Quantum Simulation

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Quantum Simulation 1.0

All Science

Design Materials

Advanced Materials

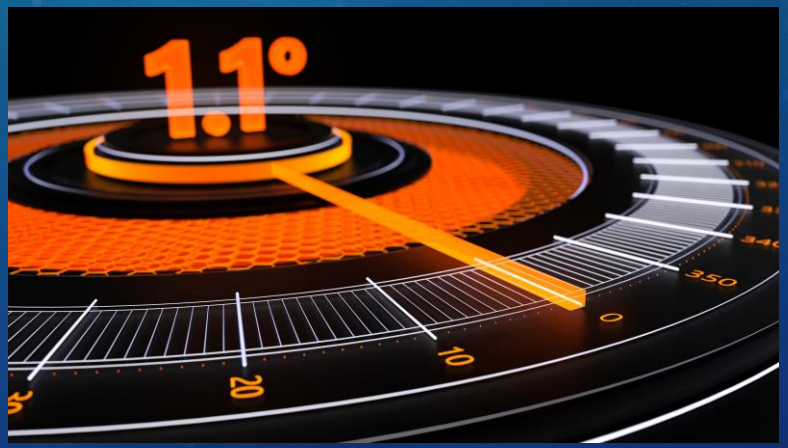
Quantum Simulation 1.0

All Science

Design Materials

Advanced Materials

What's the Magic Behind Graphene's 'Magic' Angle?



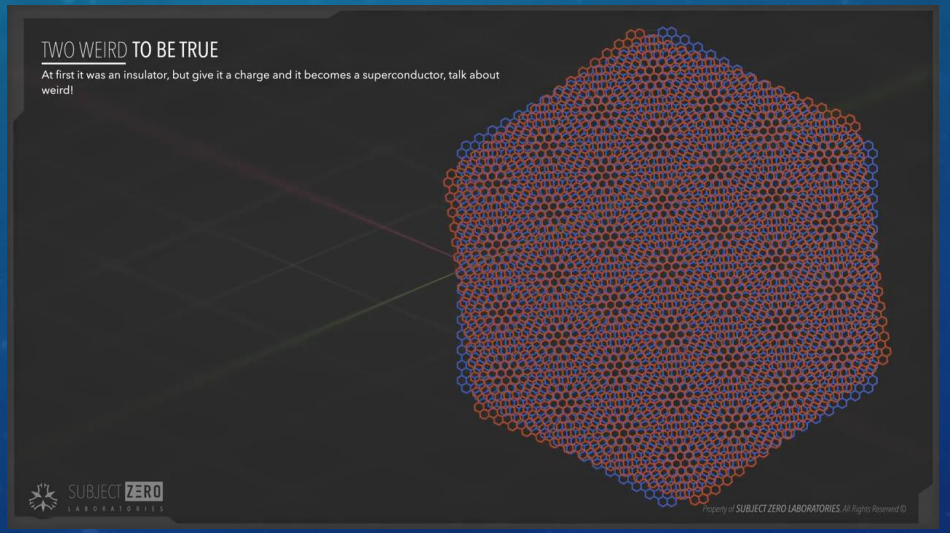
https://www.quantamagazine.o

Quantum Simulation 1.0

All Science

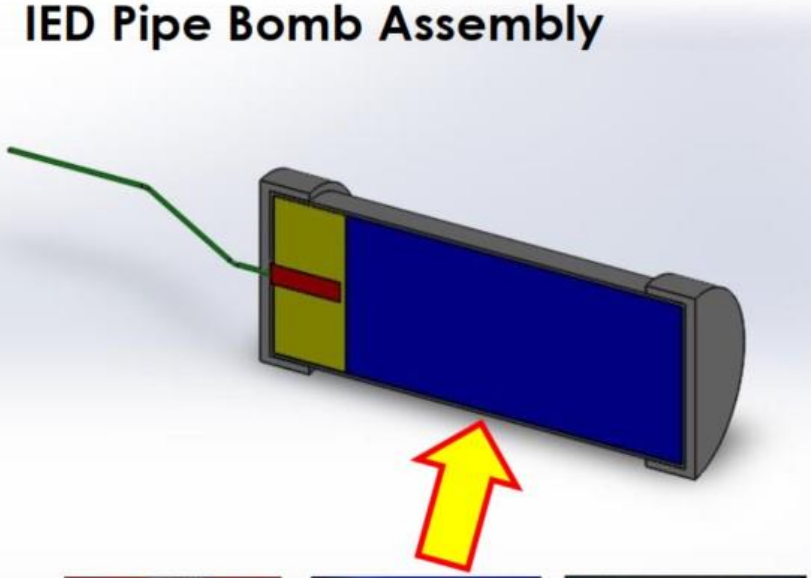
Design Materials

Advanced Materials



Subject Zero Science

Improvised Explosive Device (IED)



