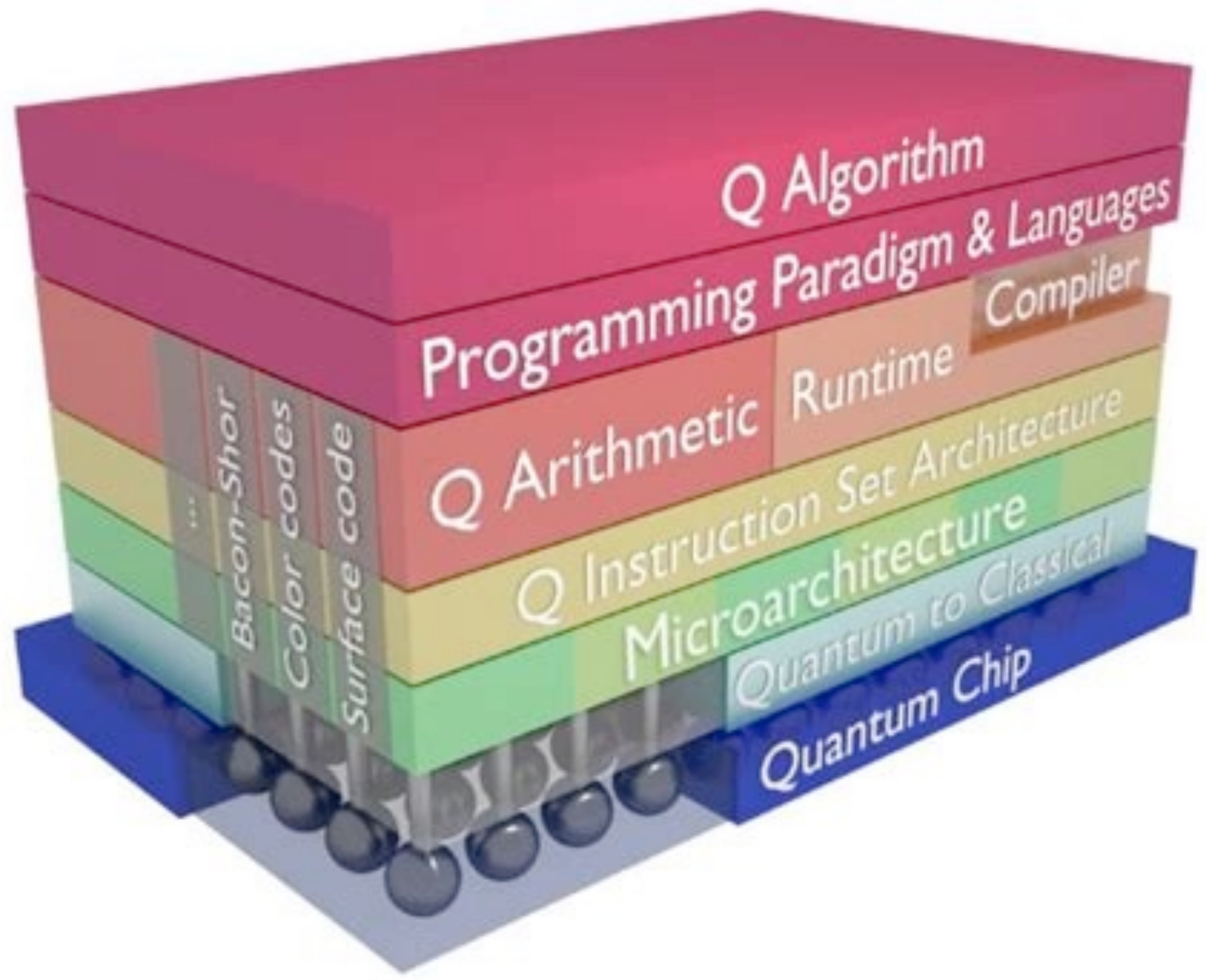




Image credit: Alberto Maldonado Romo

Time

# Quantum computing algorithm workflow >




**Quantum computers cannot replace conventional traditional computers.**

**Problems and their solutions are mapped in a particular way.**

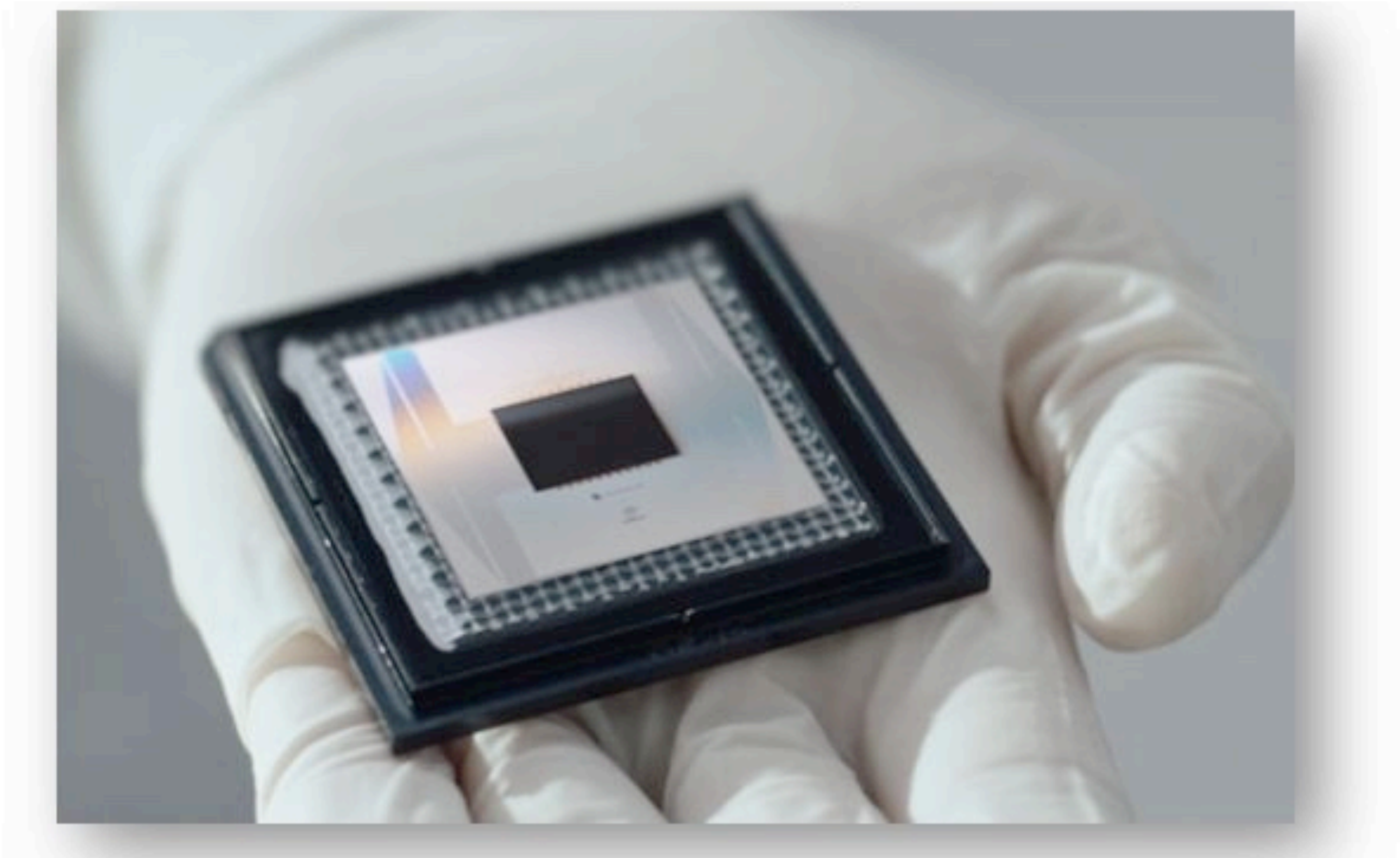
**Logistics, finance, portfolio optimization, quantum simulations, chemistry, battery design, material simulations, drug design, healthcare, …etc**

