Simulating Chemistry with Quantum Computing

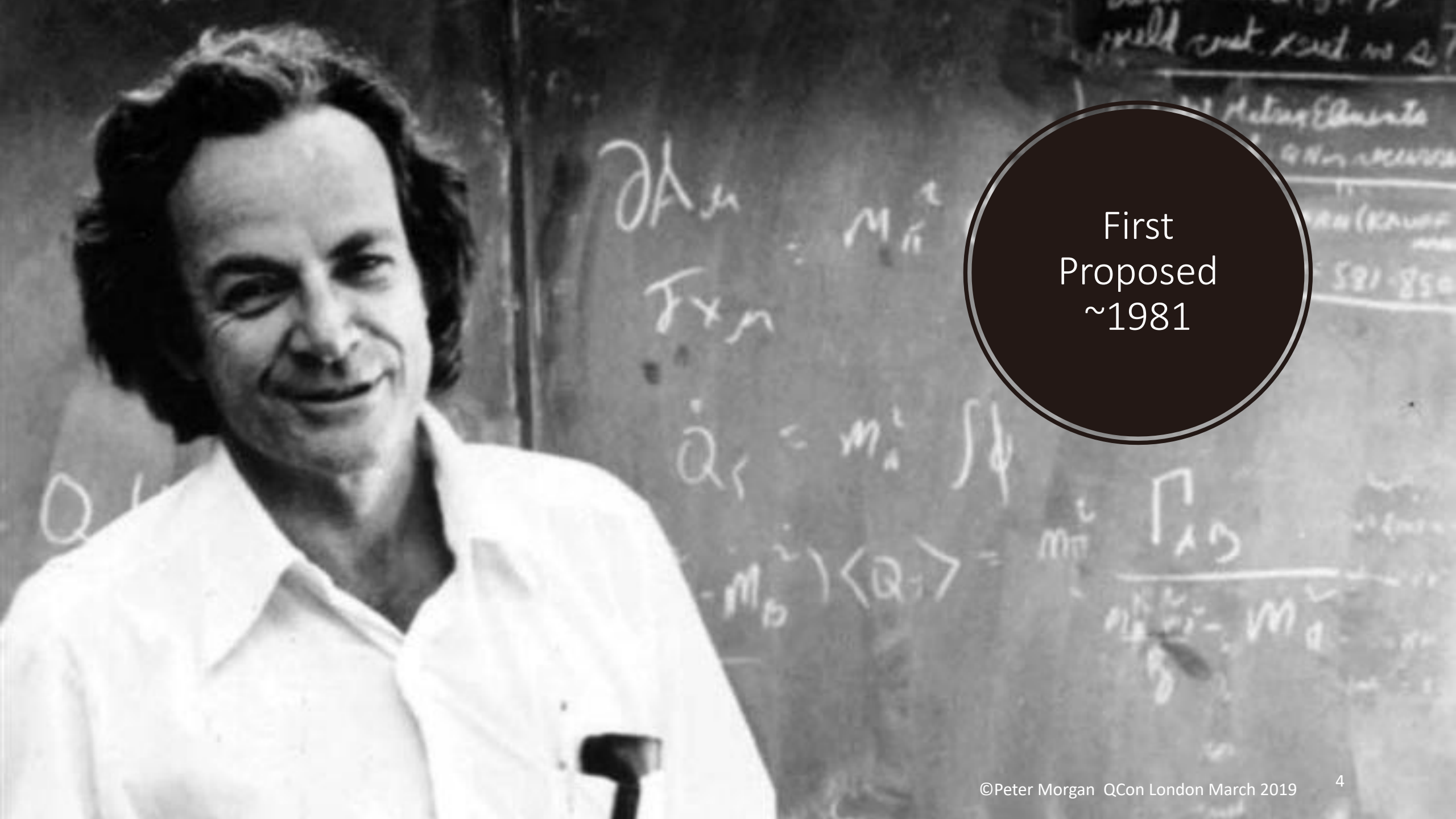
QCon by InfoQ

Peter Morgan
www.deeplp.com

Outline of Talk

- What is Quantum Computing
  - Background
  - Hardware
  - Frameworks
  - Applications
- Simulating Chemistry
  - Classical Frameworks
  - Quantum Frameworks
- Qiskit Walkthrough
  - Application
  - Code example
- Conclusions

What is Quantum Computing?



Early Pioneers - 1994

(top, left) Richard Jozsa, William K. Wootters, Charles H. Bennett. (bottom, left) Gilles Brassard, Claude Crépeau, Asher Peres. Photo: André Berthiaume.

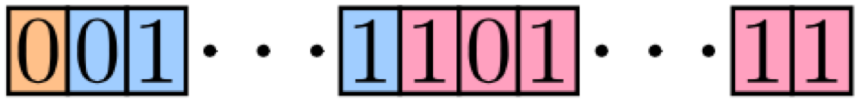
QIP 2019
@QIPConference

Following

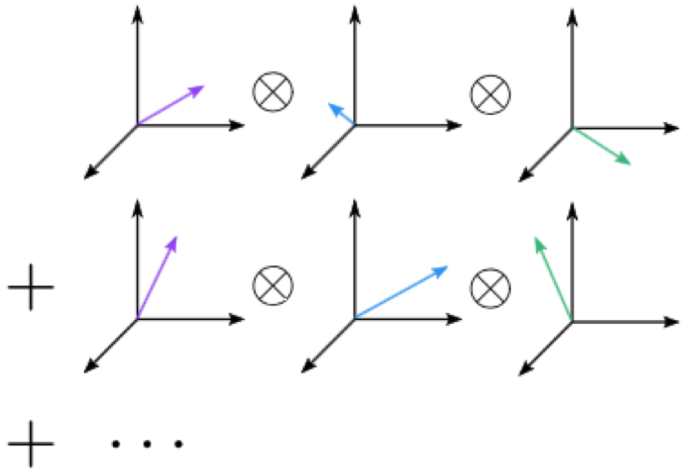
And that's a wrap for #qip2019! Thanks to everyone involved for a great conference, we hope you enjoyed it!

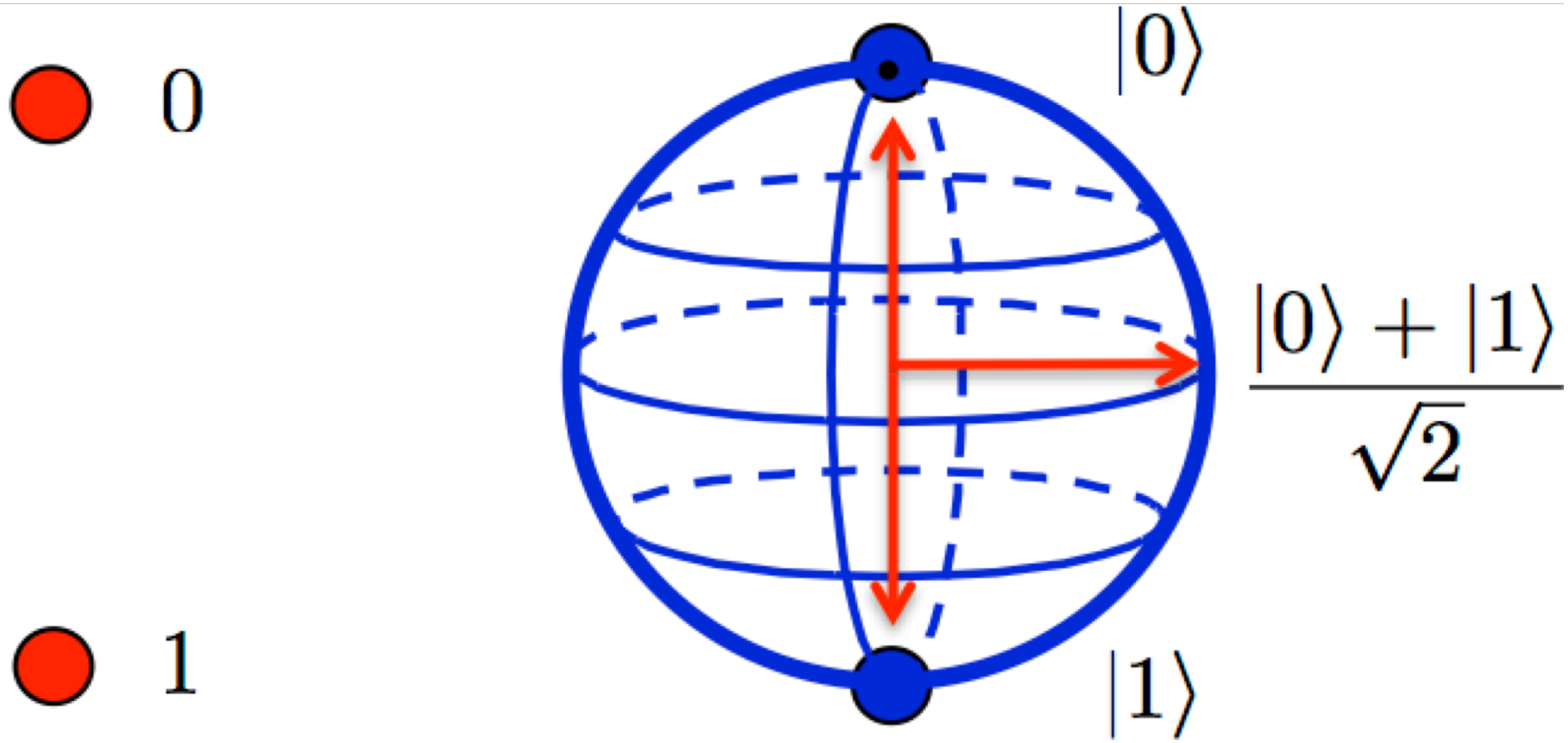
Classical vs Quantum – What's the Difference?