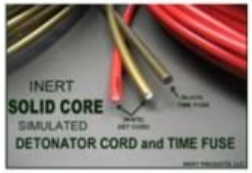

ANFO

TNT

RDX


Tetryl


Black powder



PETN

Ignition

Det cord

Booster

PETN

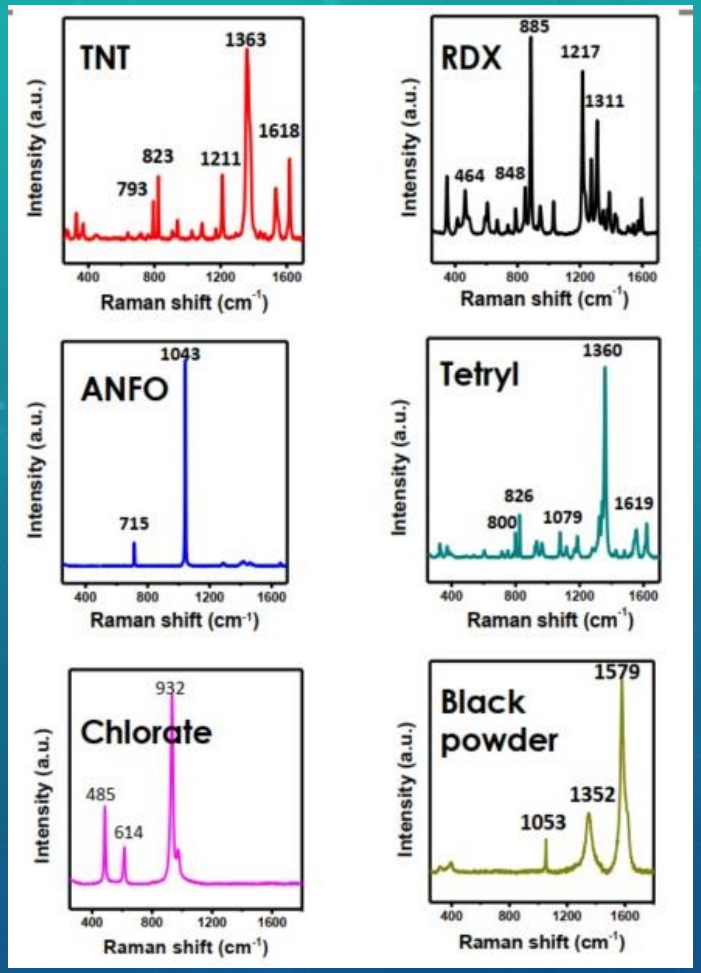
Main Charge

- TNT
- RDX
- ANFO
- Tetryl
- Chlorate
- Black Powder
- Power Gel
- Power gel & Chlorate

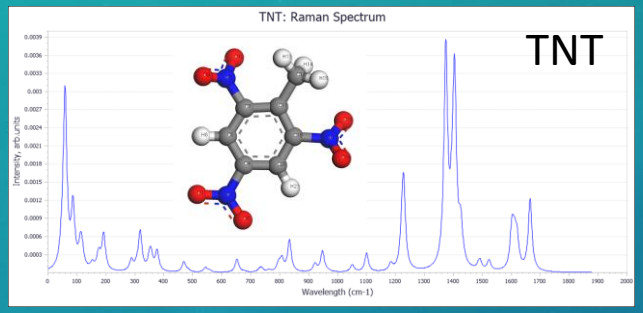
ONSPEC
NECTEC SERS Chips

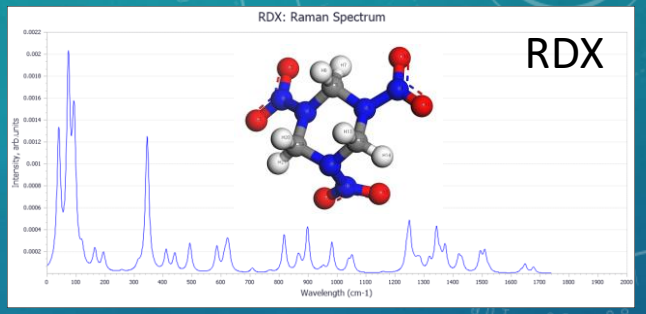
Improvised Explosive Device (IED)