# Hardware for quantum computing >

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

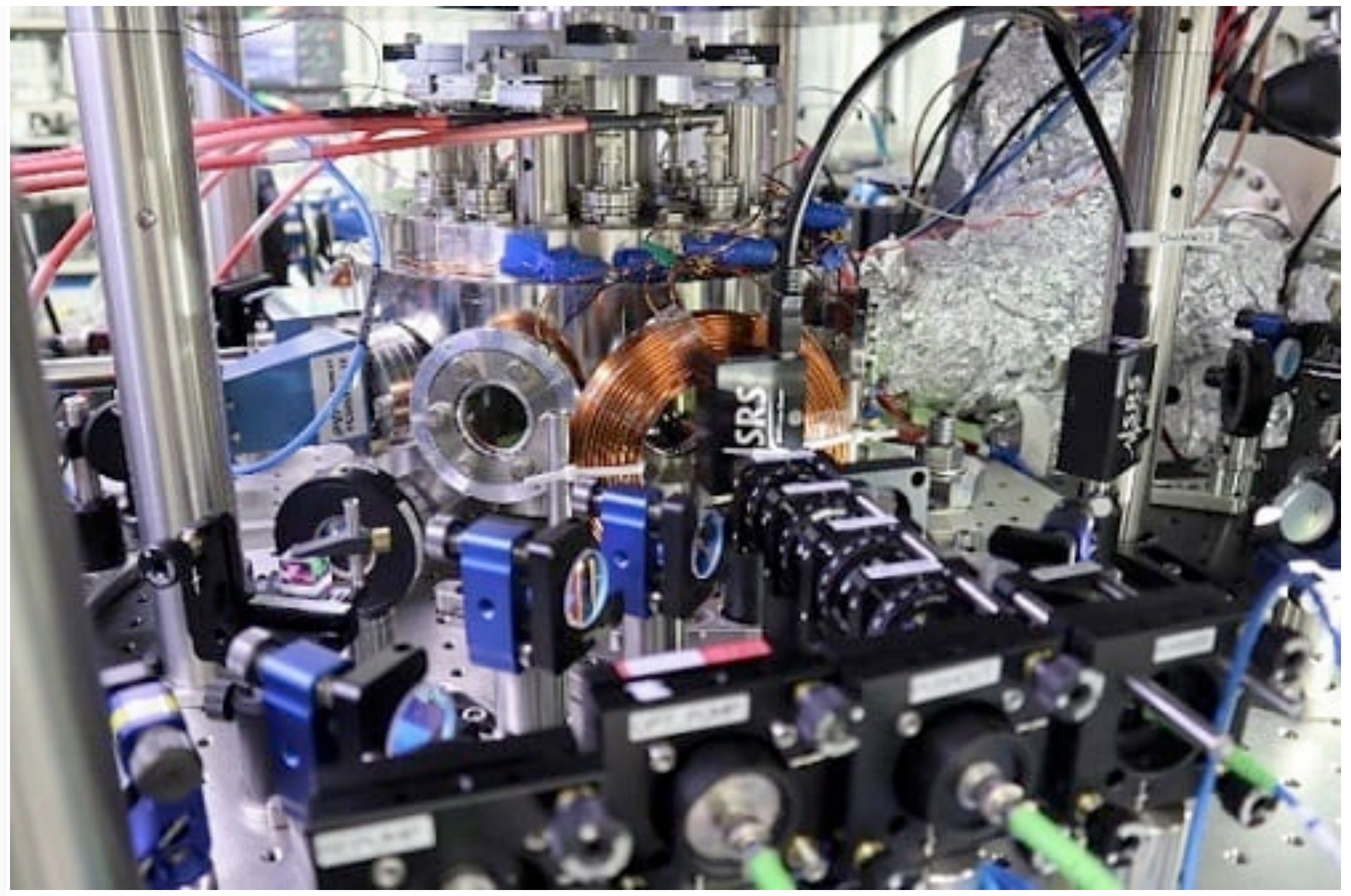

QuiX - https://www.quixquantum.com/

**Photonic quantum processor**



Google, new Willow chip

**Superconducting quantum processor**



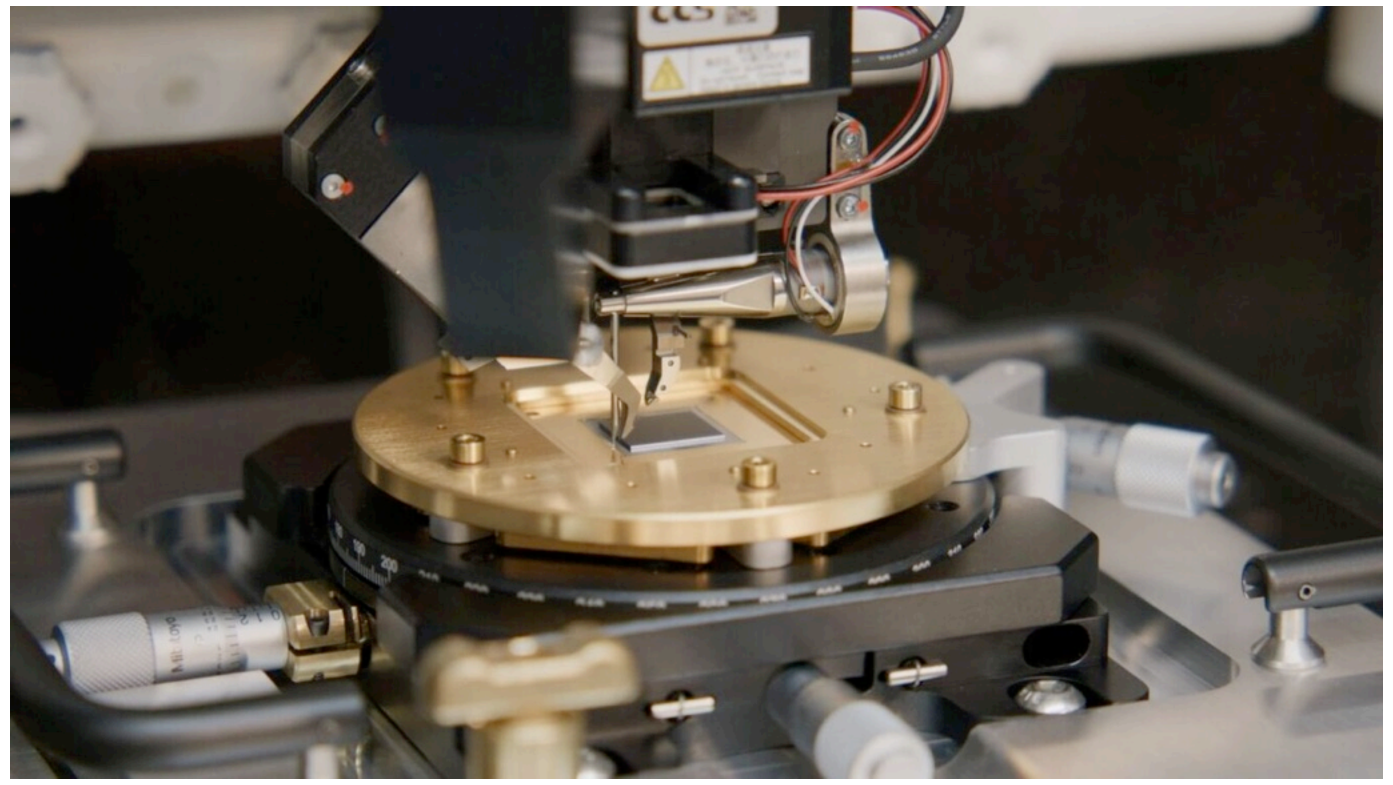
*Kenji Ohmori group at the Institute for Molecular Science. Courtesy of Takafumi Tomita.*

**Ultracold neutral atoms quantum processor**

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

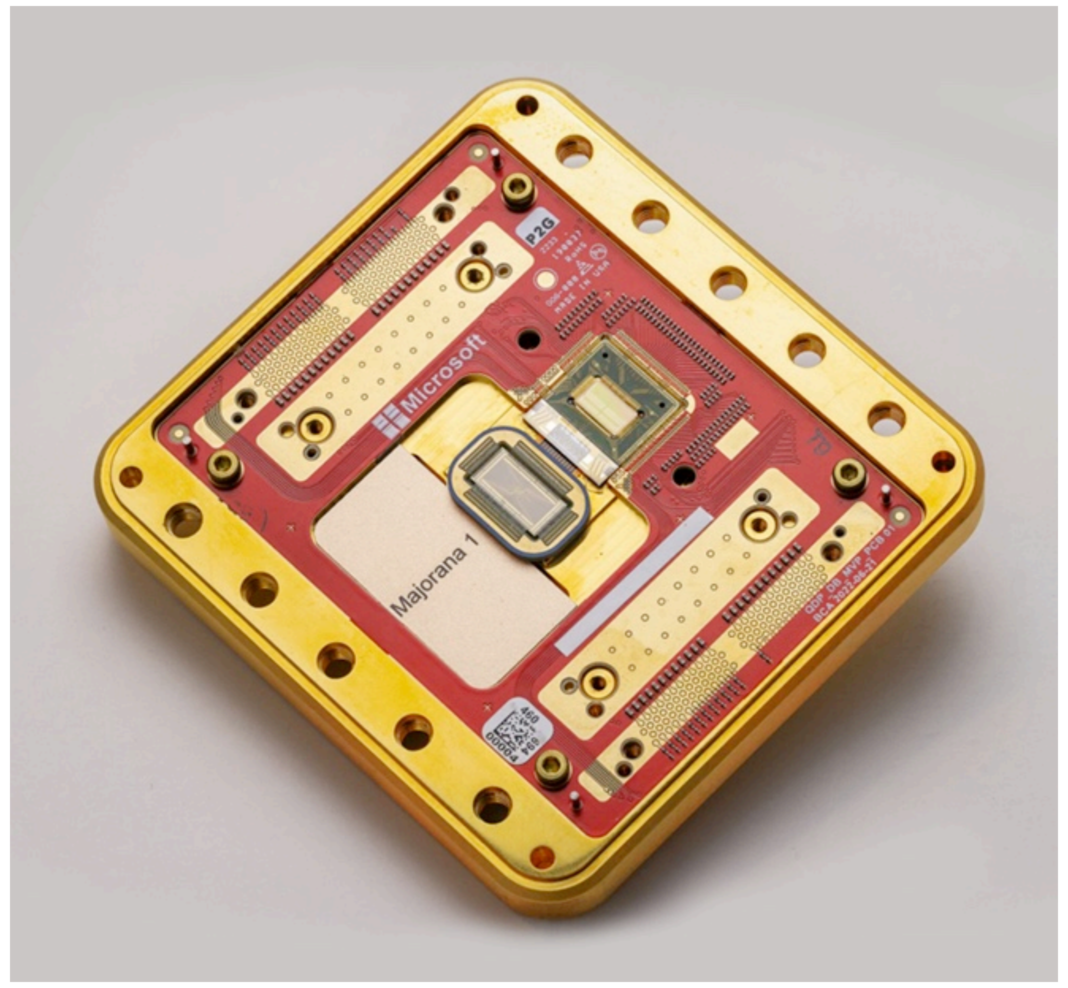
# Hardware for quantum computing >

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



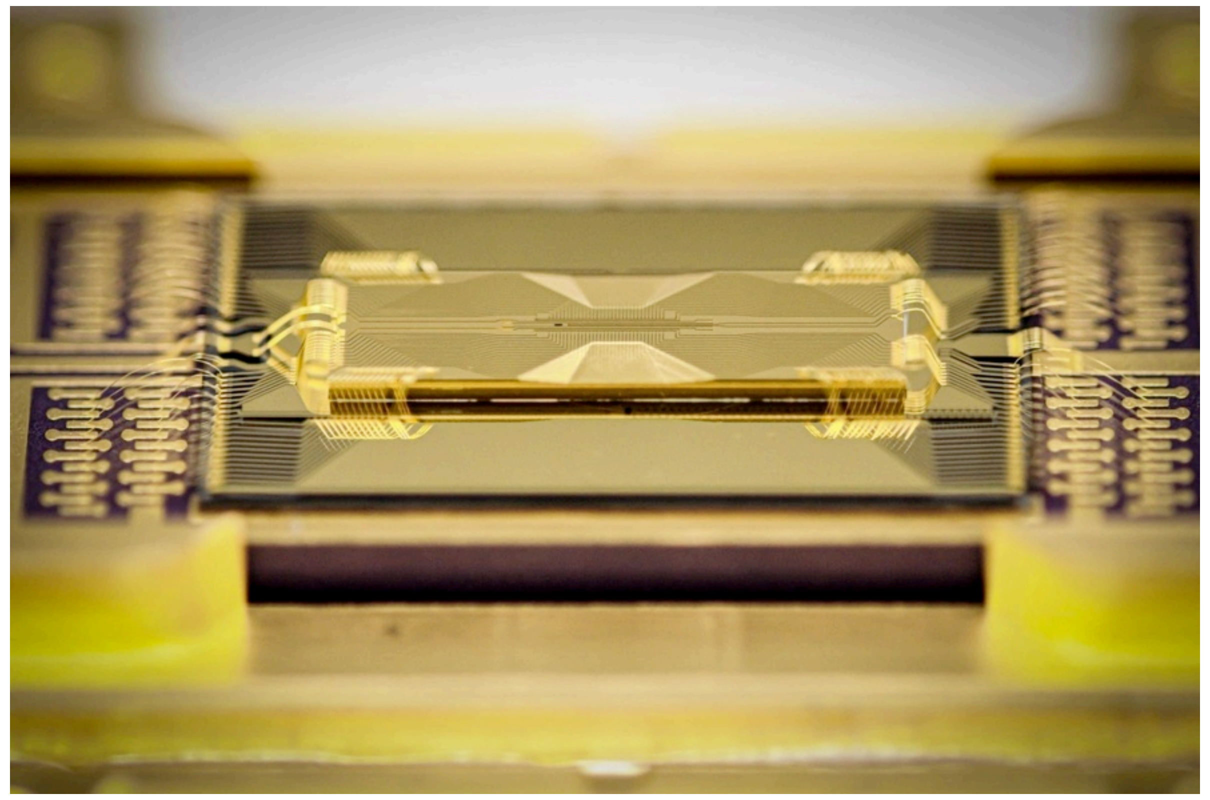
AWS- New 'Ocelot' chip

**Cat qubits**




Microsoft, Majorana 1

**Topological qubits**



IonQ

**IonQ’s trapped ion technology**

## 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)

~ 2 qubits

- hard to scale

**Raspberry pi**

Quantum circuit emulator

~ 100 euros


**NVIDIA Jetson Orin Nano Super Developer Kit**

Quantum circuit emulator +

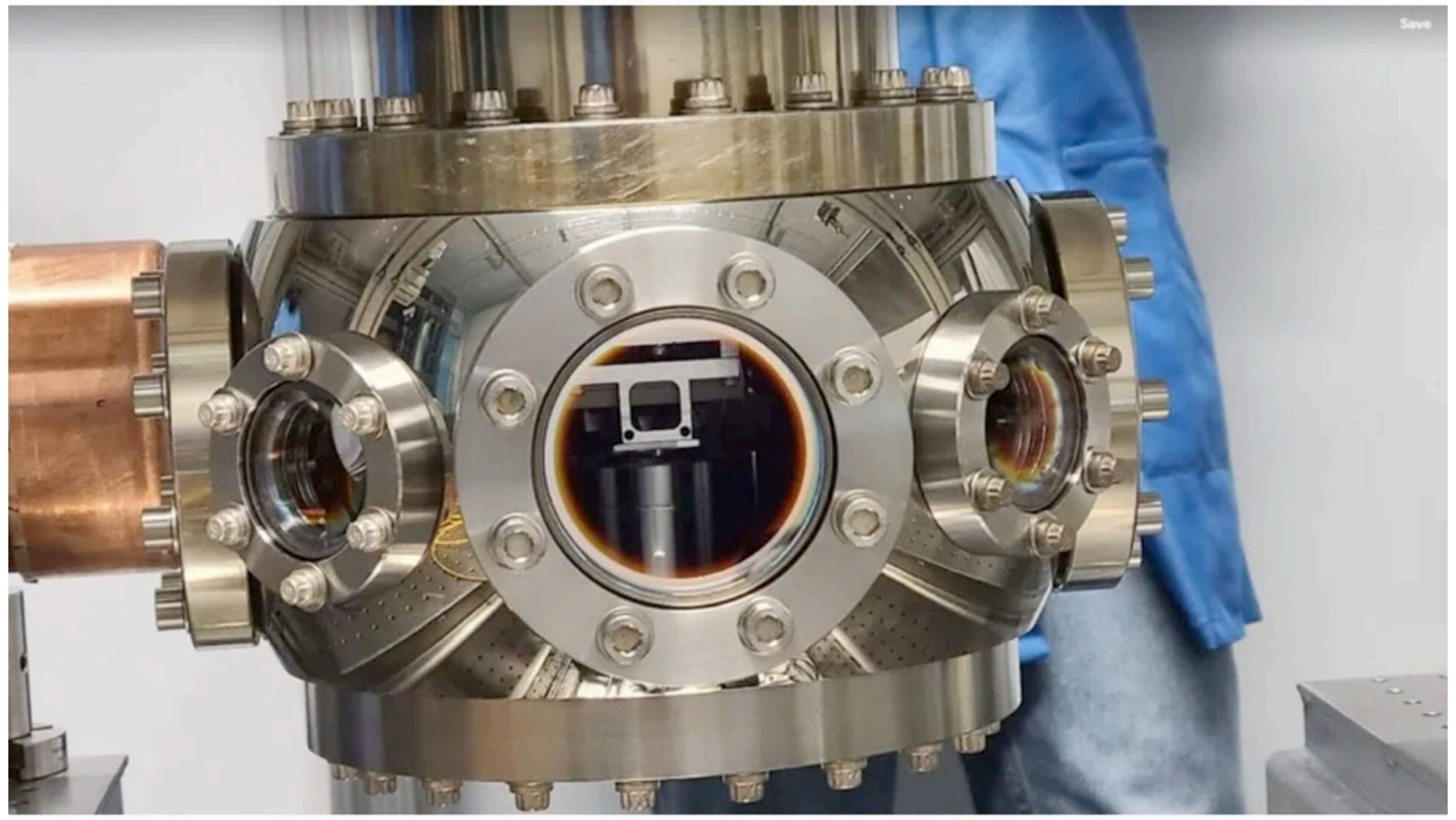
AI applications

~ 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.