Classical information



Quantum information





Classical Bit **Qubit**

Quantum States

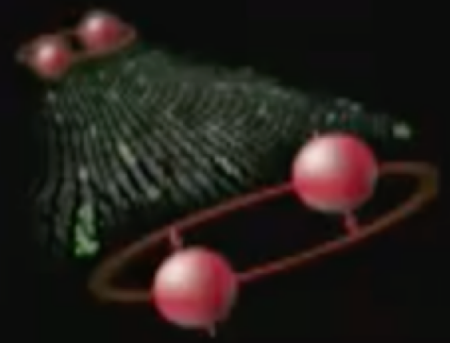
$$|+_{\theta_j}\rangle = \frac{1}{\sqrt{2}}\left(|0\rangle + e^{i\theta_j}\,|1\rangle\right)$$

$$|-_{\theta_j}\rangle = \frac{1}{\sqrt{2}}\left(|0\rangle - e^{i\theta_j}\,|1\rangle\right)$$

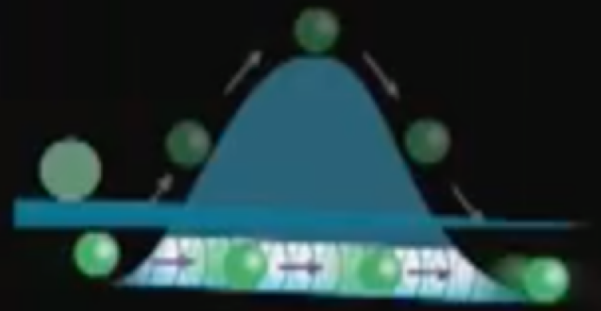
Quantum Weirdness

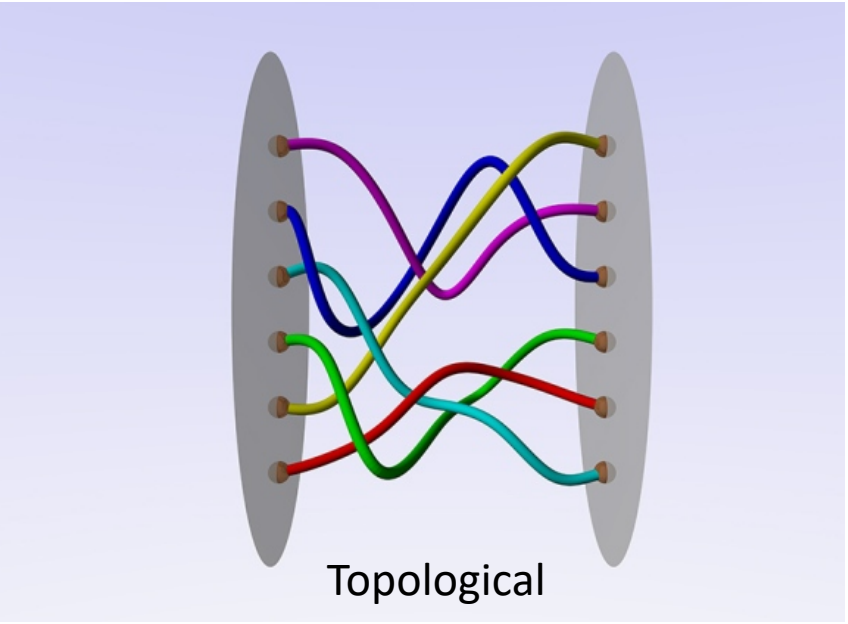
Superposition

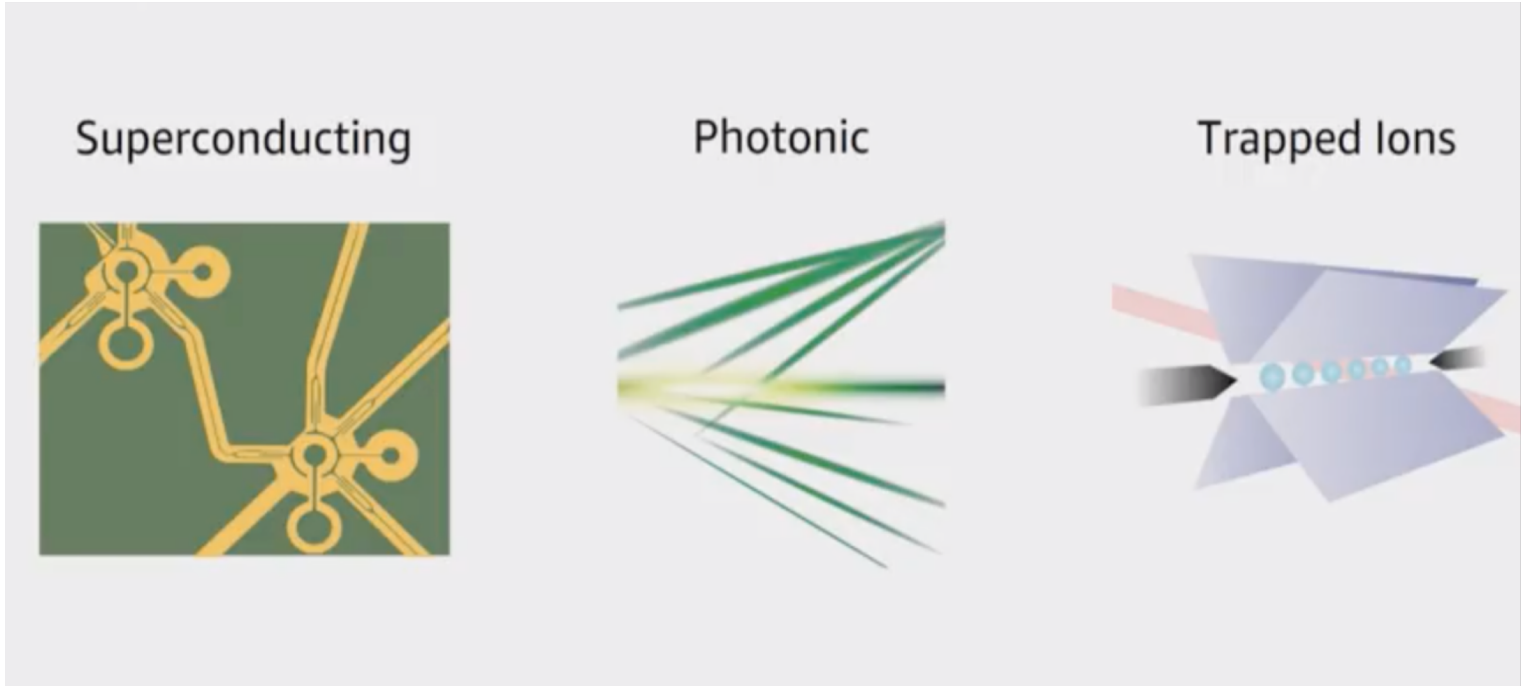
Entanglement

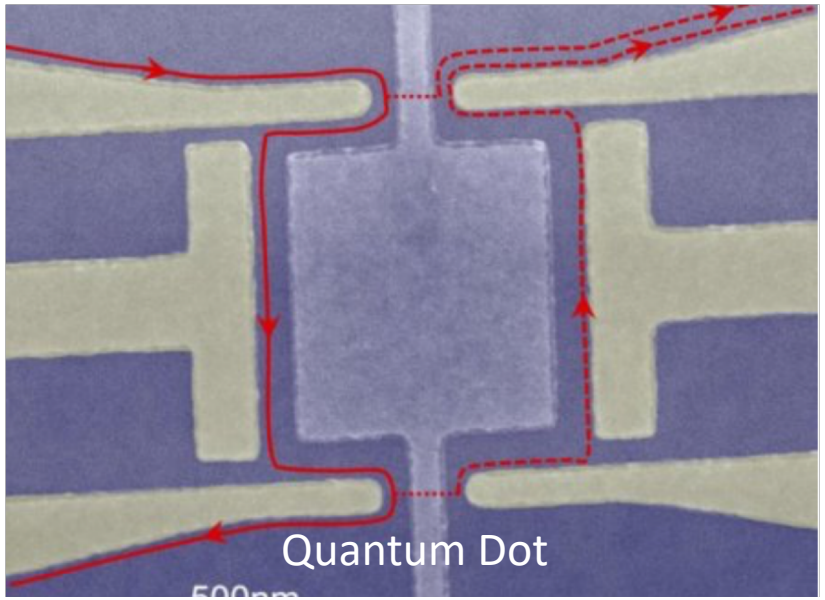


Quantum Tunneling