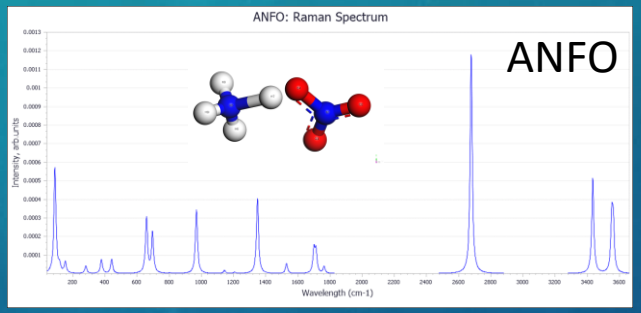
Raman Spectrometer

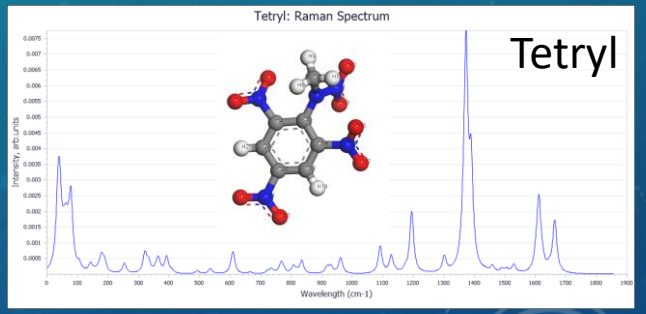


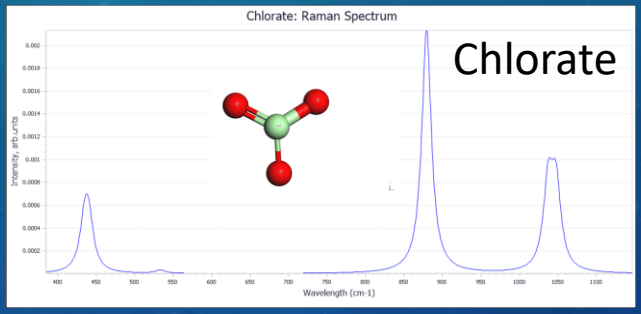
Simulation Results

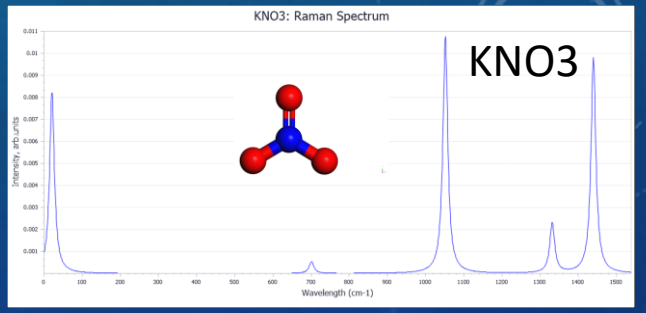




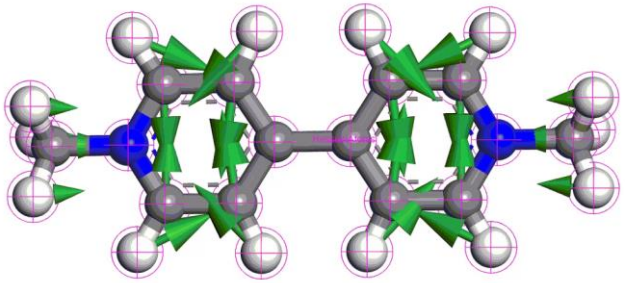