INTERESTING ENGINEERING



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

By Aman Tripathi

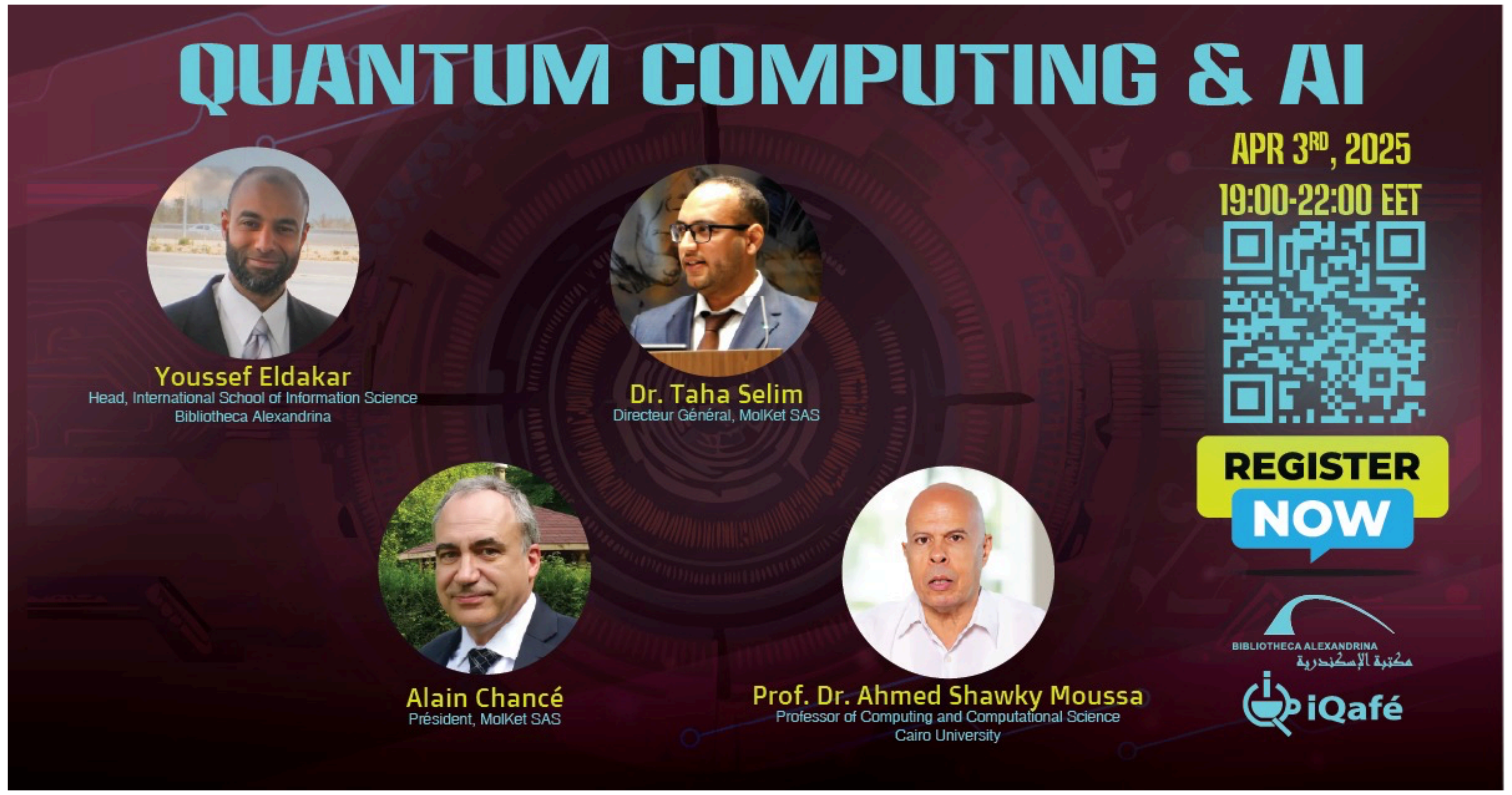
Jan 17, 2025 | 12:59 PM

## Three editions: Dec 2024, Feb & March 2025


**Quantum AI and HPC**


**Quantum Encryption and AI foundation models**

**Quantum modeling and AI agents**



# Quantum AI monthly series >

## Three editions: Dec 2024, Feb & March 2025


Quantum systems and hardware


Quantum education and ecosystem

Quantum communications and encryption

# Quantum Leap >



Quantum AI: The Next Leap in Physics Intelligence, Research, Ecosystem, and Building Community, Taha Selim

# Intro to quantum computing & quantum algorithms


# Quantum activités >


# DryRun Hackathon >


# HACKATHONS as a way to foster quantum ecosystems >

# HACKATHONS as a way to foster quantum ecosystems >

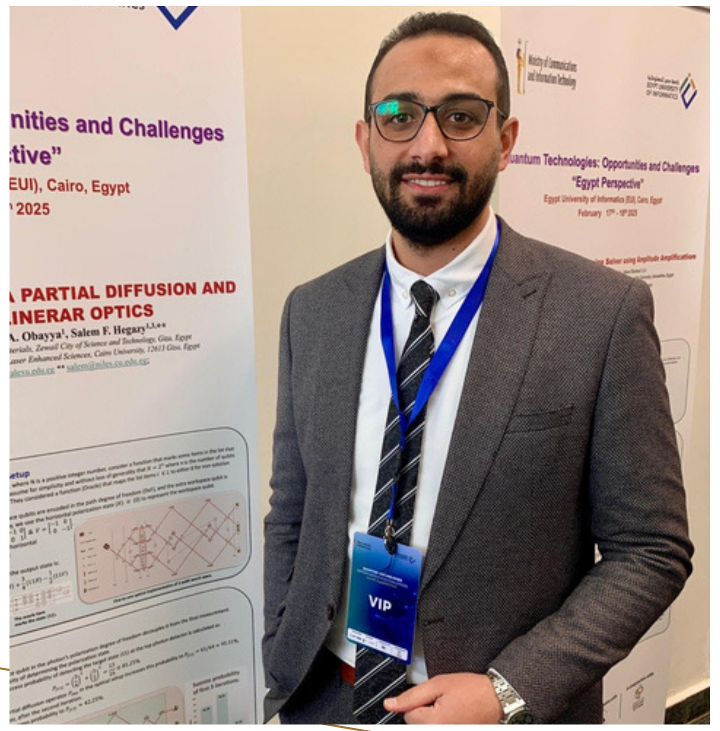
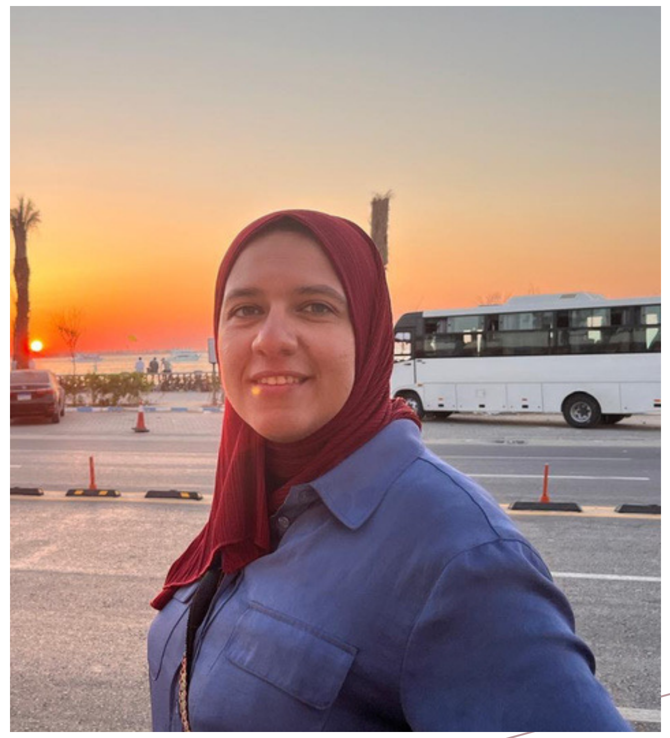
## *Hackathon Overview*

**Hackathon mentor team**








Largest community startup : )