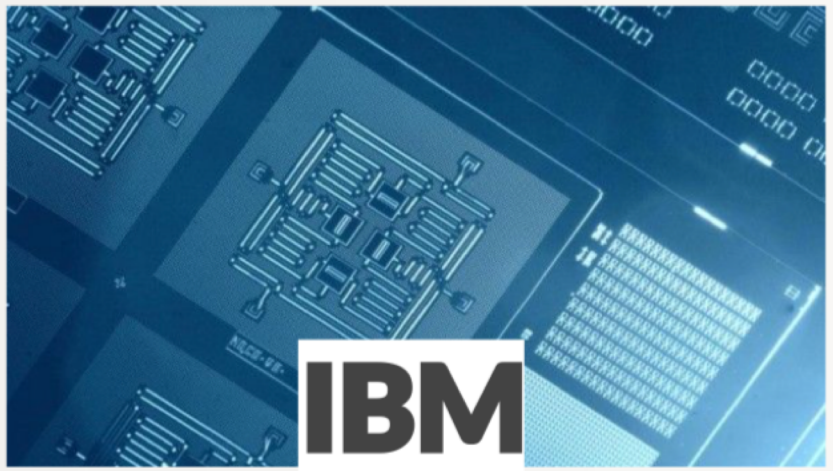


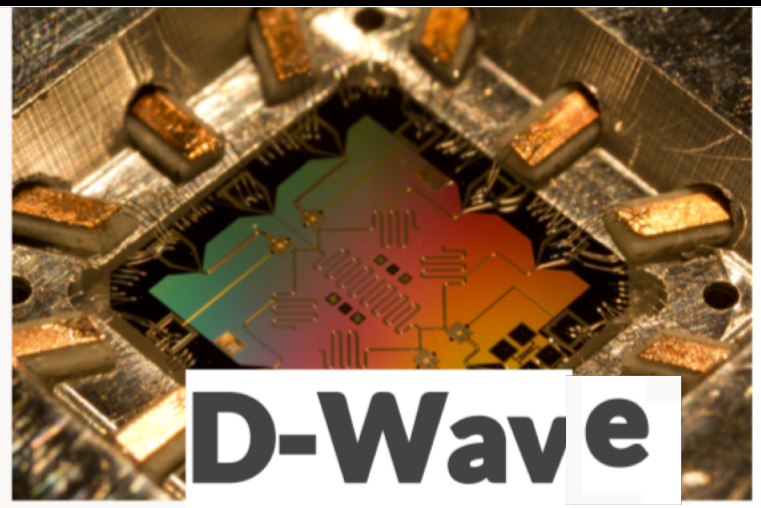


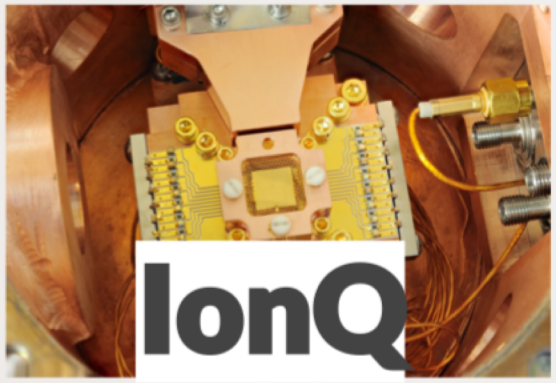


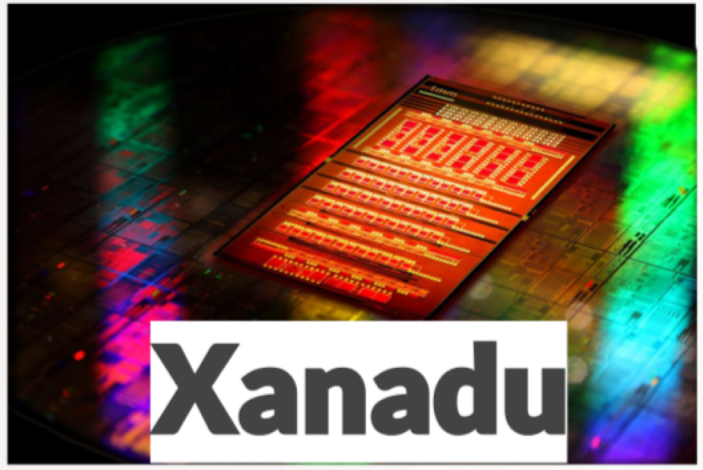
Types of Hardware

Hardware Companies







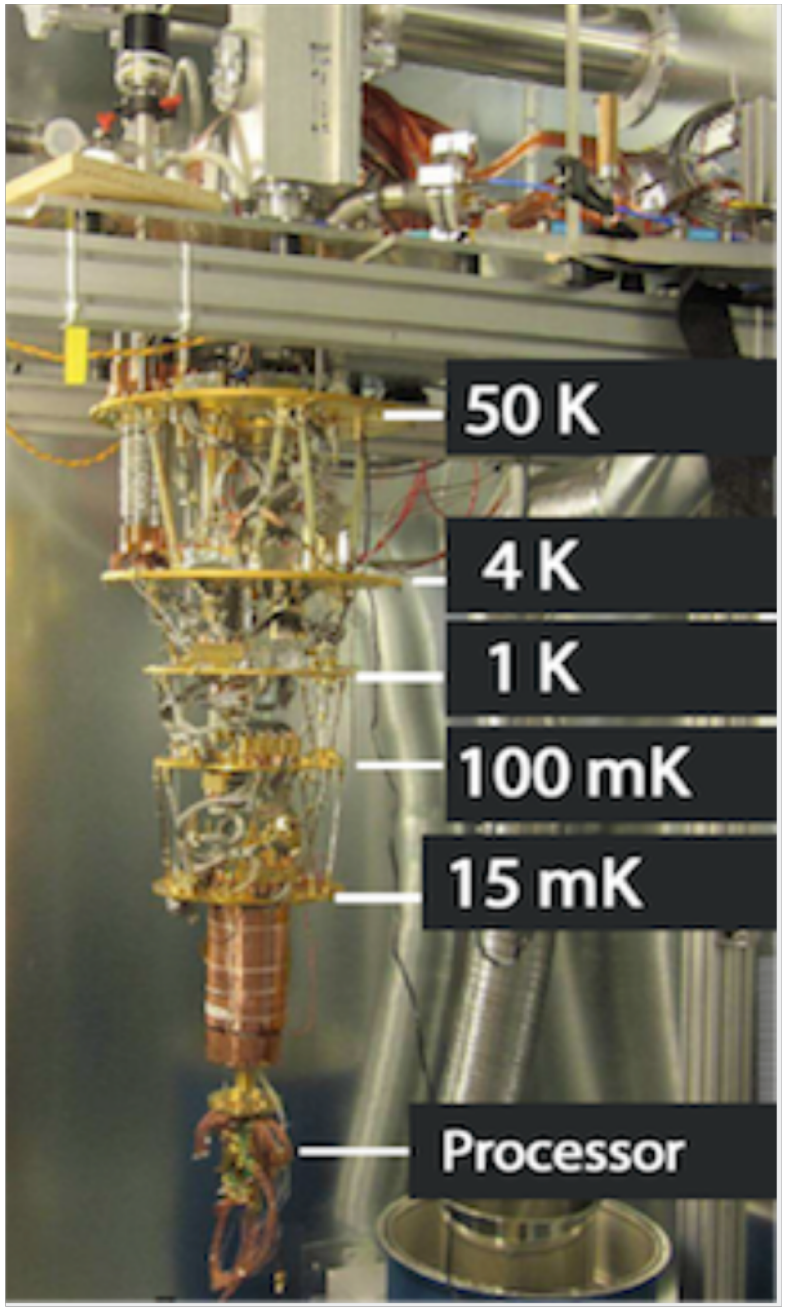


IBM Q System One

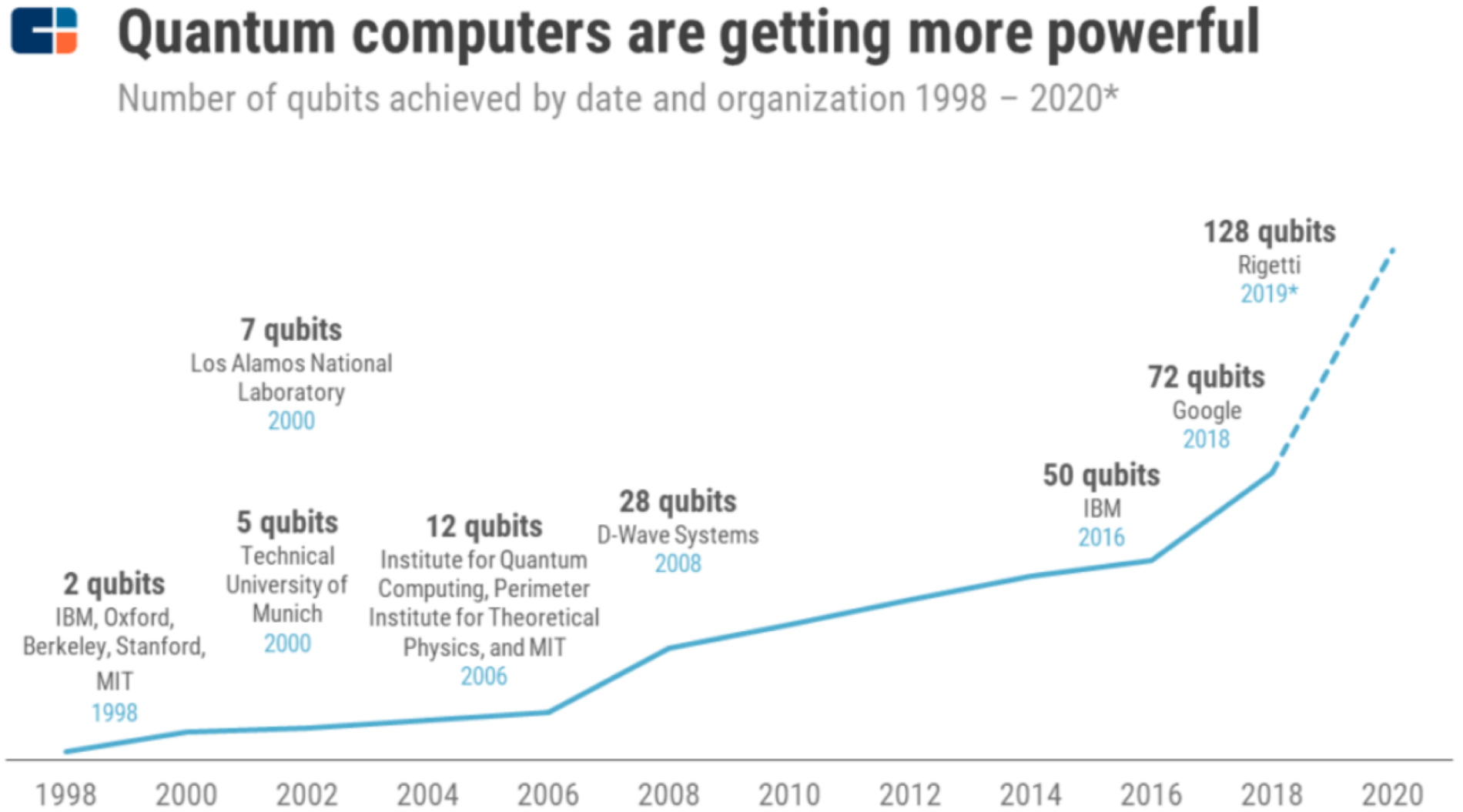
Inside

Outside

Cyrogenic System



Qubit Timeline



Quantum Computing

Grover's algorithm (1996)

Quantum simulator proposed (1981)

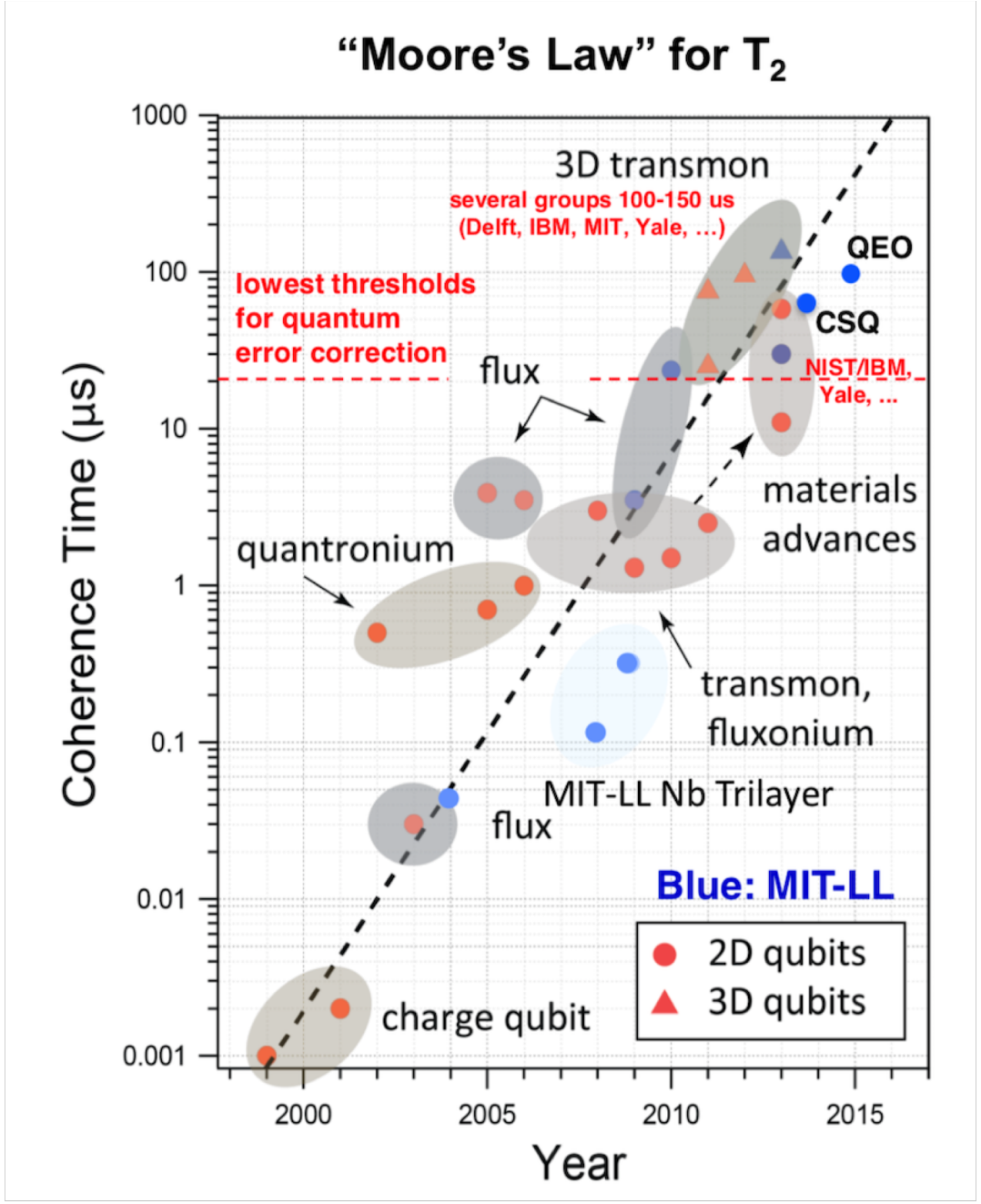
Shor's algorithm & CSS error correction (1994-95)