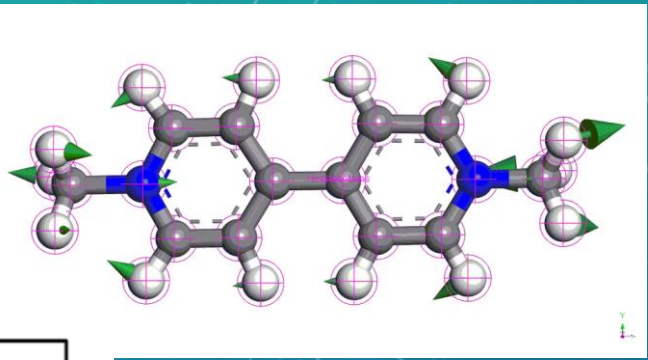




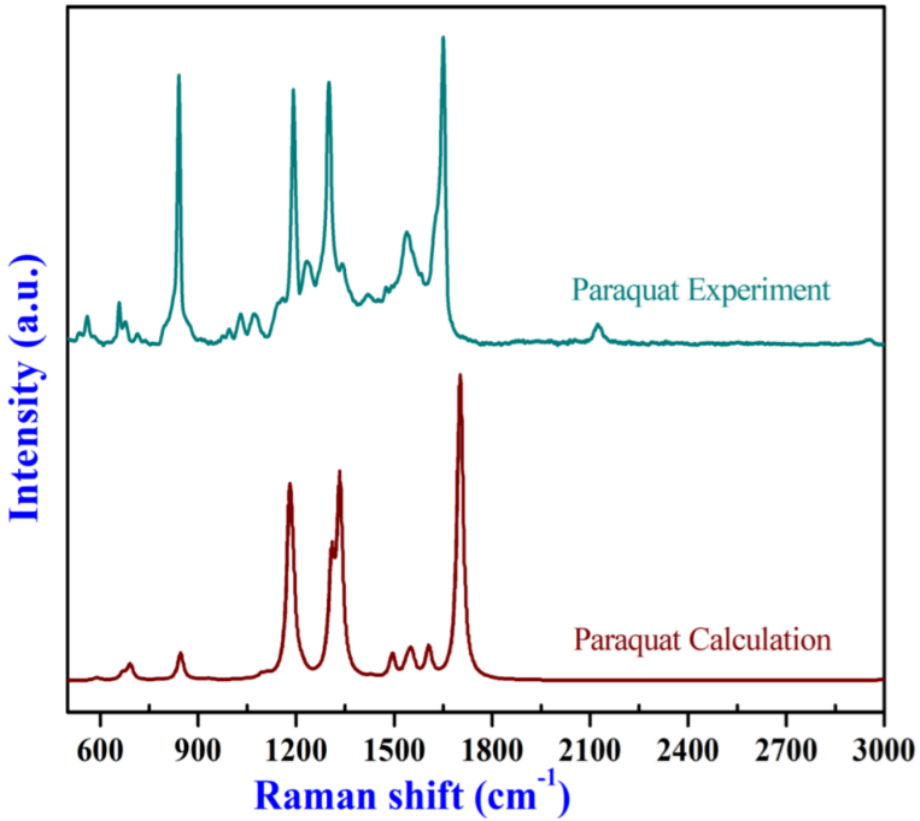
Herbicide:
Paraquat



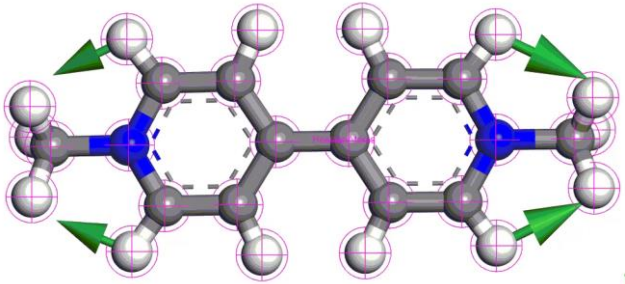
840.75 cm^{-1}



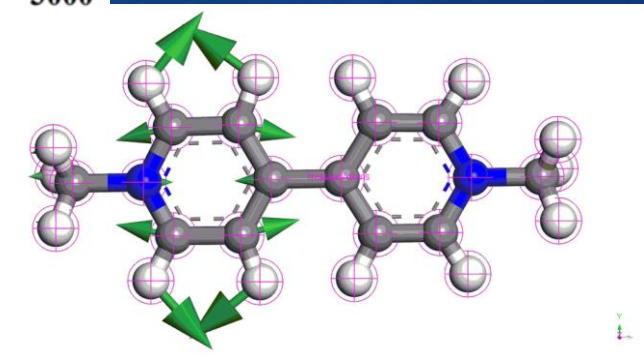
1186.53 cm^{-1}



1297.08 cm^{-1}

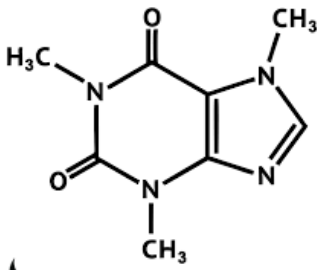