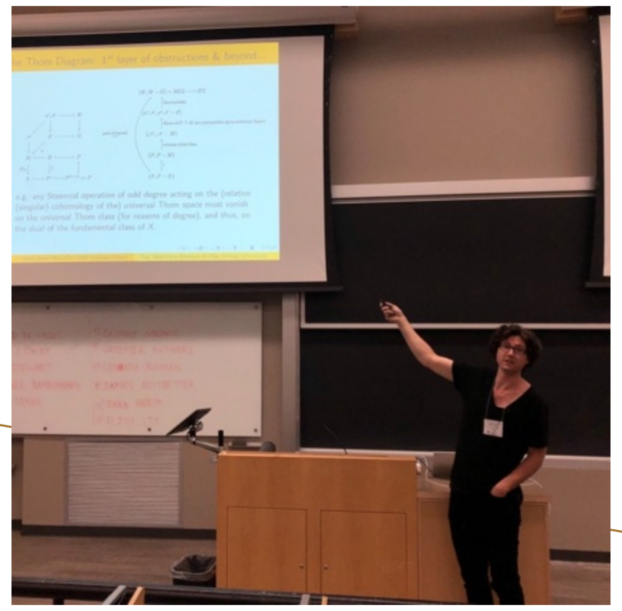
# *Hackathon Overview*

Hackathon mentor team

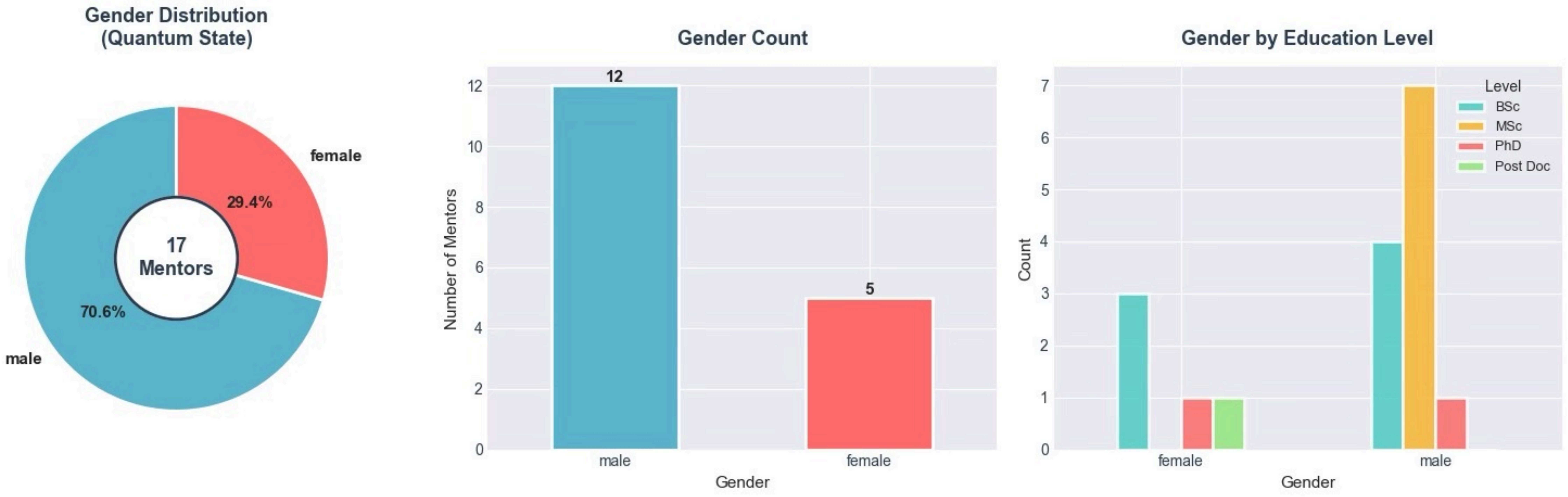




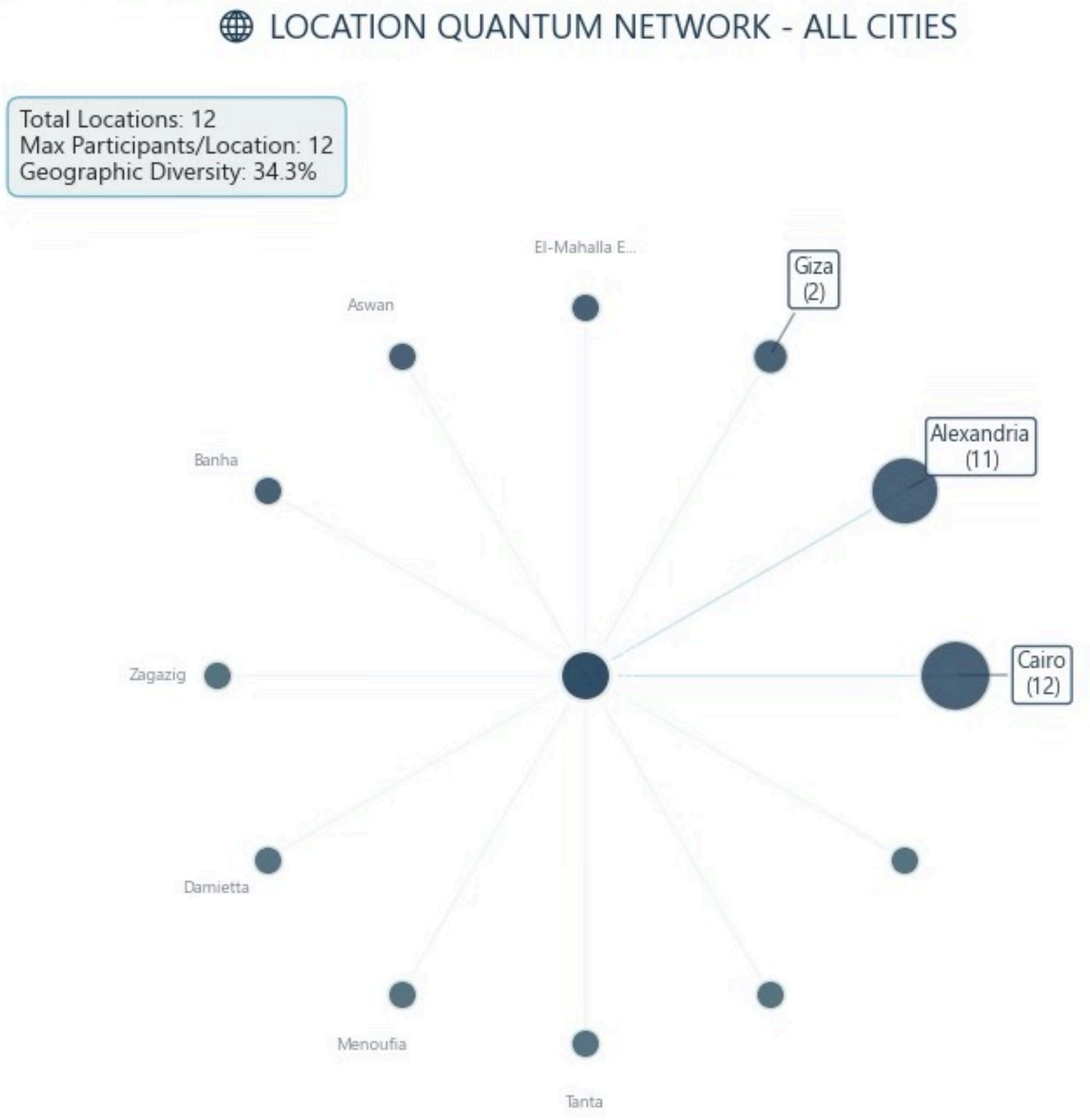



# Alexandria Quantum Hackathon statistics >



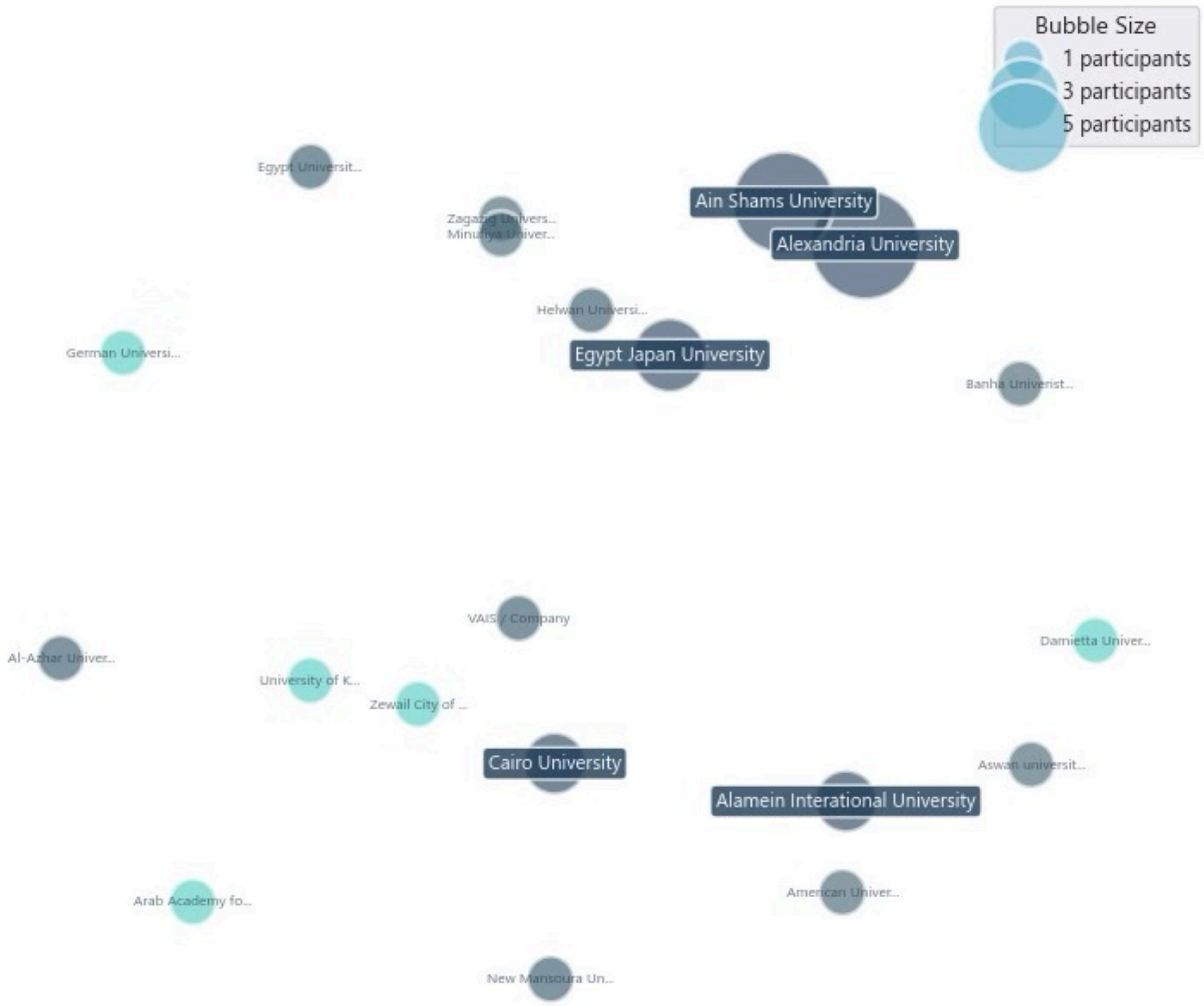
# Alexandria Quantum Hackathon statistics >

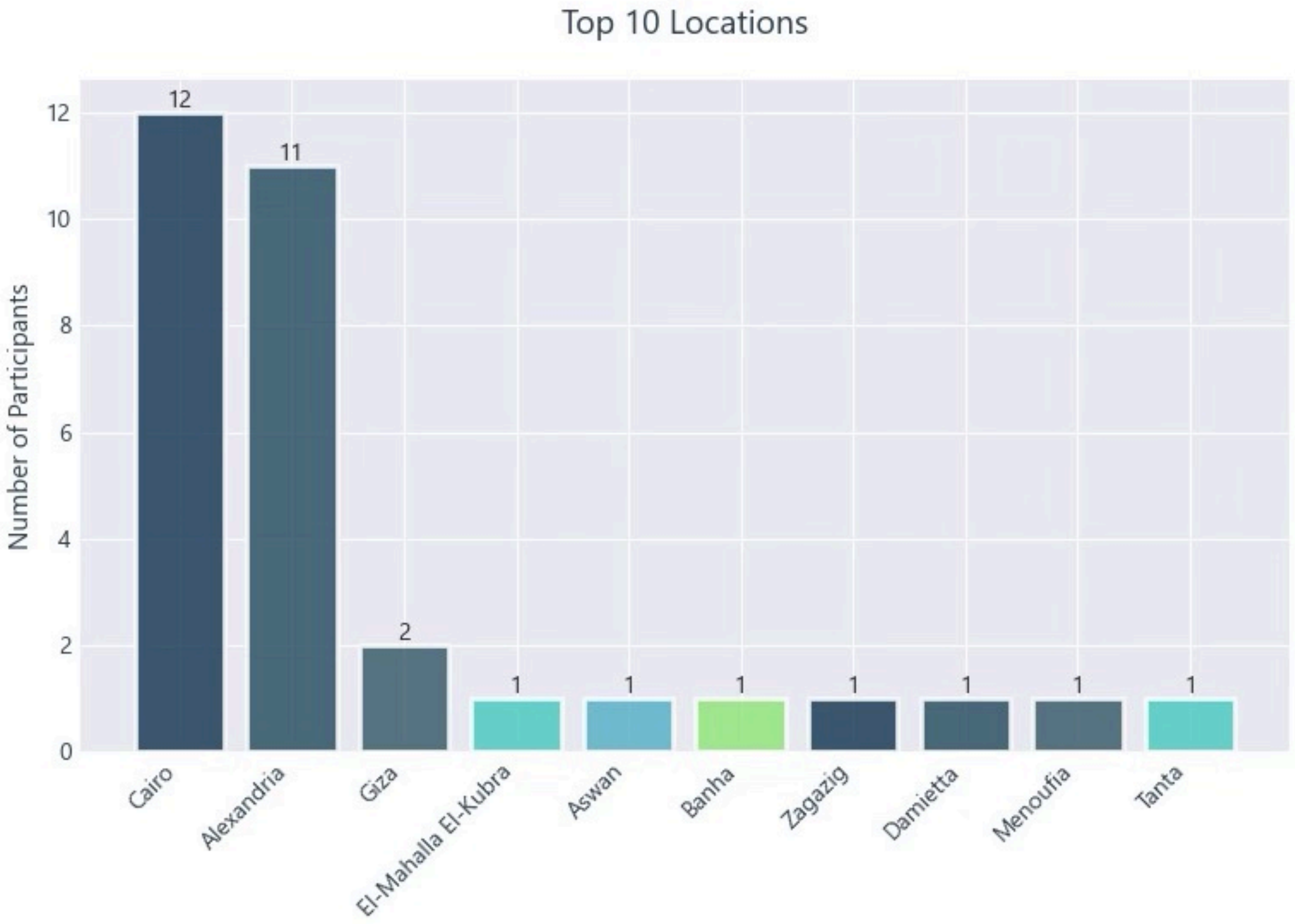
# Alexandria Quantum Hackathon statistics >