Quantum annealing & adiabatic QC (1998-2000)

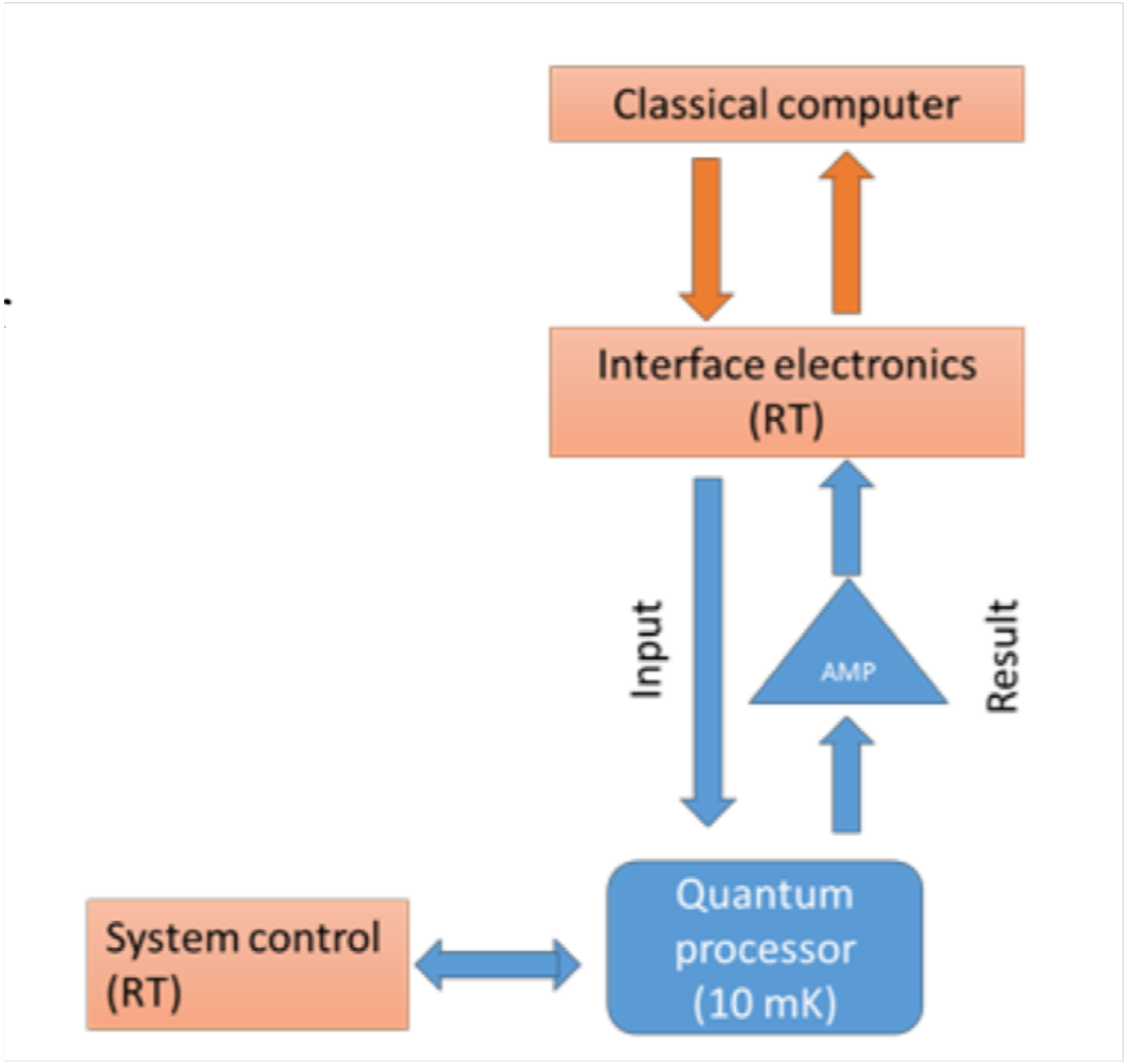
Few-qubit processors & error detection (2012-2016)

Cloud-based quantum computers (2017)

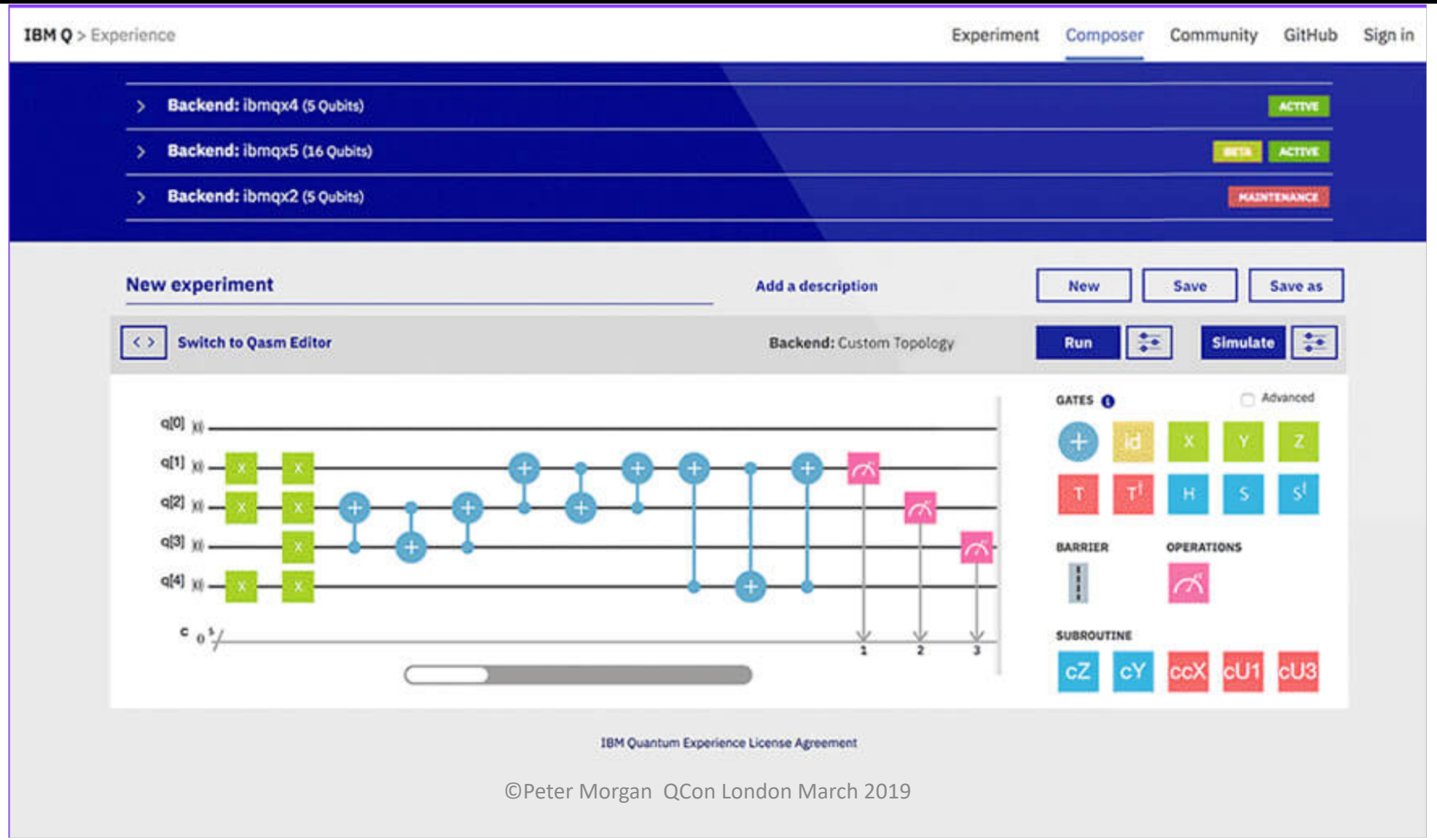
Coherence Time



Quantum Computer Architecture



Quantum Gates & Circuits



Quantum Algorithms

AHQC Algorithm	Goal(s)	Optimization Problem
Variational Quantum Eigensolver (VQE) [20, 23]	Estimate molecular properties (e.g. energies)	Minimize expected energy
Quantum Approximate Optimization Algorithm (QAOA) [5]	Estimate maximum cut of a graph	Maximize expected cut size
Quantum Autoencoder (QAE) [7]	Design a circuit for compressing a quantum data set	Maximize average fidelity
Quantum Variational Error Corrector (QVECTOR) [29]	Design device-tailored quantum error correction scheme	Maximize average fidelity
Variational Quantum Classification [11, 13, 15]	Find a circuit that classifies classical data points	Maximize log likelihood
Variational Quantum Factoring (VQF) [30]	For a given biprime find its prime factors	Minimize quartic boolean polynomial

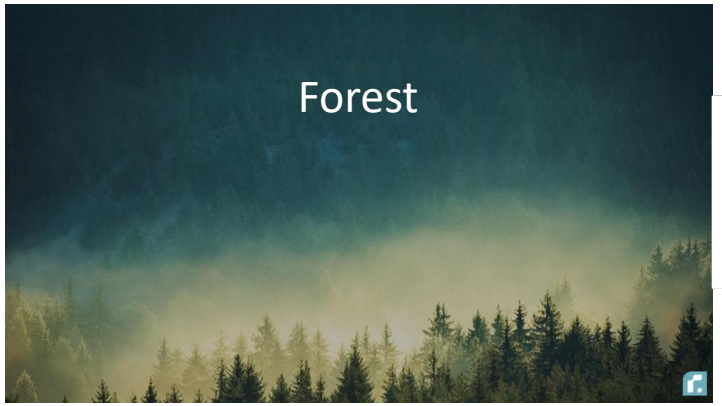
Qiskit

Cirq

Microsoft QDK

XANADU

STRAWBERRY FIELDS



OpenFermion

Frameworks

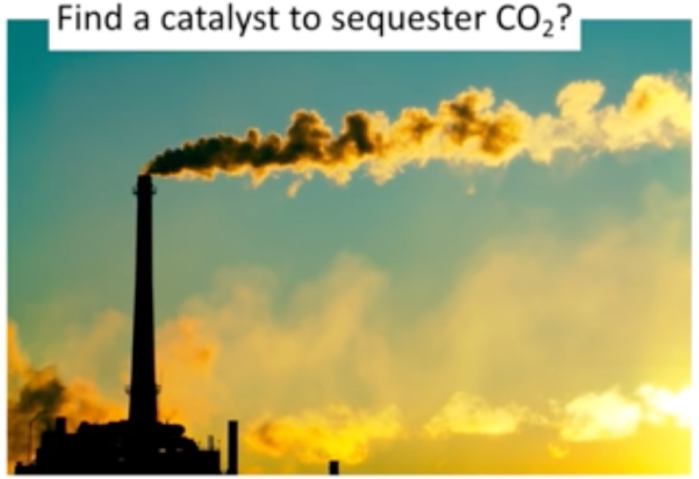
Applications

Quantum simulation

Design new materials or drugs?

Quantum chemistry

Find a catalyst to sequester CO_2?