1683.03 cm^{-1}

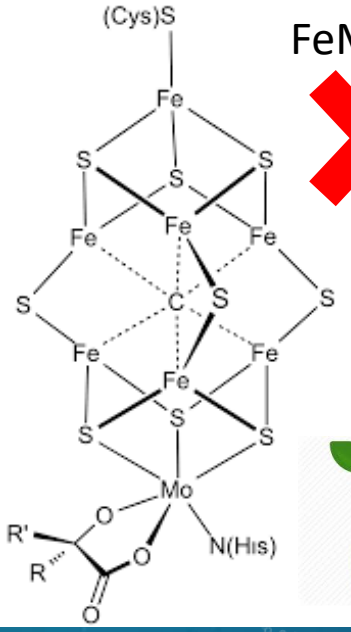


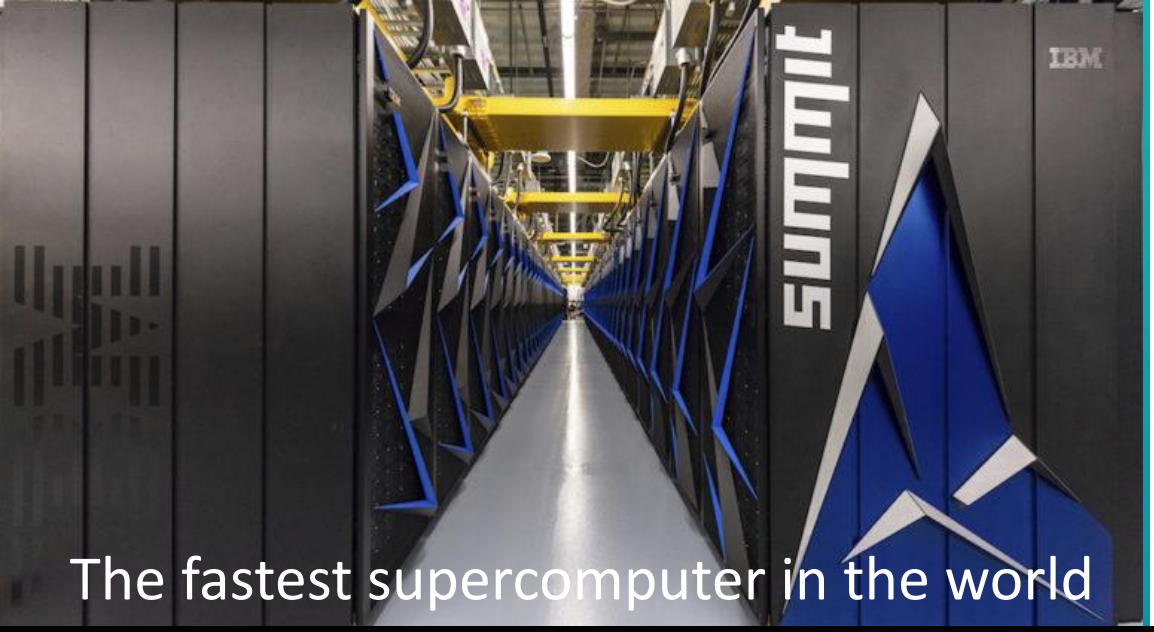
The fastest supercomputer in the world

Caffeine



FeMoco





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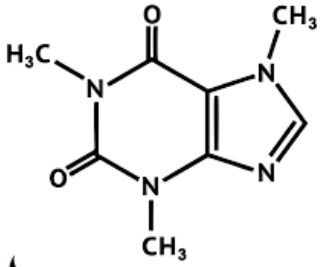