ALL INSTITUTIONS - QUANTUM FIELD VISUALIZATION


INSTITUTIONAL QUANTUM BUBBLE NETWORK



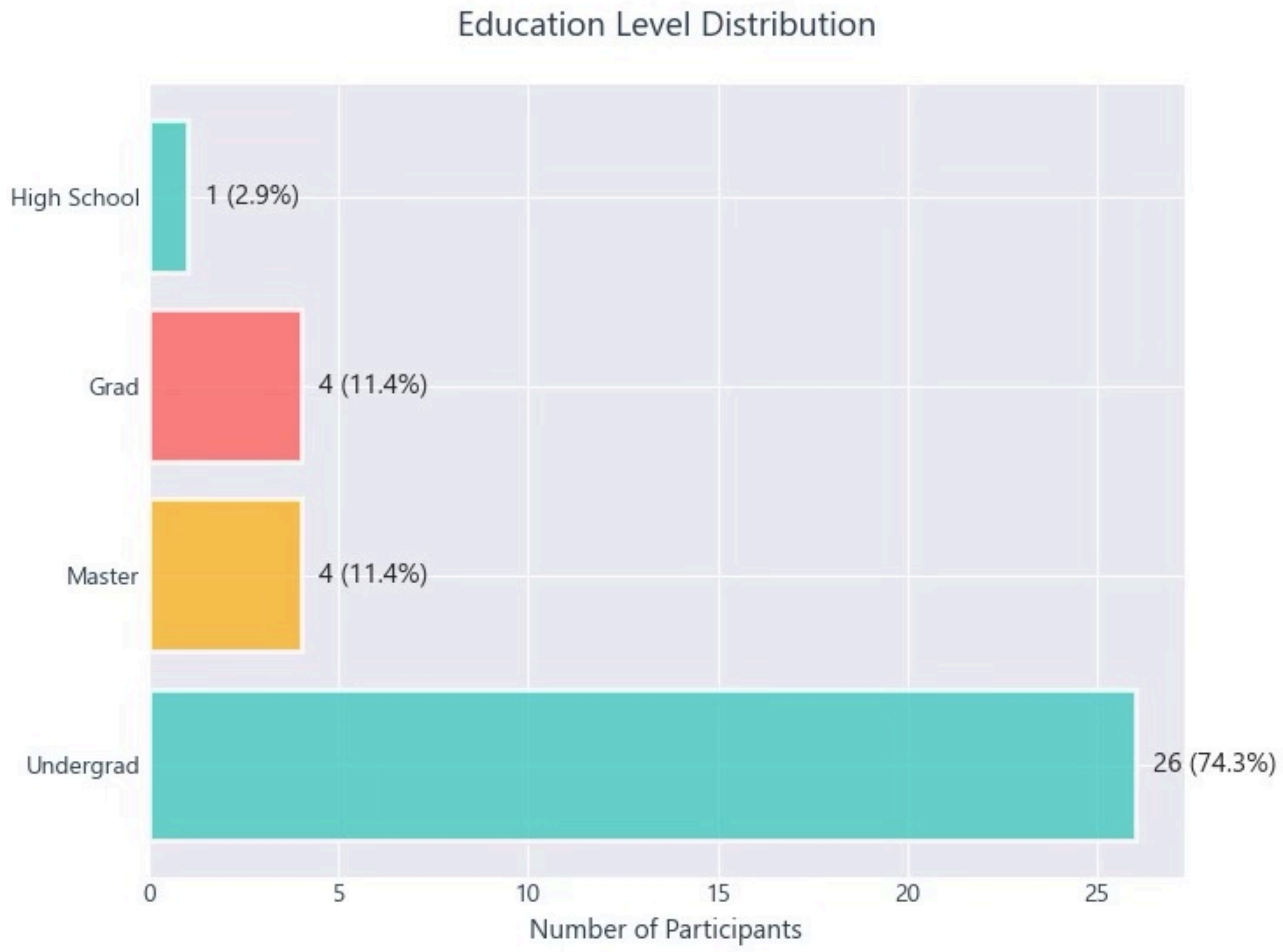
# Alexandria Quantum Hackathon statistics >

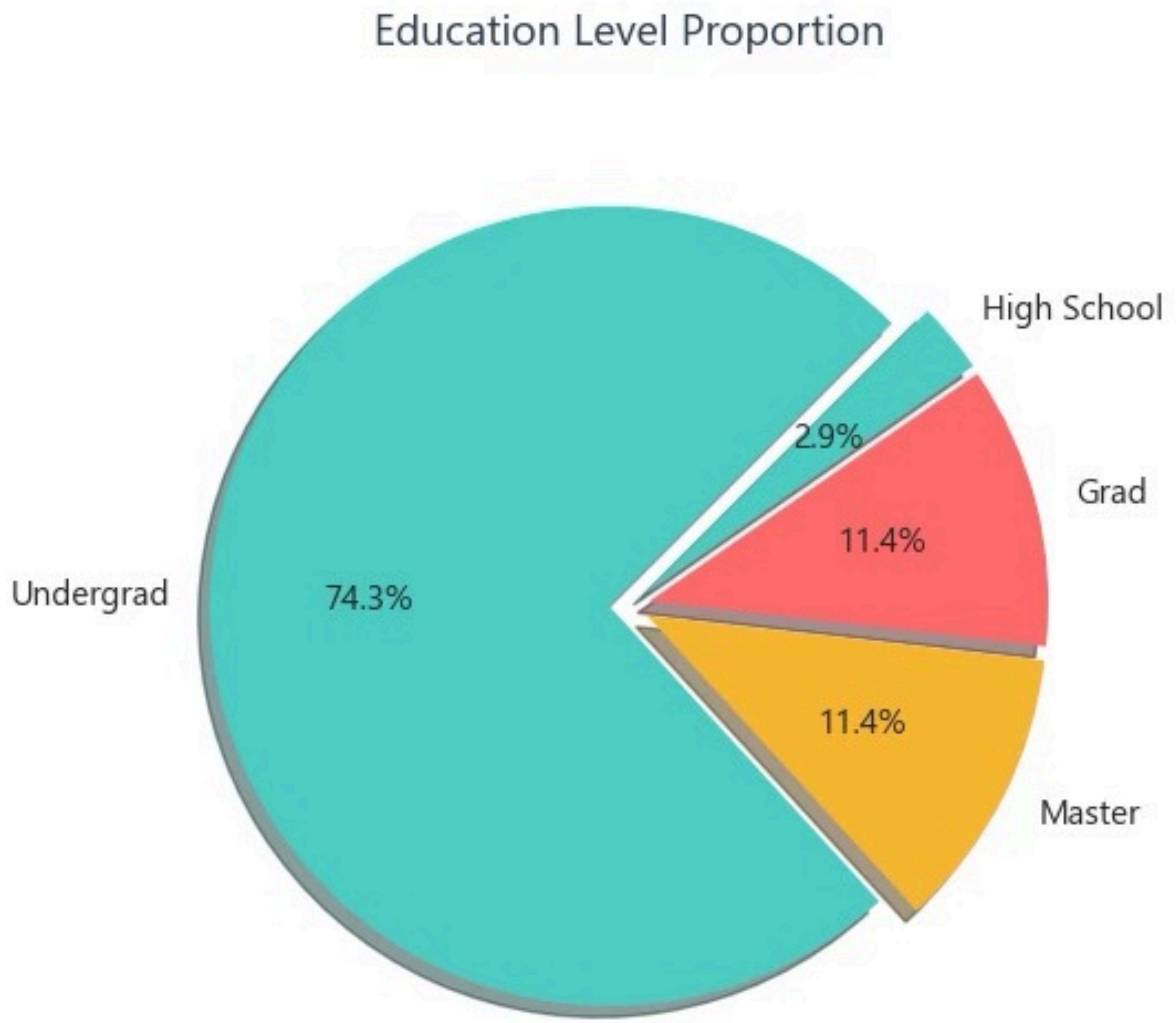



### Geographic Diversity Metrics

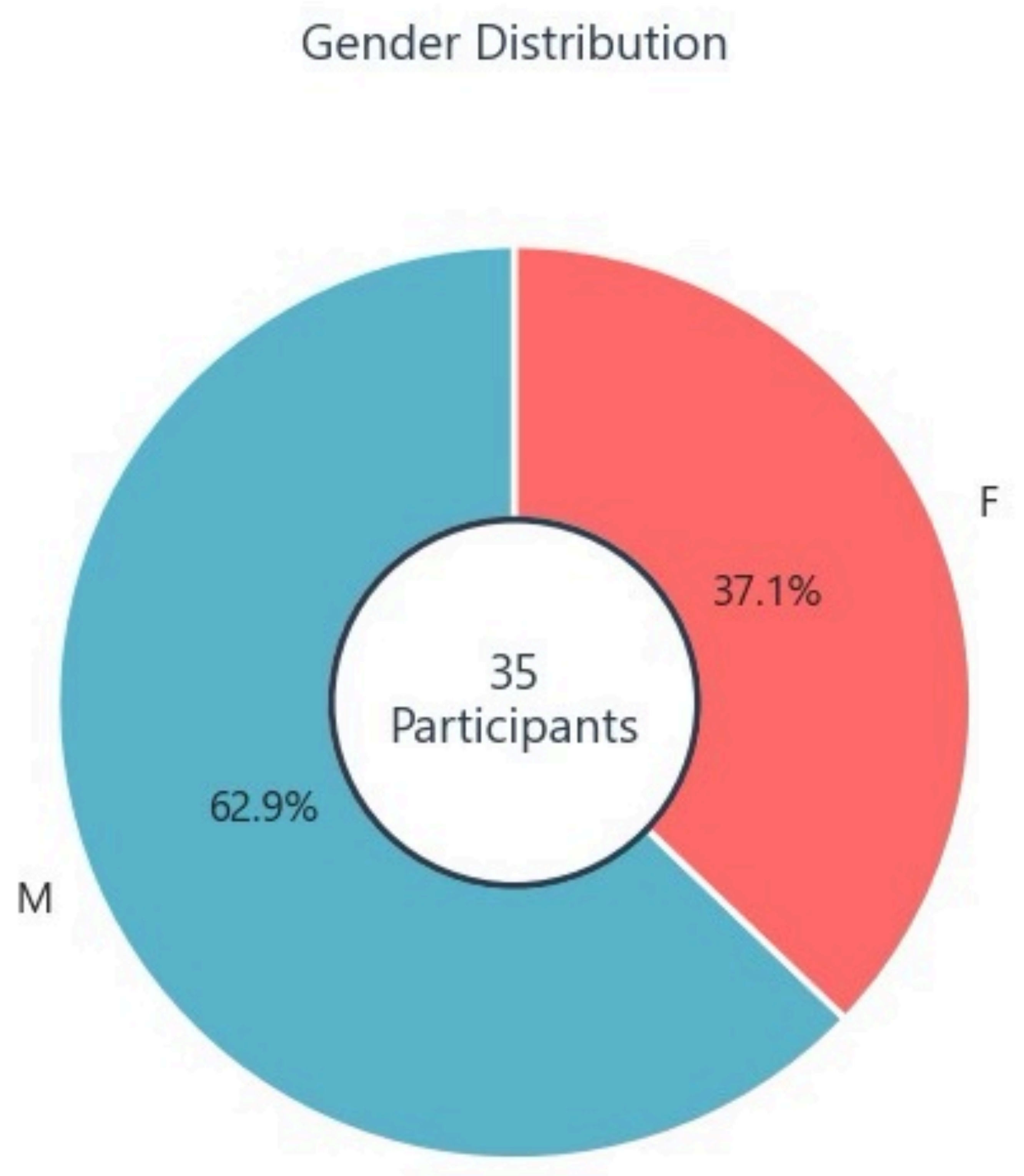
- Total Unique Locations: 12
- Most Common Location: Cairo (12)
- Locations with 1 participant: 9
- Locations with 2+ participants: 3
- Geographic Spread Index: 34.3%