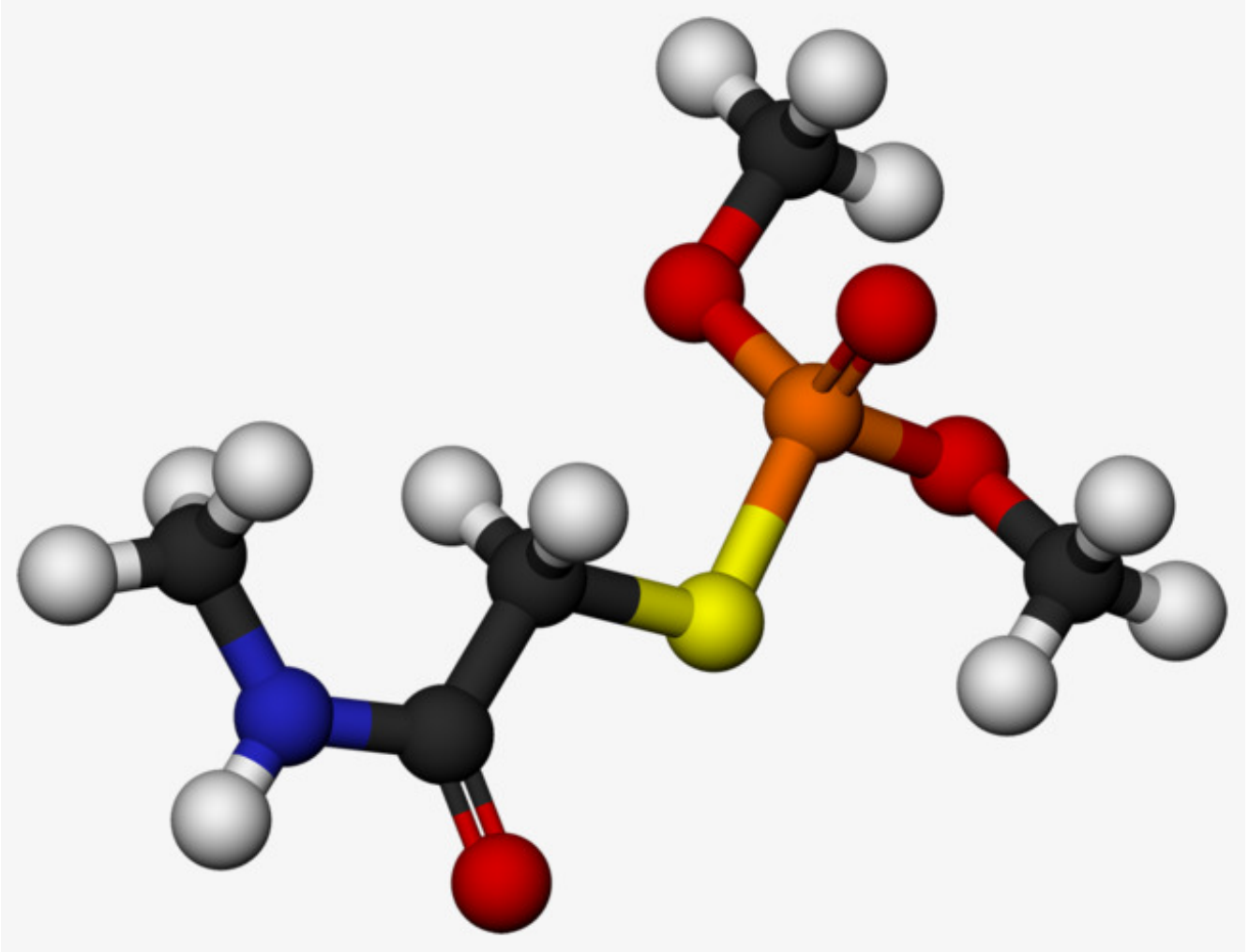
Machine learning

Cryptography

Startups

Simulating Chemistry

"Nature isn't classical, dammit, and if you want to make a simulation of nature, you'd better make it quantum mechanical..."
Richard Feynman - Simulating Physics with Computers, 1981.

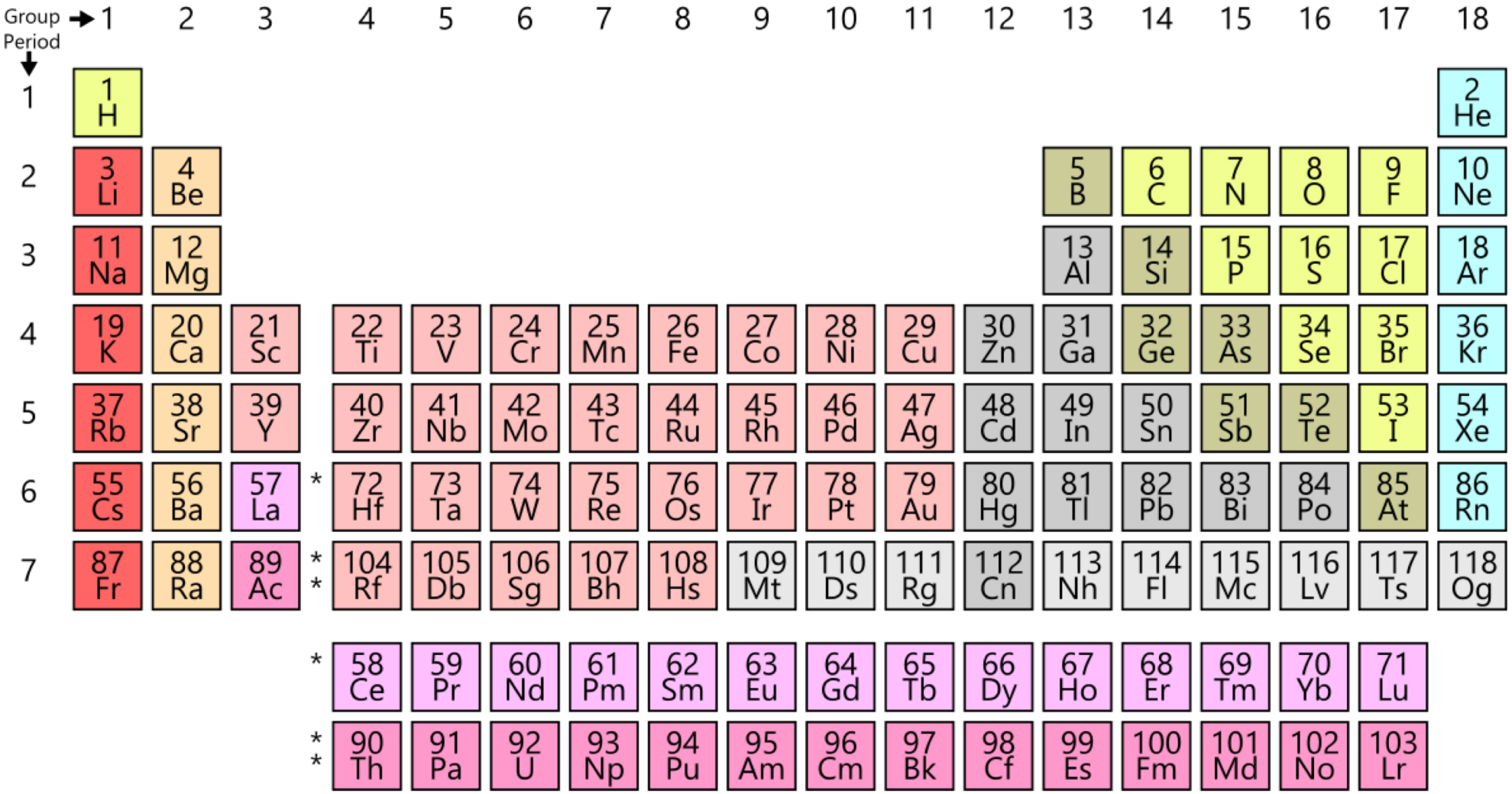


Applications

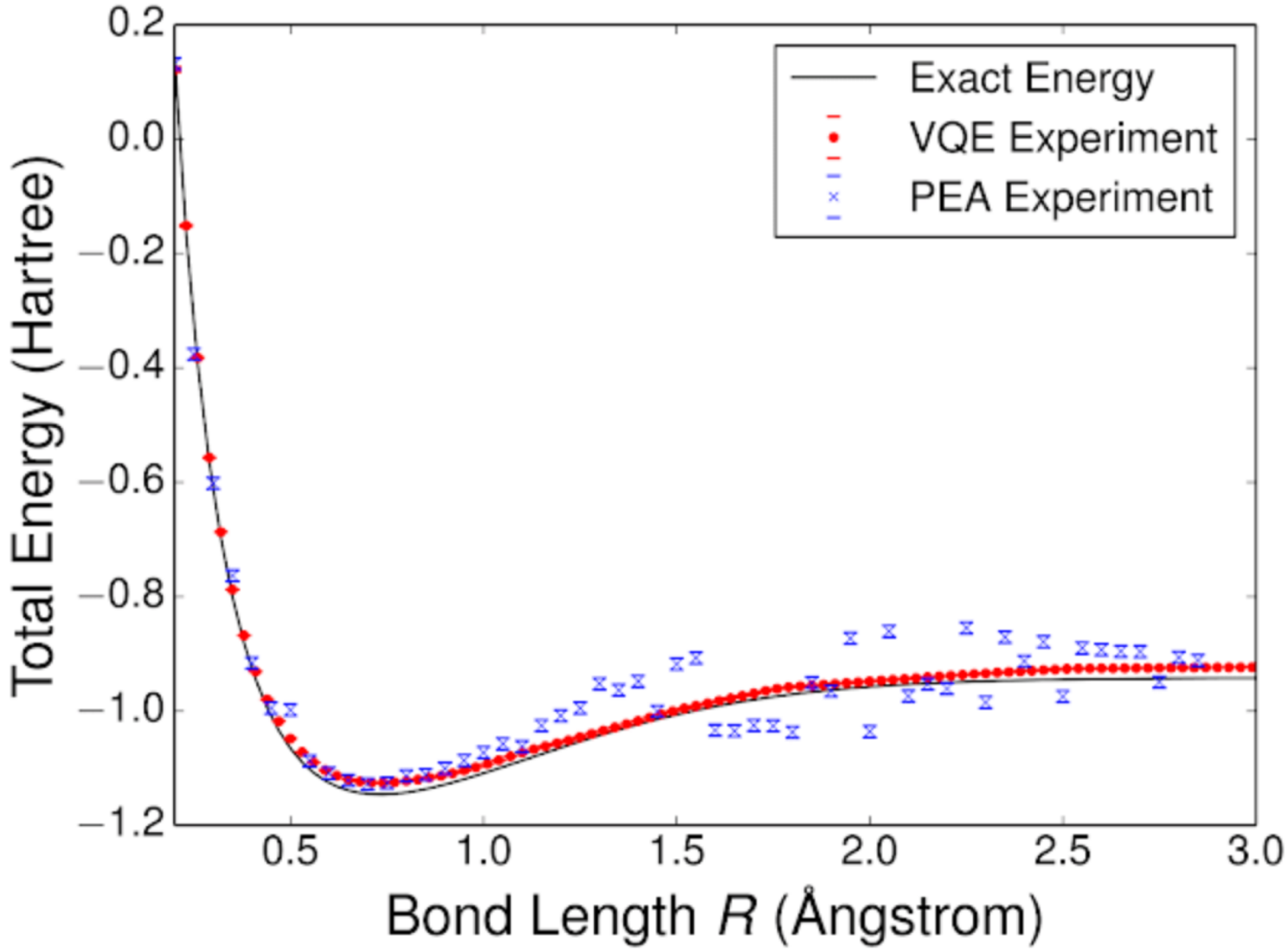
Enabling the design of

- New materials
- Medicines
- Industrial catalysts
- High temperature superconductors