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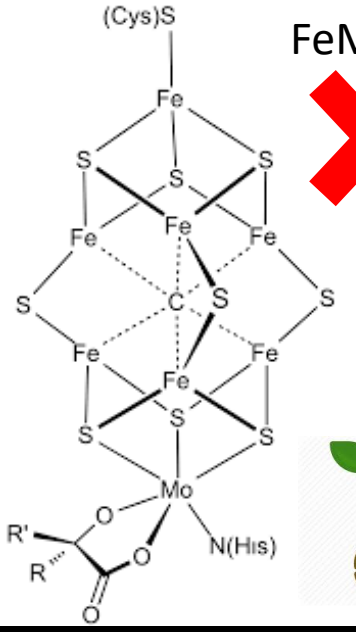
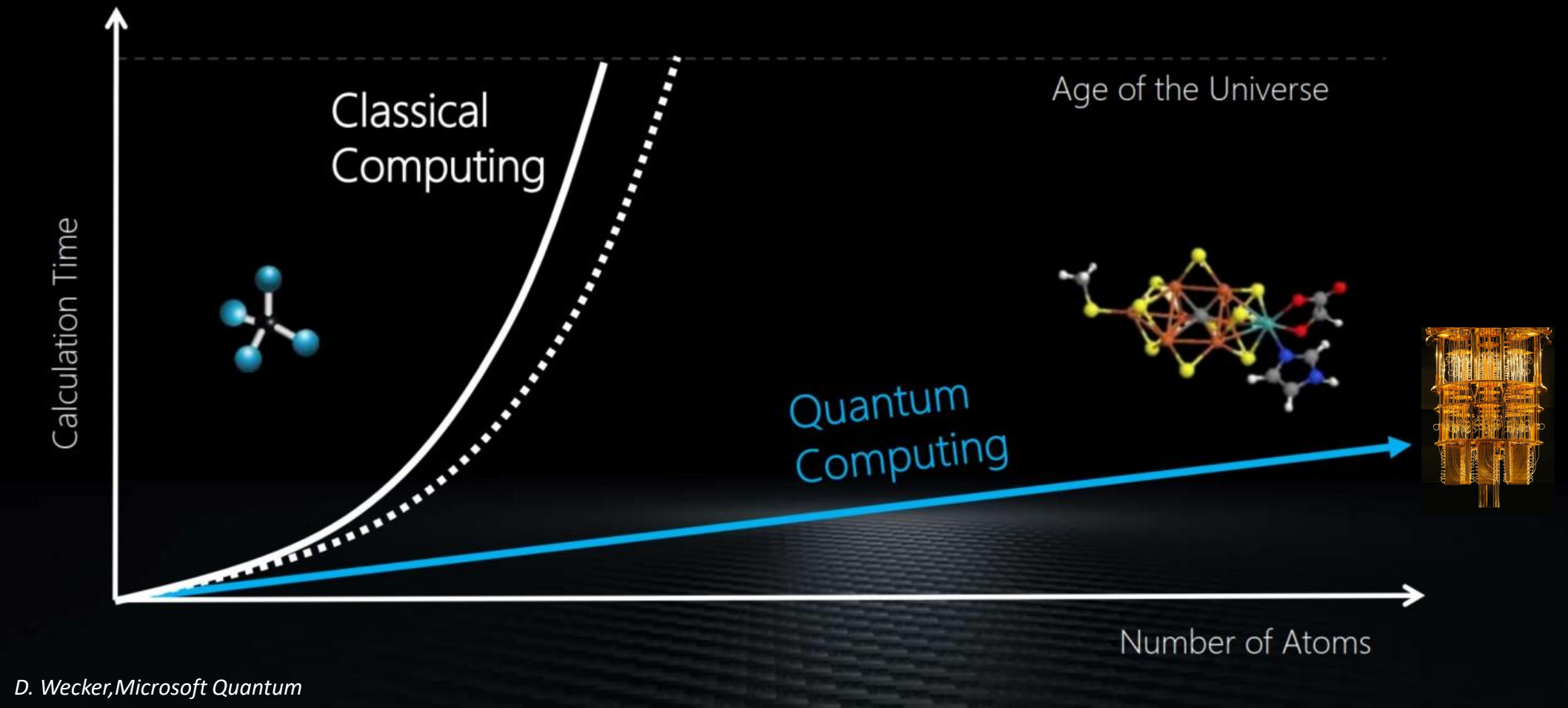
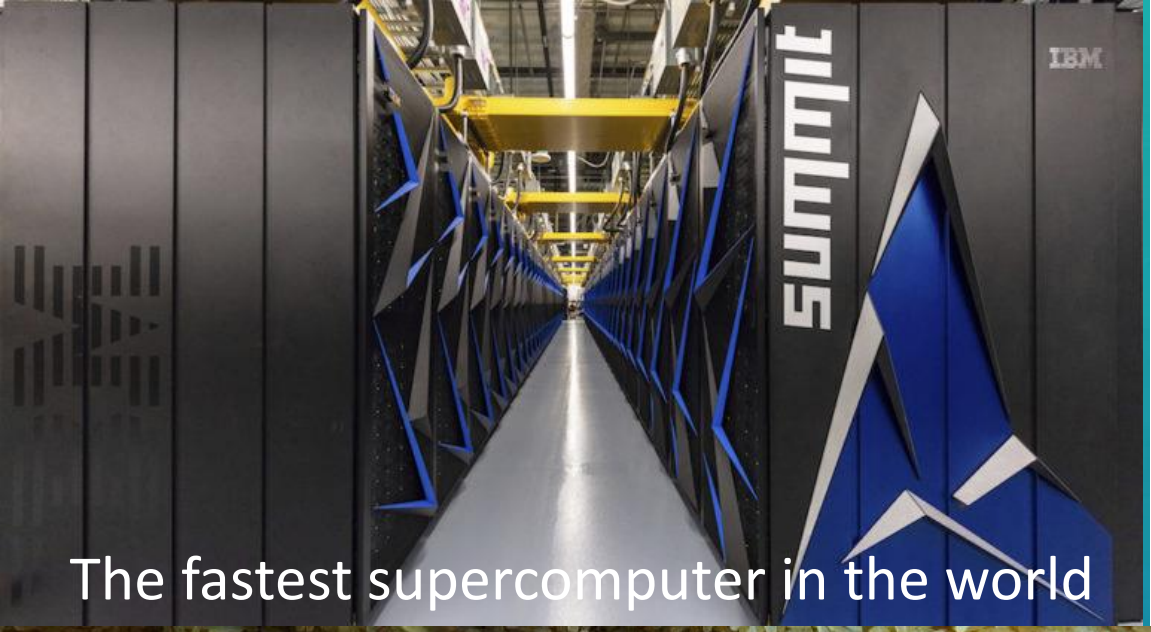