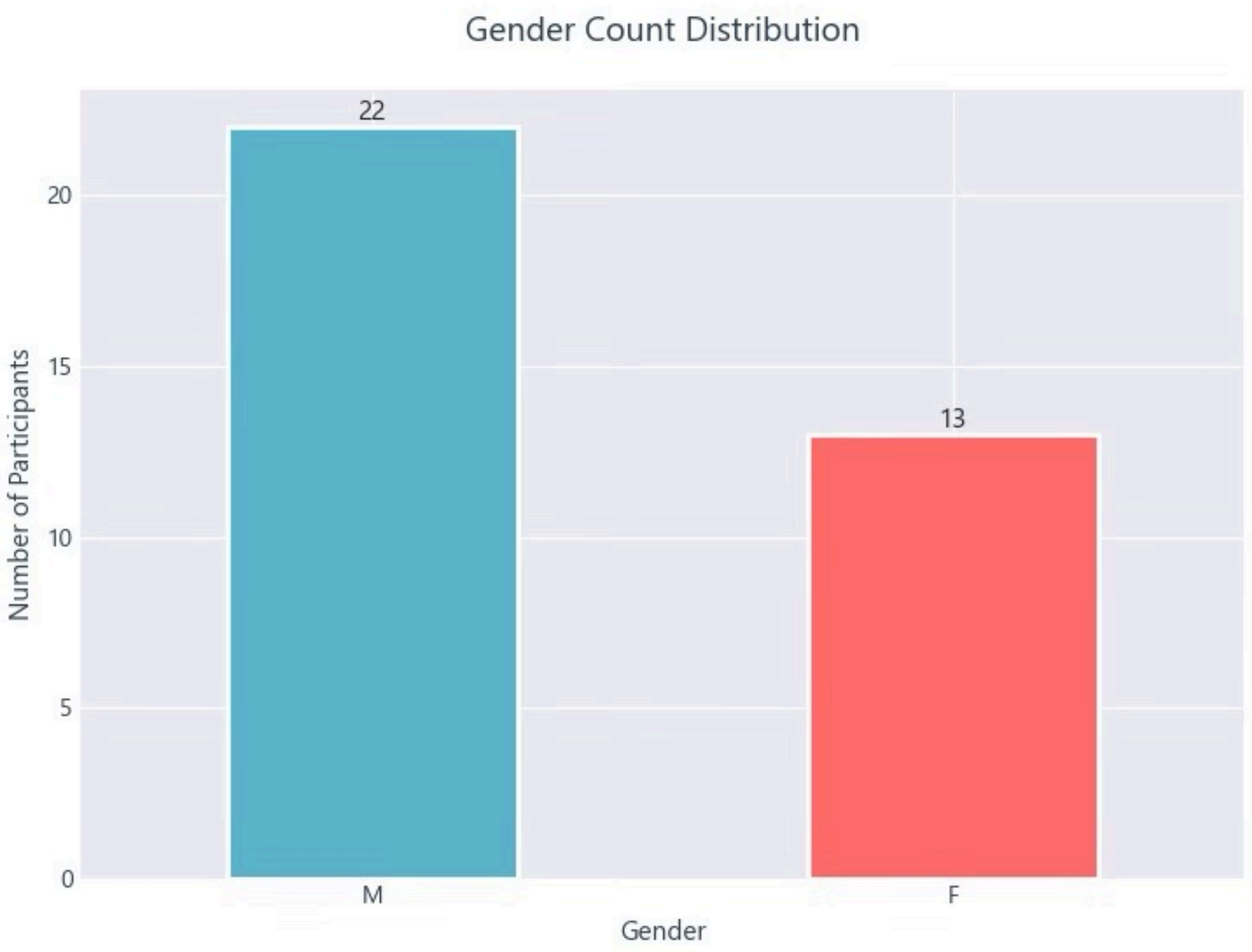
# Alexandria Quantum Hackathon statistics >



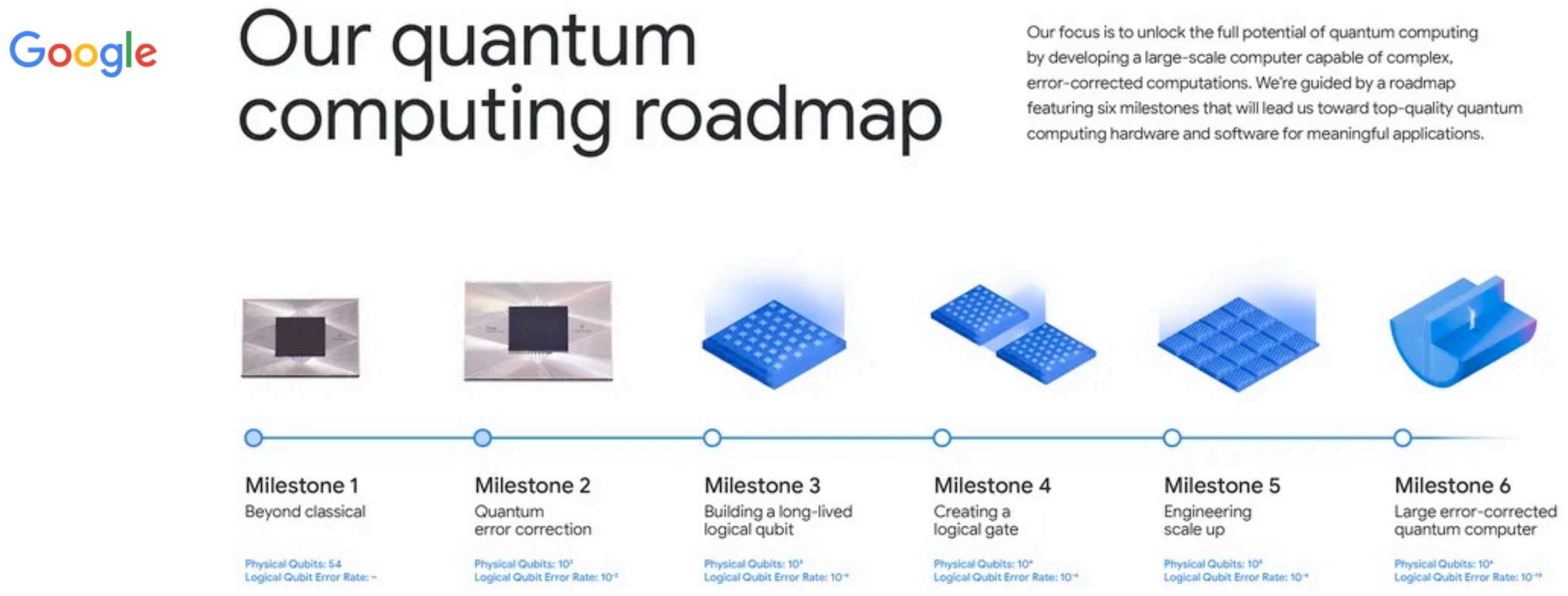



# Alexandria Quantum Hackathon statistics >



# Google quantum roadmap >




**Source:**

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

# Google quantum roadmap >

IBM Technology Roadmaps Client value

IBM Technology Atlas

The future of computing is quantum-centric.

## Quantum Roadmap

**Strategic milestones**

All information being released represents IBM's current intent, is subject to change or withdrawal, and represents only goals and objectives.

*You can learn more about the progress of individual items by downloading the PDF in the top right corner.*

### 2024

**Expand the utility of quantum computing.**

We will improve the quality and speed of quantum circuits to allow running 5,000 gates with parametric circuits.

### 2025

**Demonstrate quantum-centric supercomputing.**

In 2025, we will demonstrate the first quantum-centric supercomputer by integrating modular processors, middleware, and quantum communication. We will also enhance the quality, execution, speed, and parallelization of quantum circuits.

### 2026

**Automate and increase the depth of quantum circuits.**

We will enable quantum circuits with 7,500 gates through circuit quality improvement.

### 2027

**Scale quantum computing.**

We will scale qubits, electronic infrastructure, and software to footprint, cost, and energy usag quality of quantum circuits will to allow running 10,000 gates.

IBM

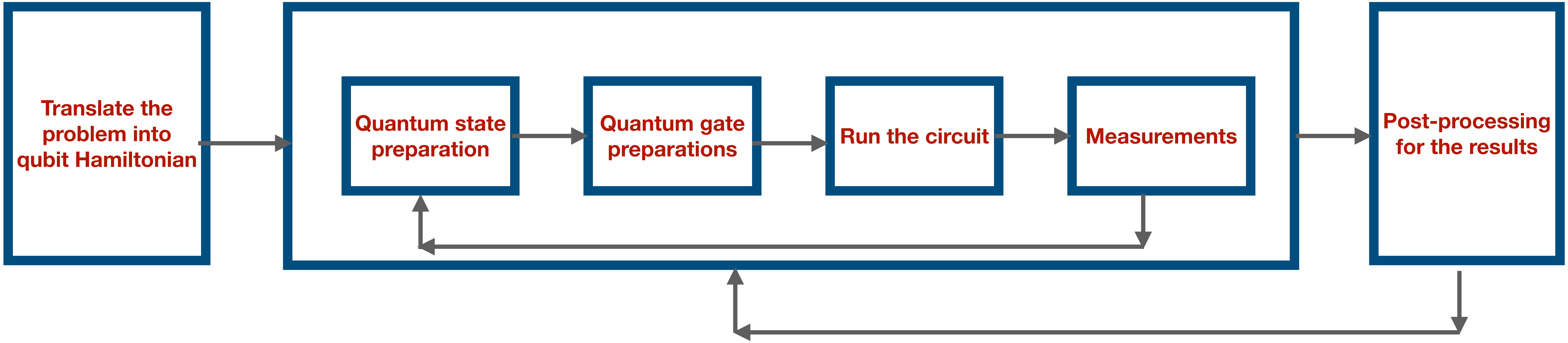
**Sources:**

https://www.ibm.com/roadmaps/quantum/

https://www.ibm.com/think/topics/quantum-centric-supercomputing

# 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.**

# Is there a Moore's law for quantum computing? >

Moore's empirical law cannot easily be translated to an equivalent in quantum computing.

- Qubit lifetimes
- Qubit fidelities
- Physical qubits
- Logical qubits

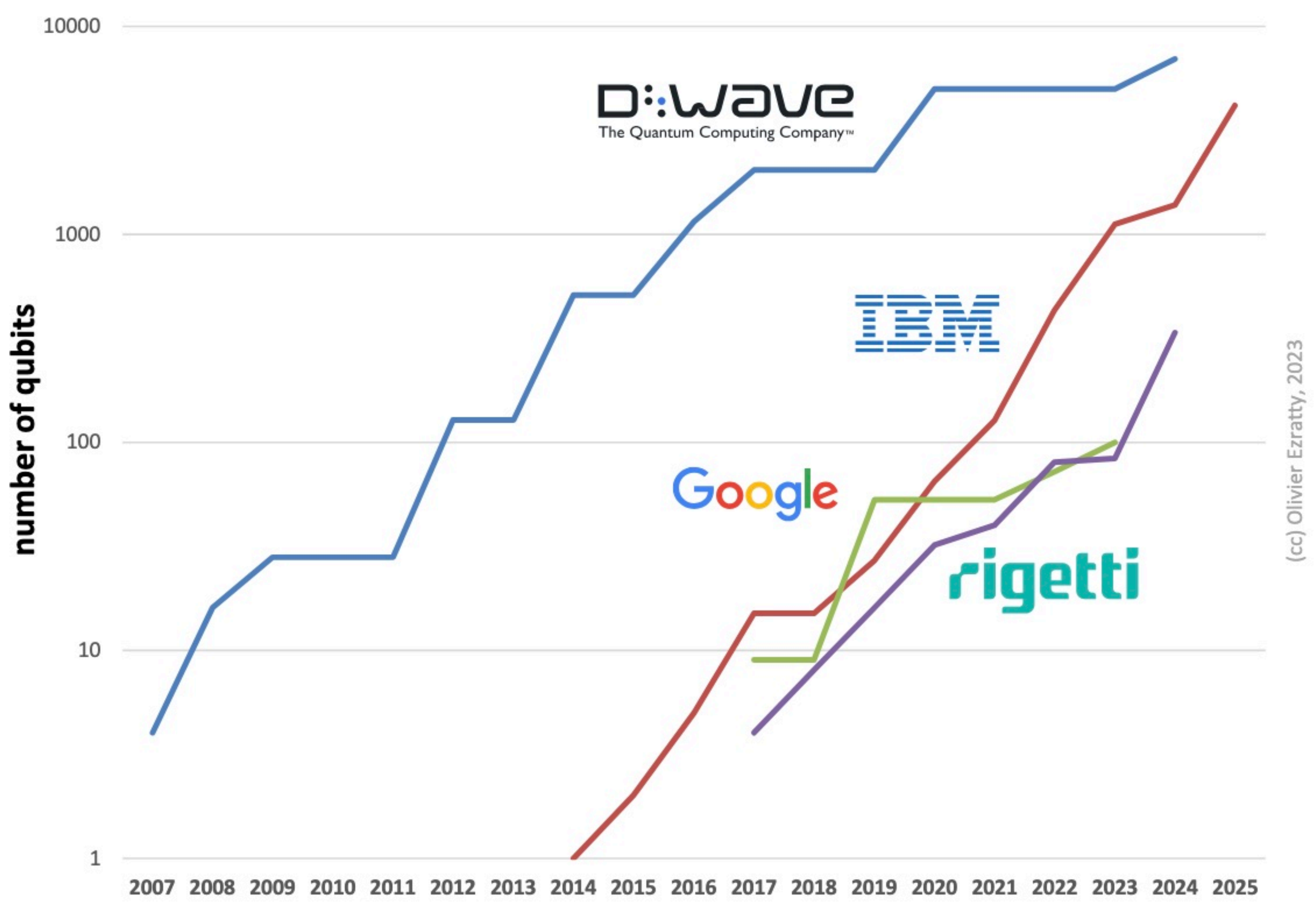



Figure 6: evolution of the number of physical qubits with D-Wave, IBM, Google and Rigetti. Compilation: Olivier Ezratty.