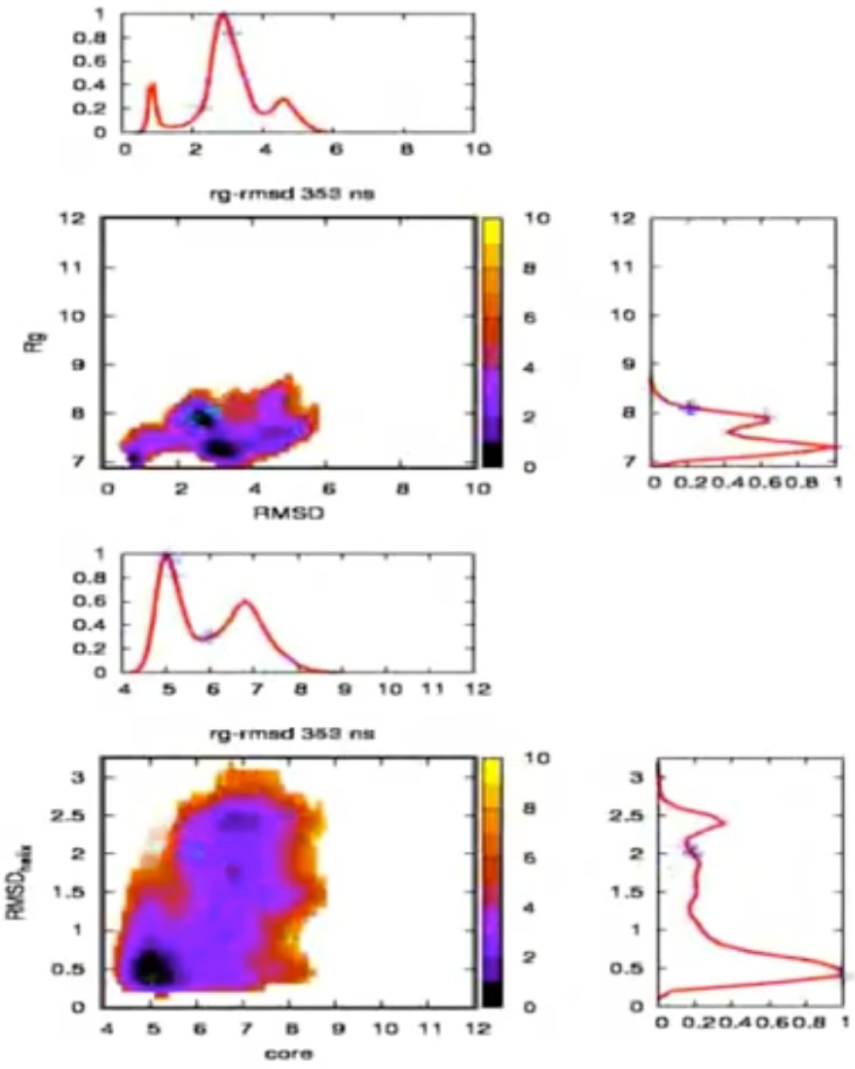
Periodic Table

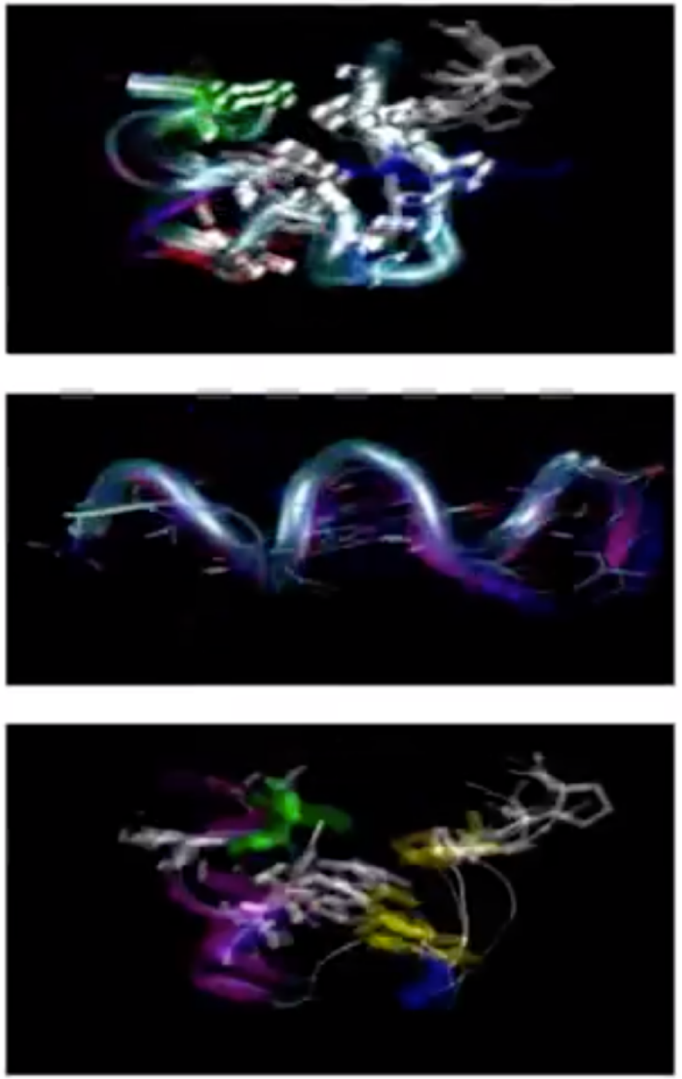


Molecular Energy Levels (Static)

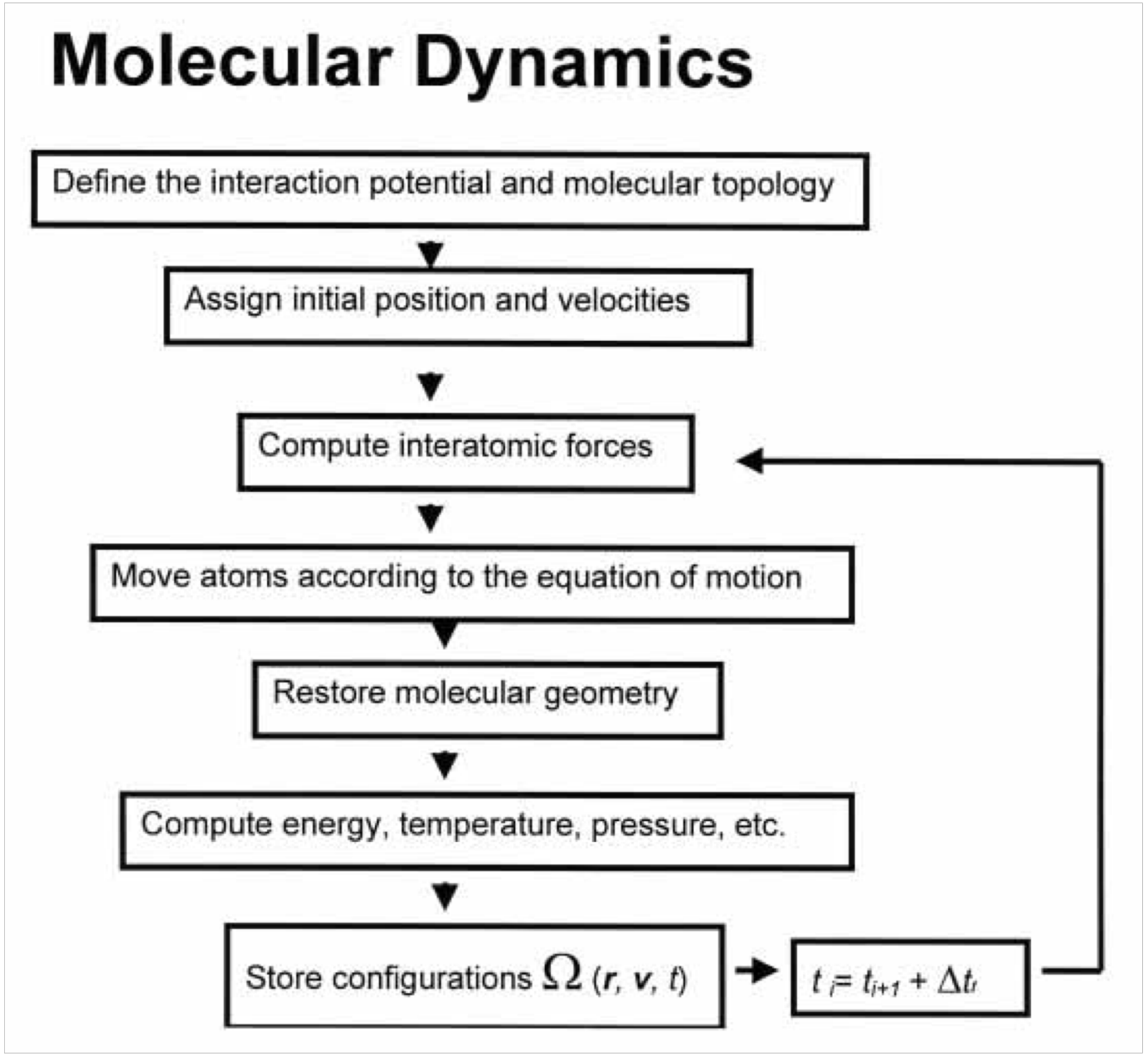


Molecular Dynamics (e.g, protein folding)