D. Wecker,Microsoft Quantum



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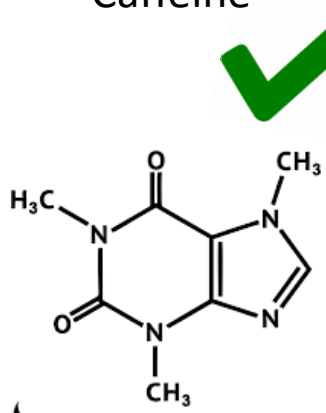

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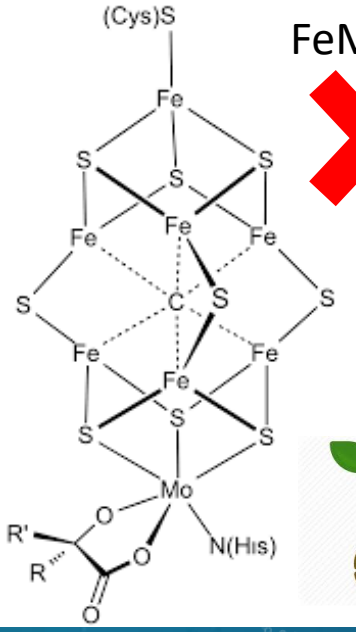


D. Wecker,Microsoft Quantum

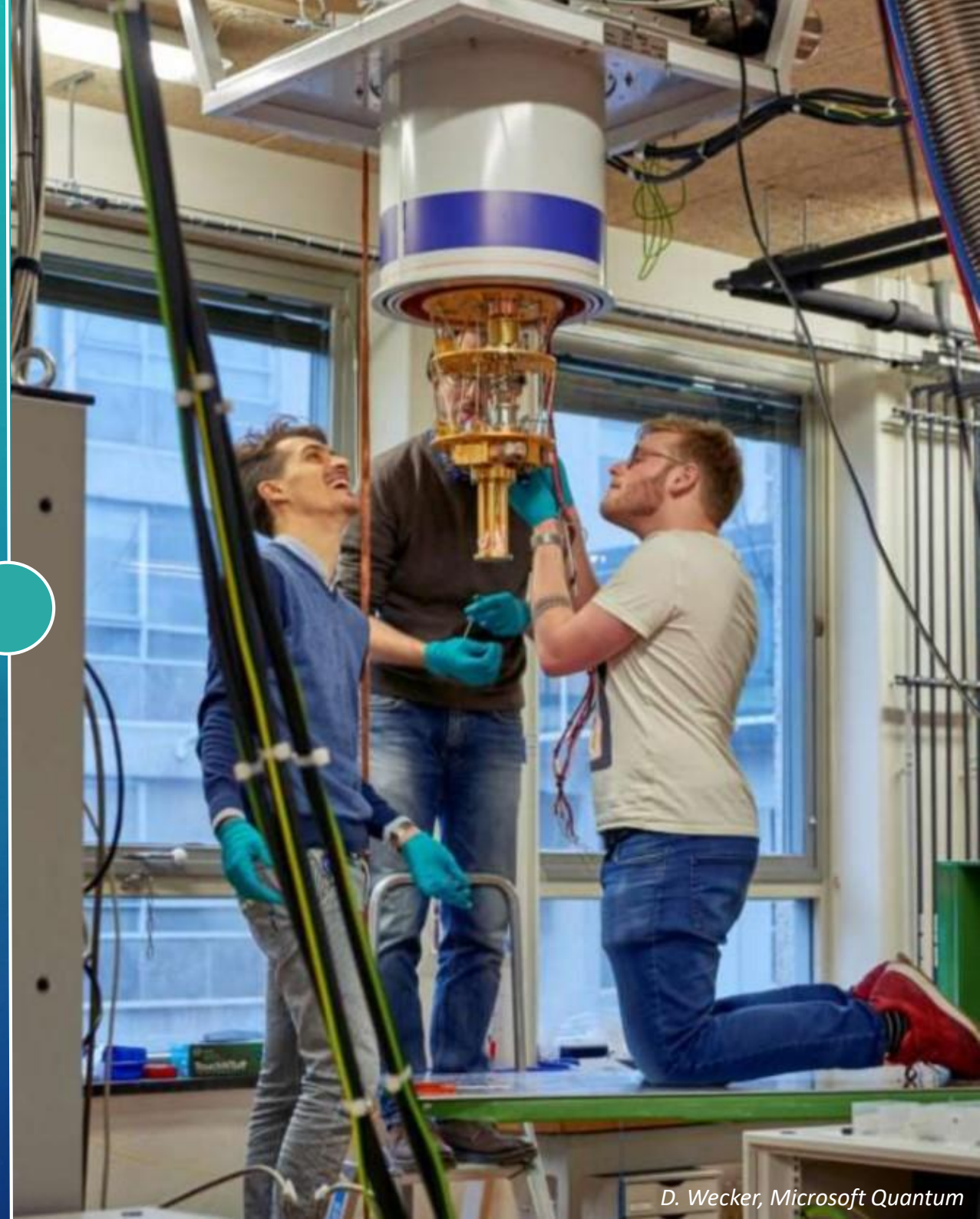
Exponential Scaling