**Sources:**

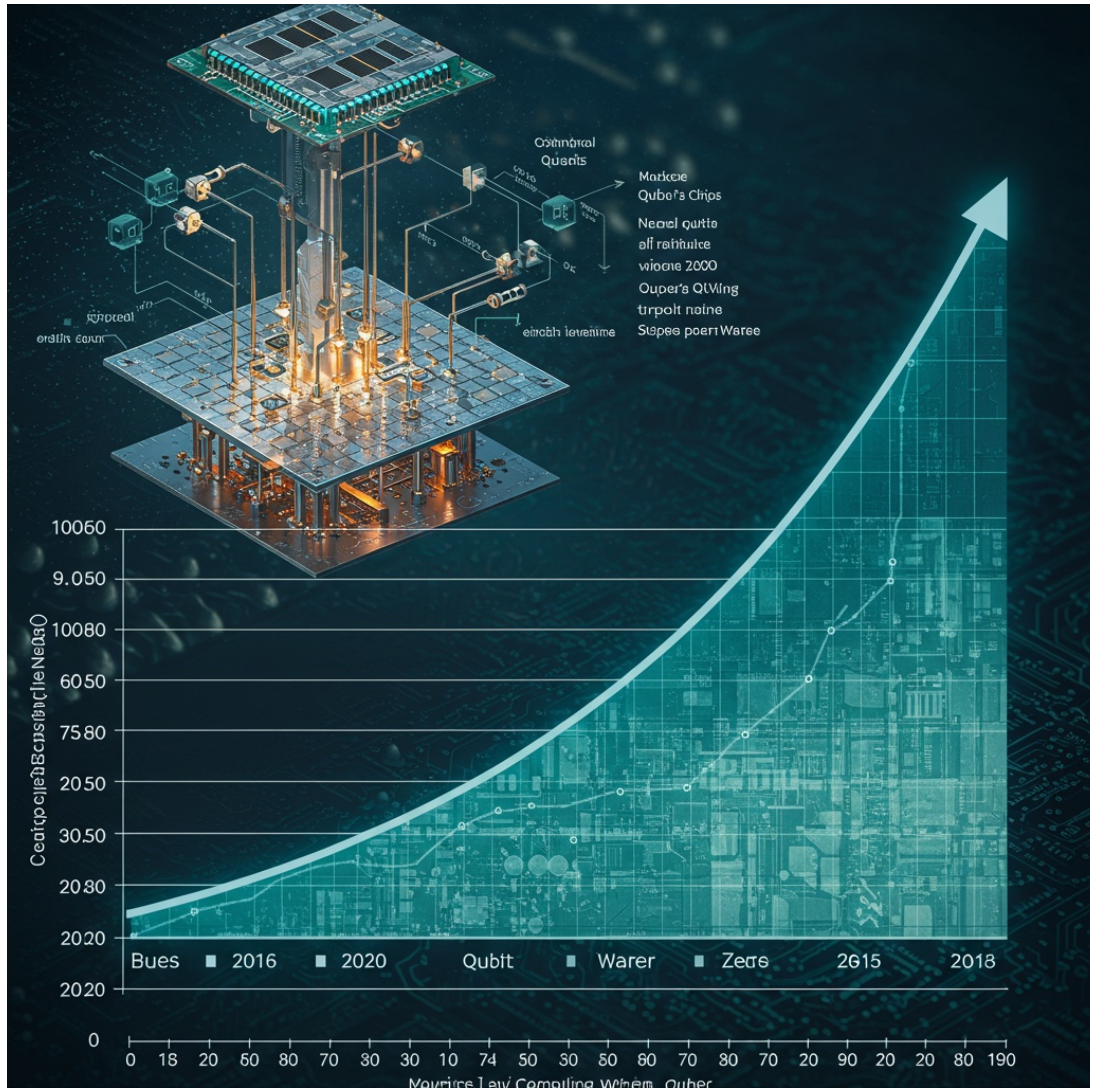
https://arxiv.org/pdf/2303.15547

https://www.oezratty.net/wordpress/2024/understanding-quantum-technologies-2024/

# Is there a Moore’s law for quantum computing? >

## Moore’s empirical law cannot easily be translated to an equivalent in quantum computing.

- **Complex Metrics**: Quantum progress depends on qubit quality, connectivity, and error rates, not just qubit count like transistor density in Moore's Law.
- **Quality over Quantity**: More qubits alone aren't enough; maintaining stability and low errors is crucial and gets harder.
- **Diverse Hardware**: Various quantum technologies scale differently, unlike the uniform silicon base of classical computing.
- **Exponential Scaling**: Quantum power grows exponentially with qubits, not through physical shrinking like transistors.
- **Early Market**: No economic driver (yet). Quantum computing lacks the mass market that drove consistent growth in classical computing.



# What Quantum Advantage Really Means?>

## | What if the execution on actual quantum hardware is not available? >

# Is there a Moore's law for quantum computing? >

## You can still work and excel in quantum computing without hardware

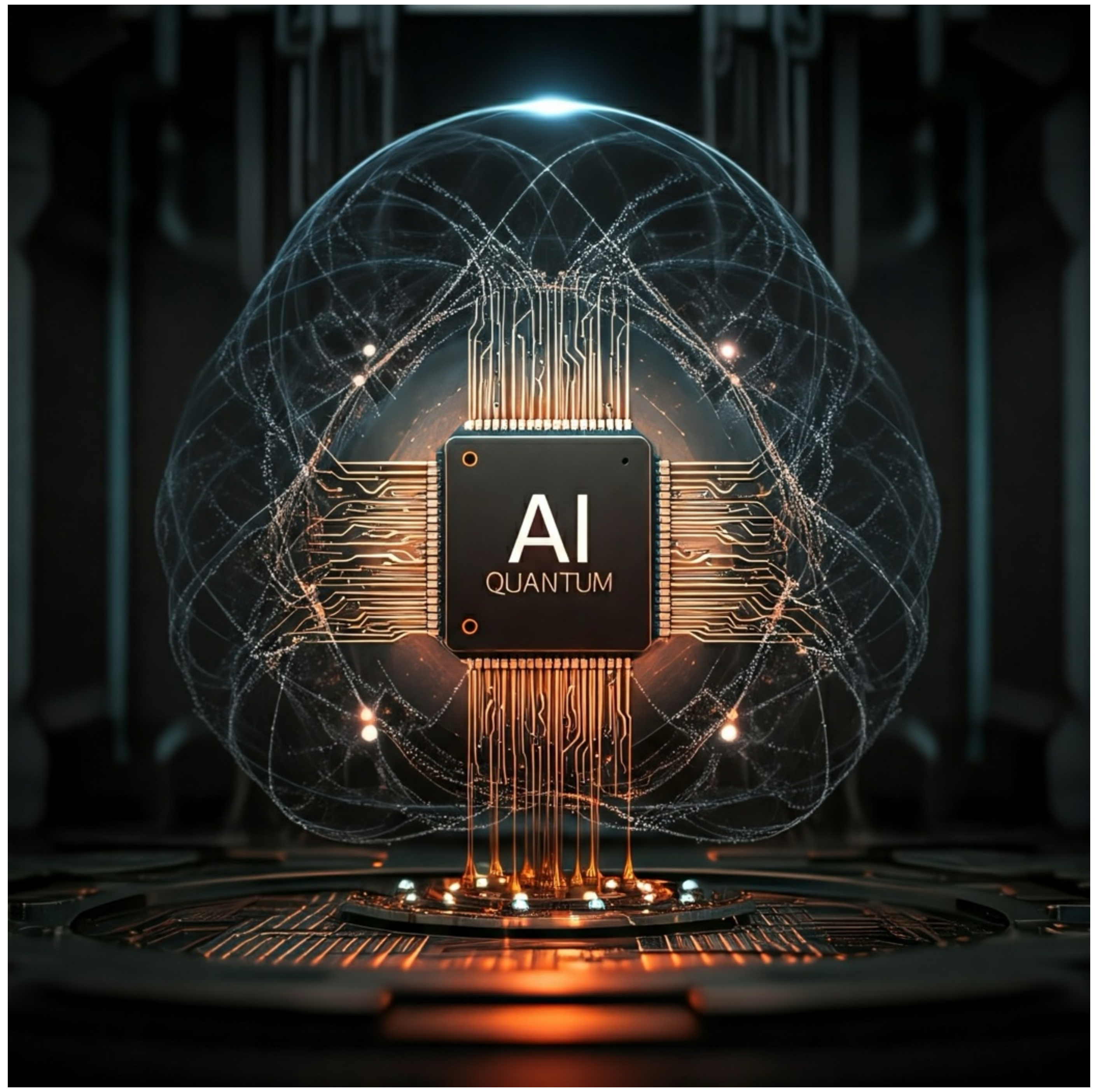
- **Use existing simulators**
- **Develop simulators**
- **Software and consultancy**
- **Algorithm development of quantum computing and use cases**
- **Research and education**
- **Provide cloud simulations services**

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

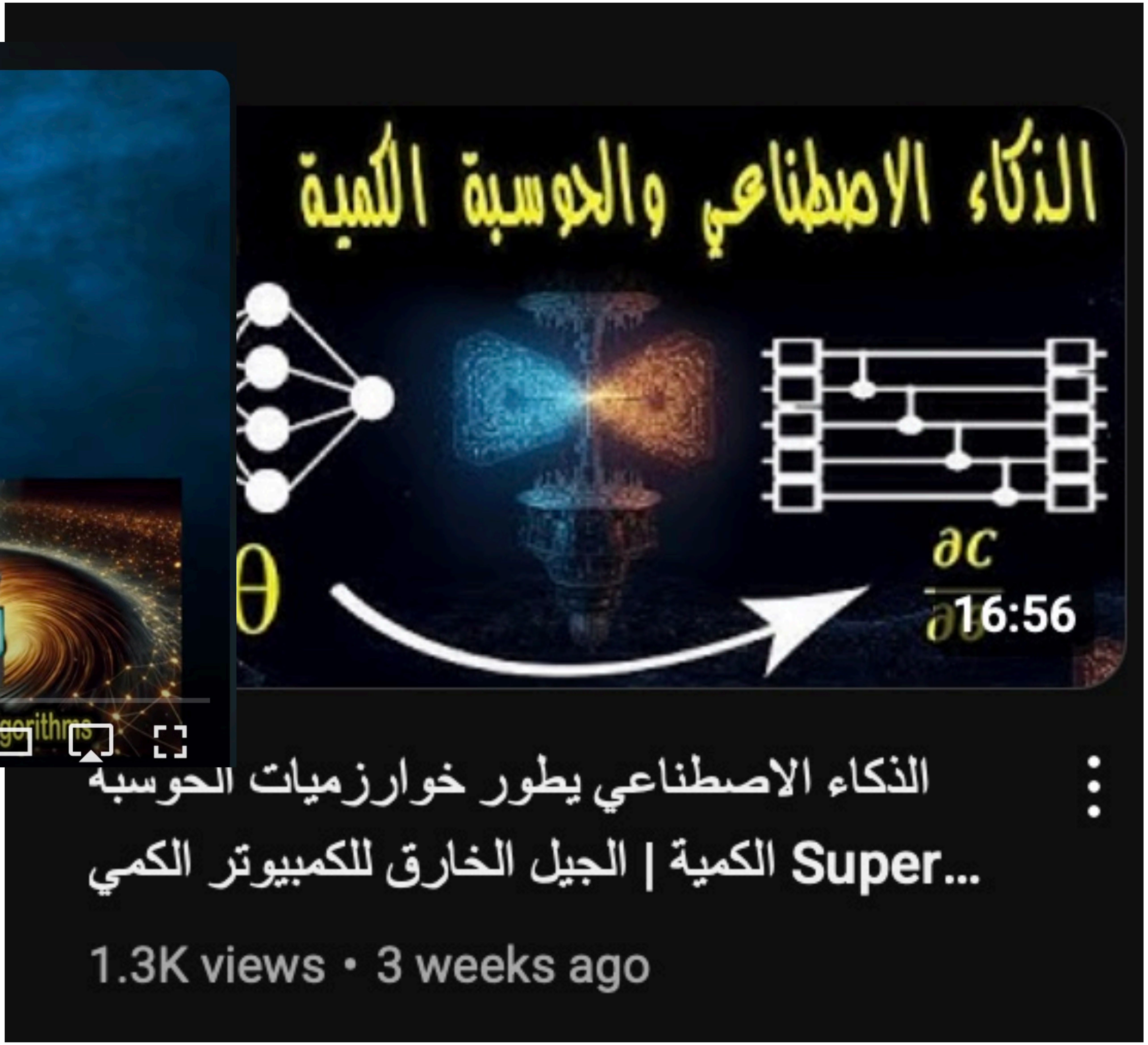
# Quantum AI in quantum computing >

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.