Molecular Dynamics Simulation Procedure



Classical Frameworks

PySFC

Gaussian 16

Psi4

NWChem

PyQuante

OpenMM

Quantum Frameworks

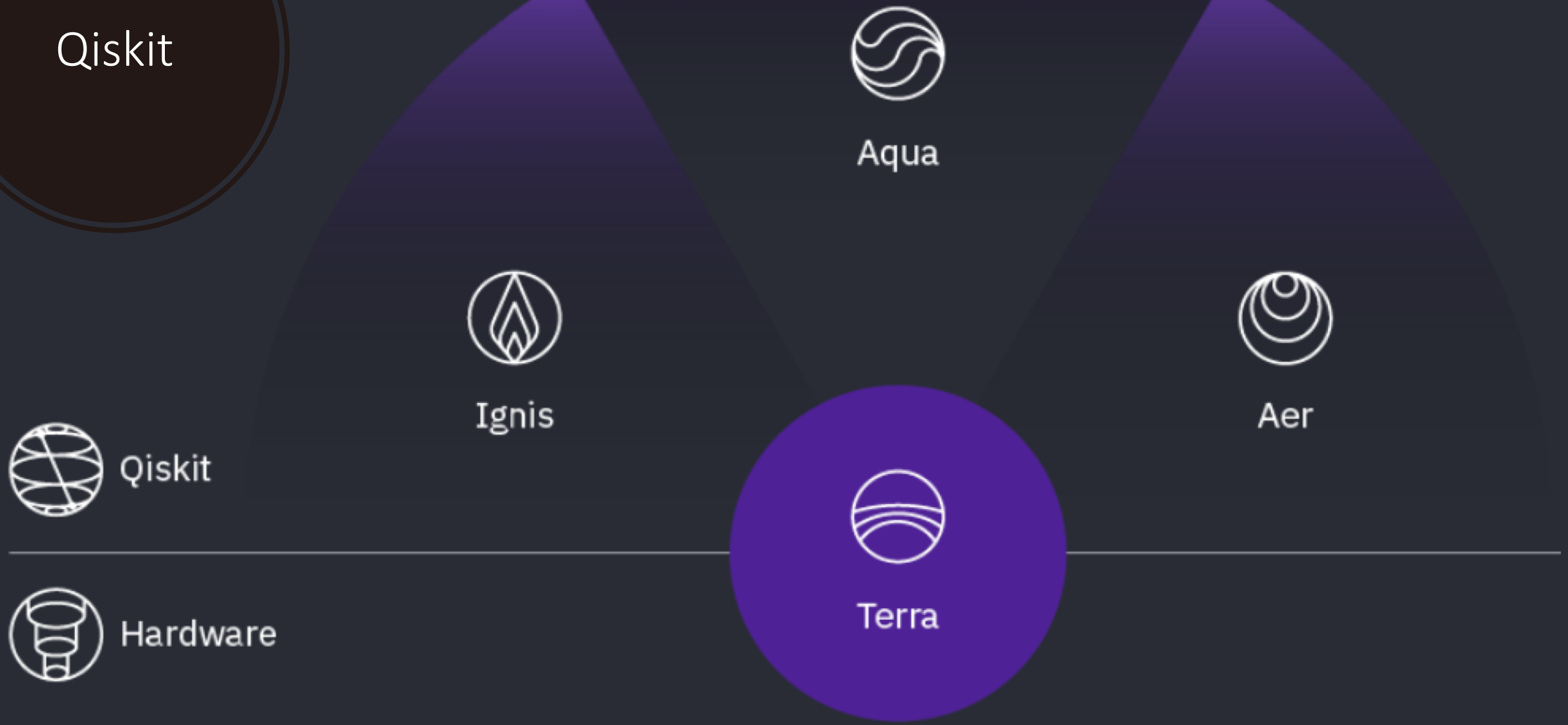
IBM Qiskit Aqua

Google OpenFermion

Microsoft QDK Chem library

Project Q FermLib

Qiskit



Qiskit Aqua

- Contains a library of quantum algorithms on which applications for near-term quantum computing are built
- Designed to be extensible - employs a pluggable framework where quantum algorithms can easily be added
- It currently allows the user to experiment on the following domains:
  - Chemistry
  - Optimization
  - Finance
  - AI
- `pip install qiskit-aqua`
- https://github.com/Qiskit/qiskit-aqua

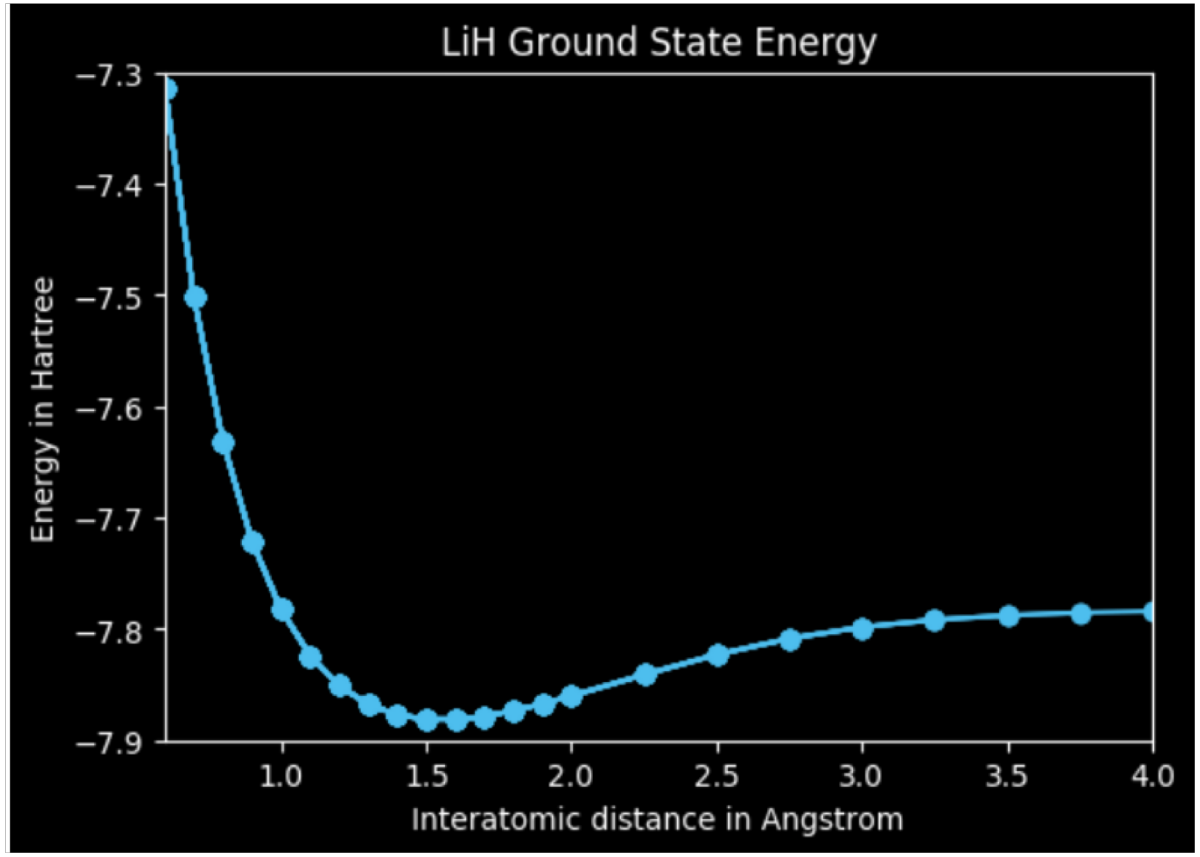
Qiskit Chemistry

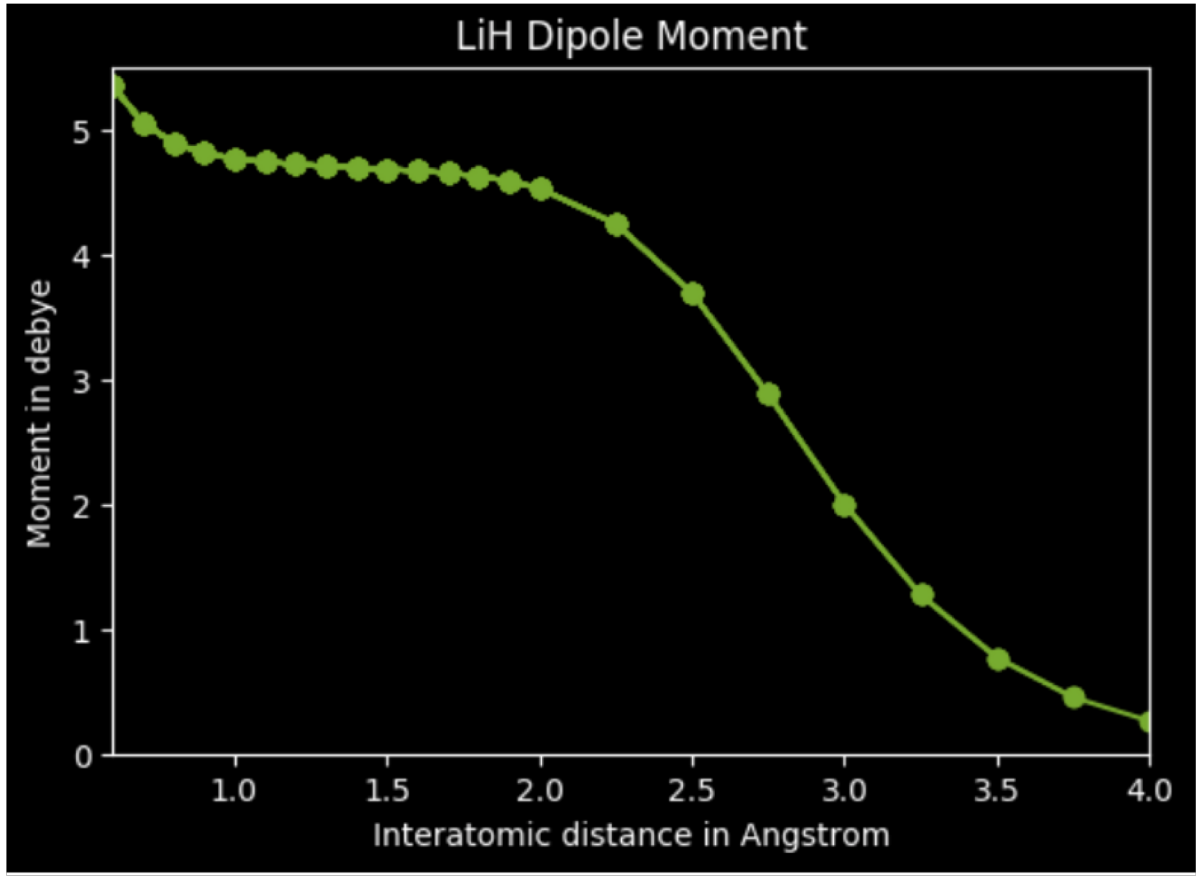
- End-to-end stack that enables experimenting with chemistry problems on near-term (NISQ) quantum computers
- Translates chemistry-specific problems defined via classical drivers into **inputs for Aqua** algorithms
- Modular and extensible
- Allows users with different levels of experience to execute chemistry experiments and contribute to the quantum computing chemistry software stack
- `pip install qiskit-chemistry`
- https://github.com/Qiskit/qiskit-chemistry

```
mport numpy as np
rom qiskit_chemistry import QiskitChemis

iskit_chemistry_dict = {
  "driver": { "name": "PYSCF" },
  "PYSCF": { "atom": "", "basis": "sto3g"
  "operator": {
    "name": "hamiltonian",
    "qubit_mapping": "parity",
    "two_qubit_reduction": True,
    "freeze_core": True,
    "orbital_reduction": [-3, -2]
```

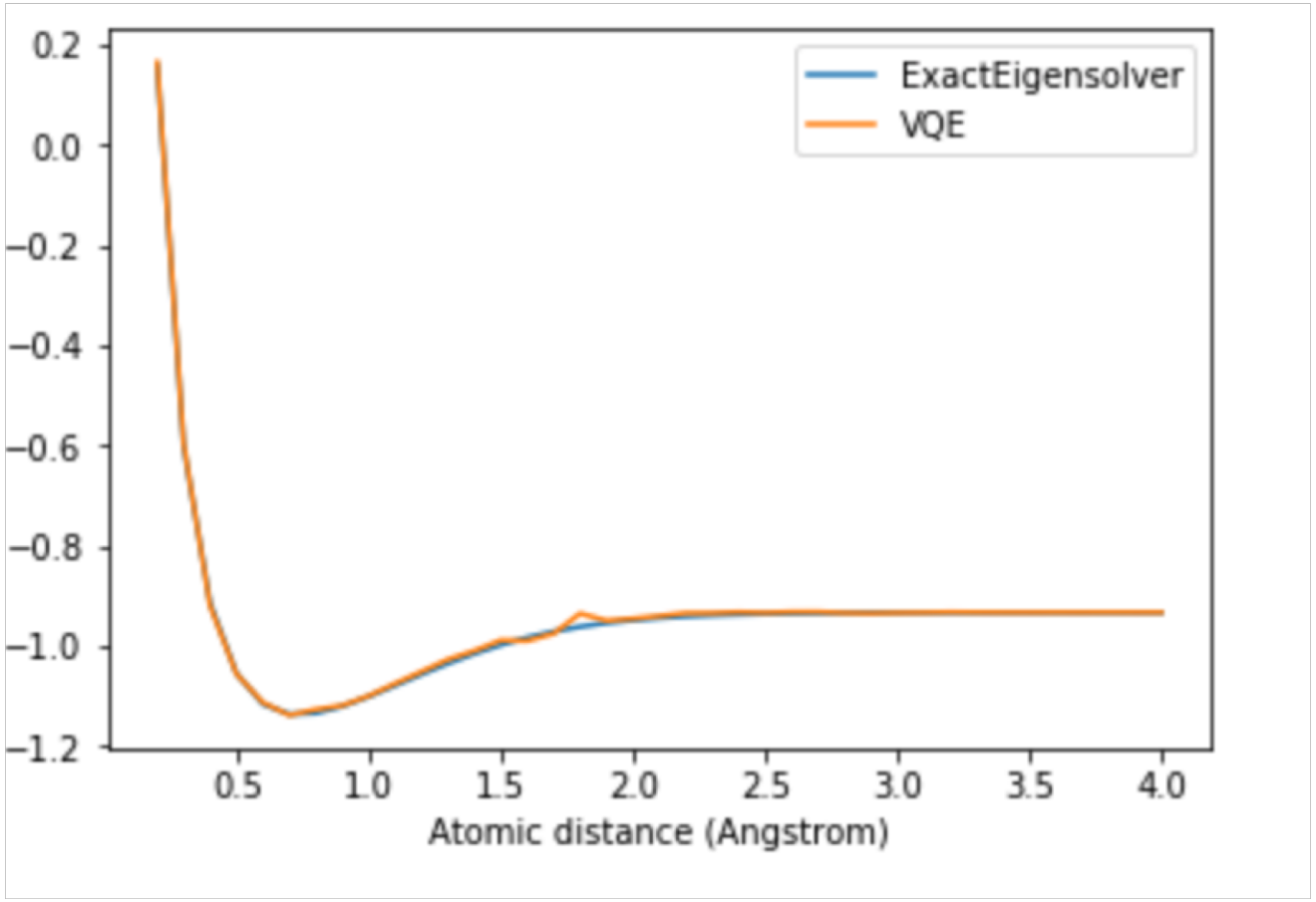
Energy Calculations





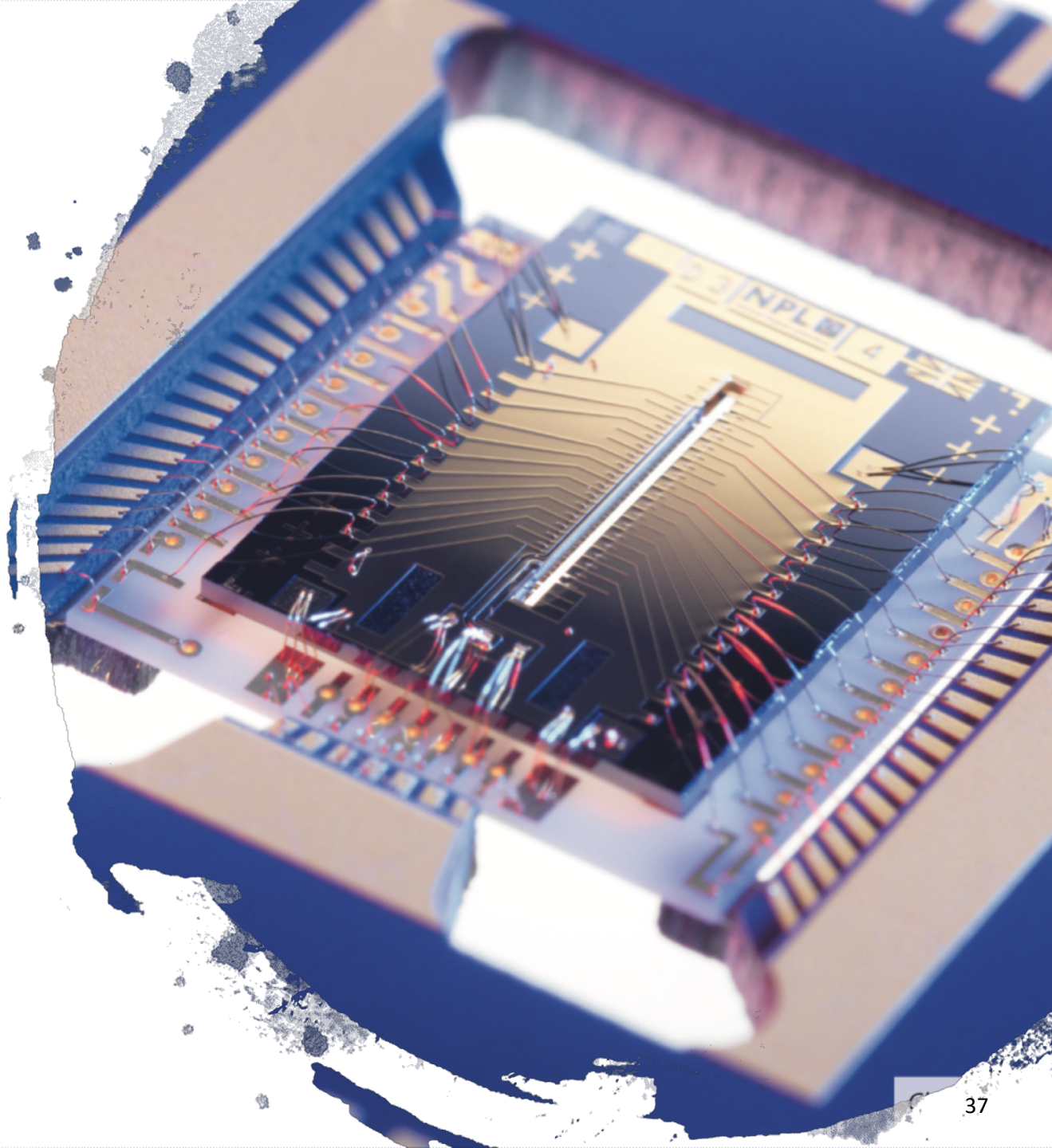
Code Demos

- Hello Quantum World https://github.com/Qiskit/qiskit-tutorials/blob/master/community/hello_world/quantum_world.ipynb
- Quantum Chemistry with VQE https://nbviewer.jupyter.org/github/Qiskit/qiskit-tutorials/blob/master/qiskit/aqua/chemistry/dissociation_profile_of_molecule.ipynb



Conclusions

- We are waiting on quantum hardware development
- Meanwhile working on software stack plus quantum algorithms
- NISQ – noisy without error correction (next 5-10 years?)
- After this error corrected, and maybe topological (error free) qubits?
- Quantum computers will revolutionize everything – including chemistry
- Nature is quantum mechanical (dammit)!



References - Blogs

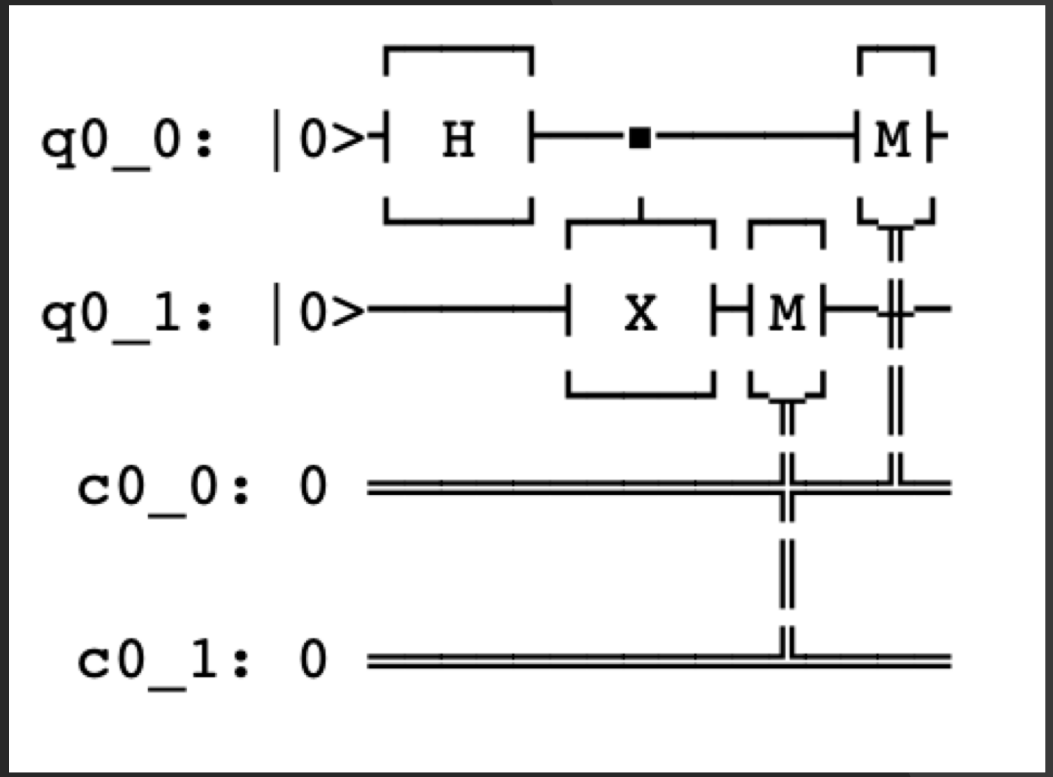
- Pistoia, M. et al, *Aqua 0.4: Improved Programmatic Interface, Better Performance, Richer Finance Applications, and More*, IBM Qiskit, Jan 2, 2019
- *Simulating nature with the new Microsoft Quantum Development Kit chemistry library*, Microsoft Quantum Team, Dec 4, 2018
- Kandala A. et al, *How to measure a molecule's energy using a quantum computer*, IBM Research, Sept 2017
- Babbush, Ryan, *Towards an exact (quantum) description of chemistry*, Google AI, July 2016

References - Papers

- McClean, J. et al, *OpenFermion: The Electronic Structure Package for Quantum Computers*, Feb 27, 2019, https://arxiv.org/abs/1710.07629
- McArdle, S. et al, *Quantum Computational Chemistry*, Jan 17, 2019, https://arxiv.org/abs/1808.10402
- Cao, Y. et al, *Quantum Chemistry in the Age of Quantum Computing*, Dec 28, 2018, https://arxiv.org/abs/1812.09976
- Olson, J. et al, *Quantum Information and Computation for Chemistry,* June 10, 2017, https://arxiv.org/abs/1706.05413

Qiskit Tutorials

- Qiskit Tutorials
  https://github.com/Qiskit/qiskit-tutorials
- Qiskit Aqua Chemistry
  https://nbviewer.jupyter.org/github/Qiskit/qiskit-tutorials/blob/master/qiskit/aqua/chemistry/index.ipynb



Any Questions?