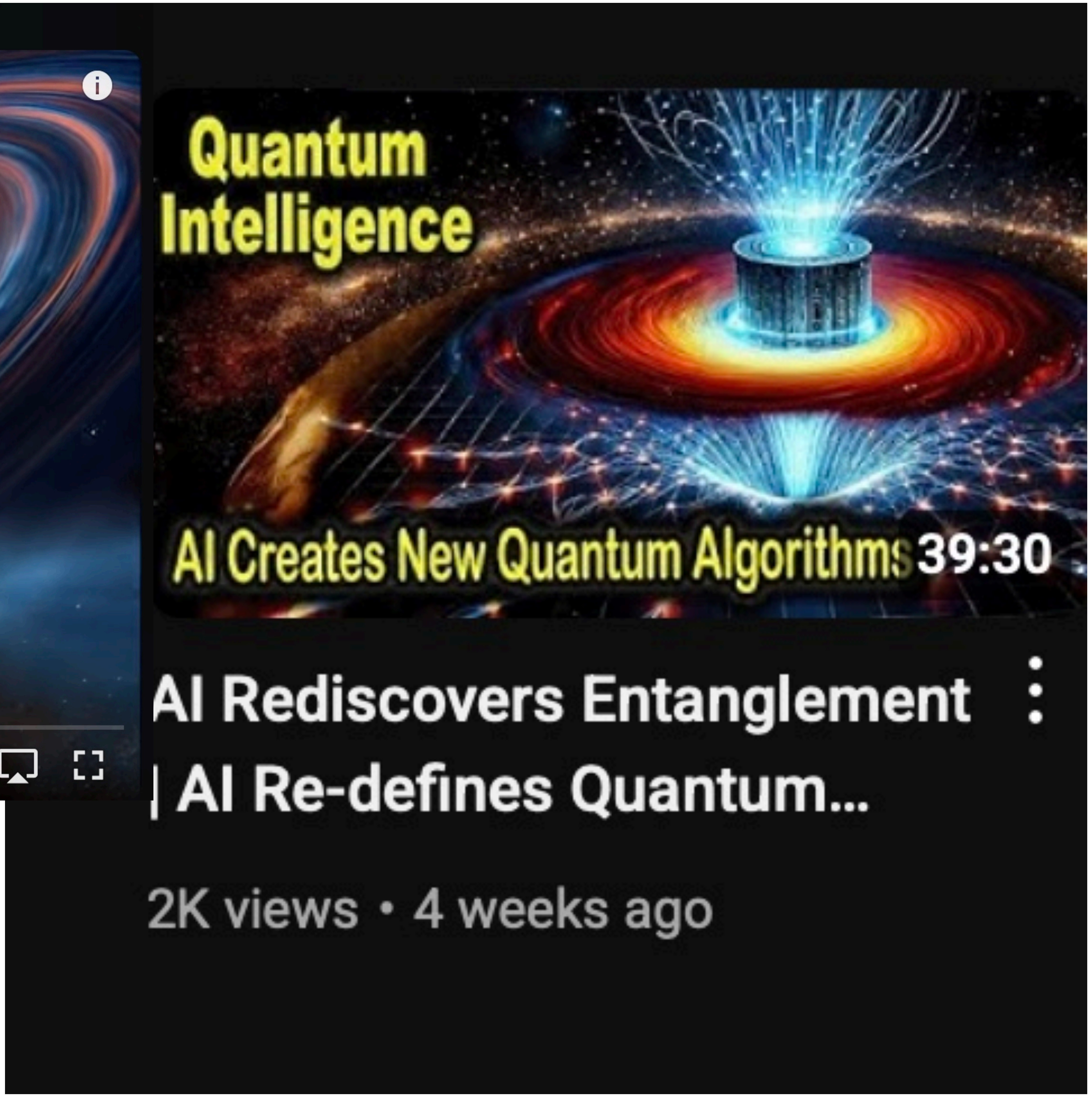
# The generative quantum eigensolver (GQE) >


**Source:**

https://www.youtube.com/watch?v=kHsSrYFv6Lc

# AI creates new quantum protocols >


**Source:**

https://www.youtube.com/watch?v=ZC_aVrM1dZs

# LLM optimizes feature maps for quantum machine learning>

Automating quantum feature map design via large language models

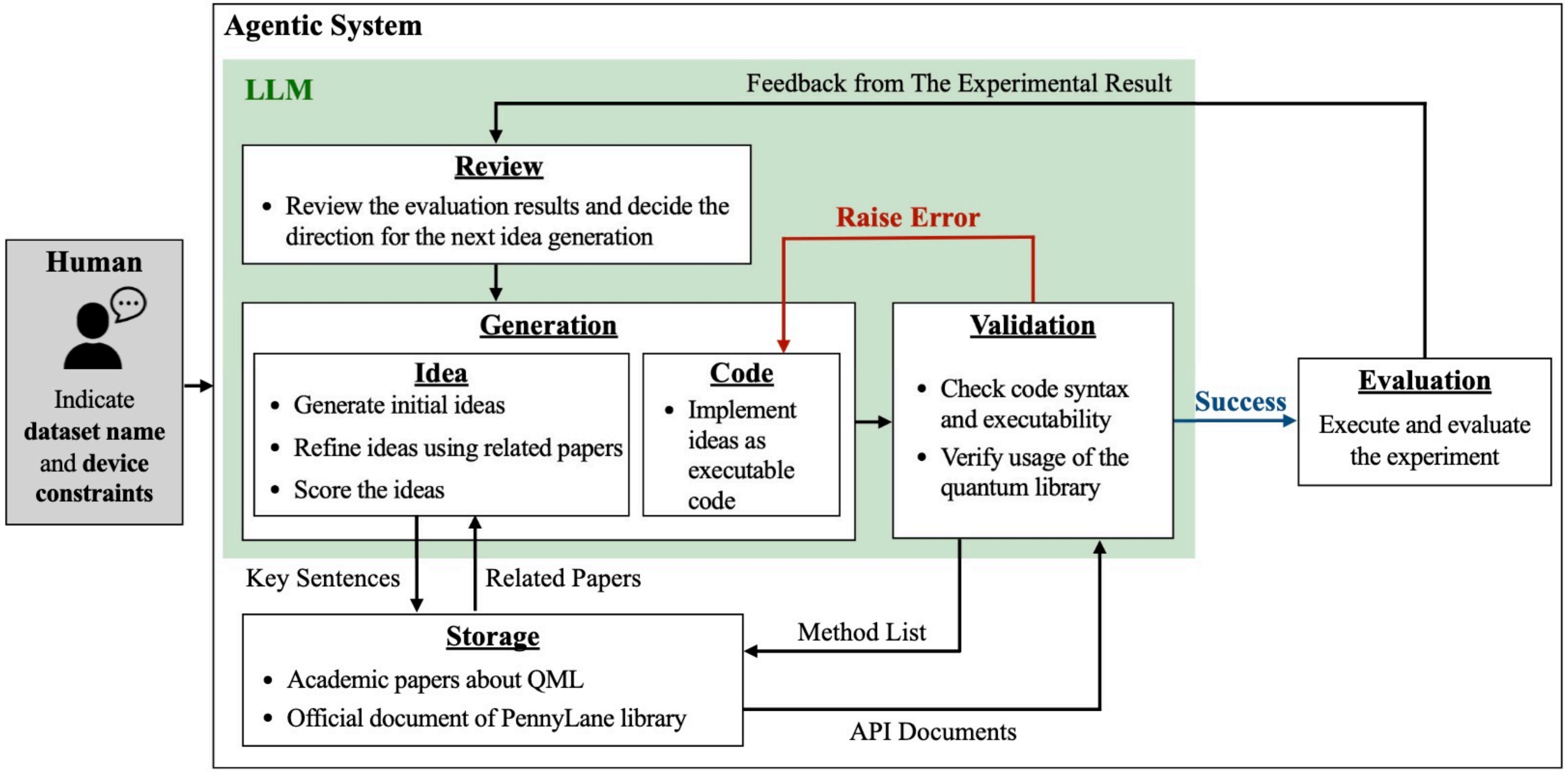


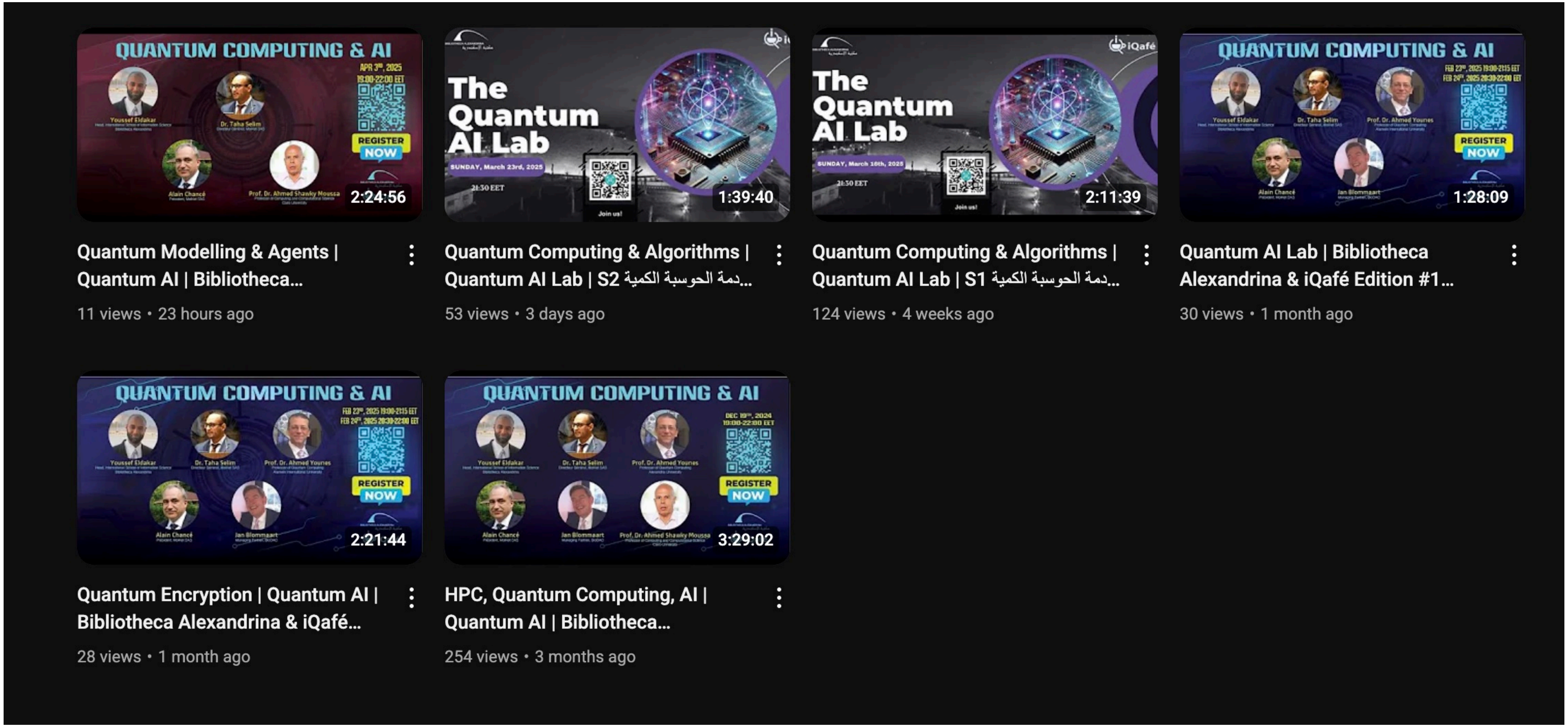

*Figure 1.* Overview of the agentic system for automatic generation of quantum feature maps. When a user provides task instructions to the system, five internal components work collaboratively to autonomously conduct experiments and improvements. As a result, the system generates an executable program that implements a quantum feature map capable of performing the task with high accuracy.

**Source:**

https://arxiv.org/pdf/2504.07396

# Quantum AI monthly series >

## Three editions: Dec 2024, Feb & March 2025



# Alexandria Quantum Hackathon and Summer courses

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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

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/

AI Index: State of AI in 13 Charts
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# References >


Olivier Ezratty, quantum computing roadmaps

https://www.oezratty.net/Files/Conferences/Olivier%20Ezratty%20QEI%20Workshop%20Jan2025.pdf

Olivier Ezratty, Is there a “Moore's law” for quantum computing?

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Olivier Ezratty, Understanding Quantum Technologies 2024

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# Thank you! >