30 qubits → 16 Gb

40 qubits → 16 Tb

50 qubits → 16 Pb

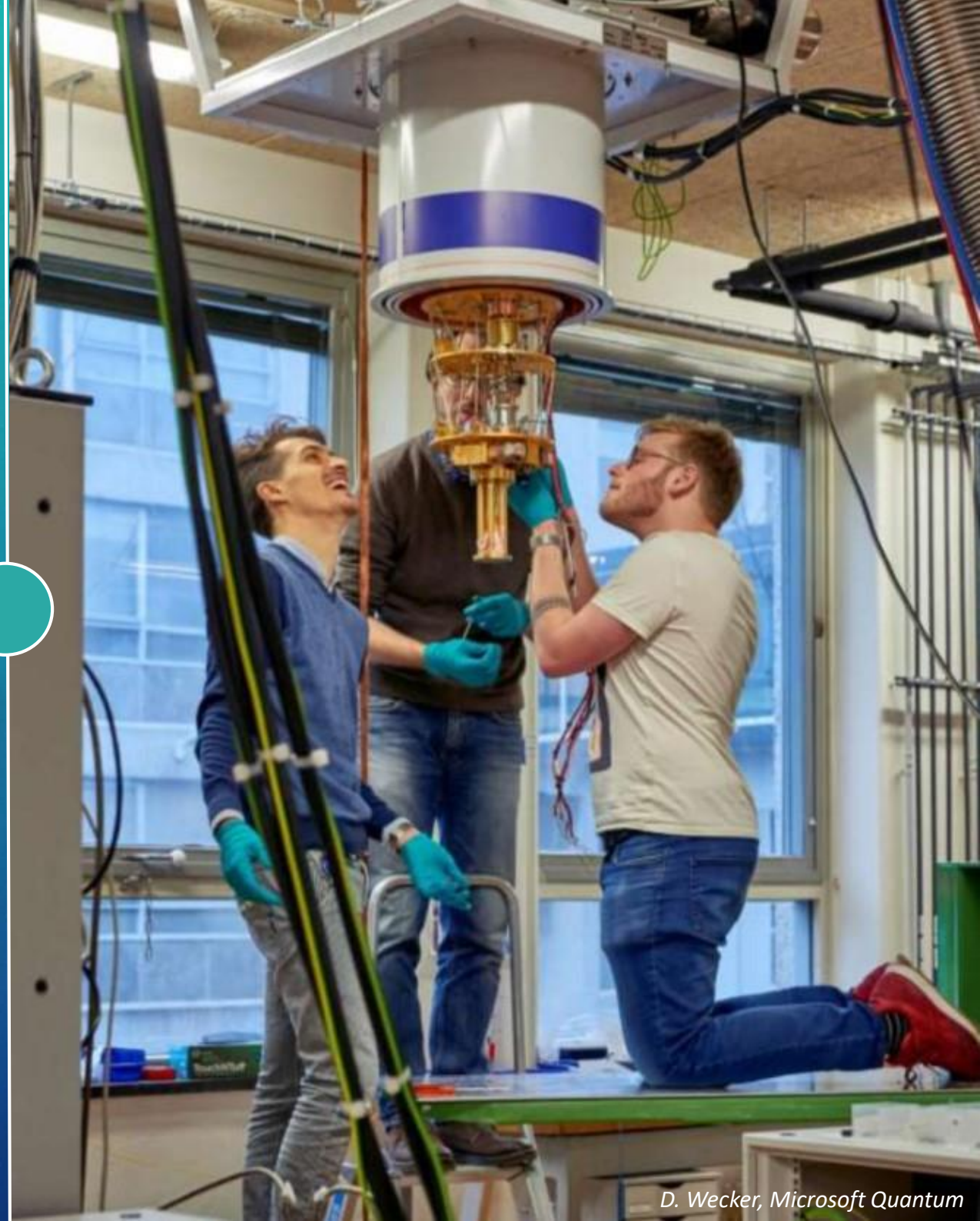
Richard Feynman:
“Shut up & calculate!”



D. Wecker, Microsoft Quantum

Richard Feynman:
“Shut up & calculate!”

Quantum 2.0:
“Shut up & engineer!”



D. Wecker, Microsoft Quantum

Quantum Engineering = Future Technology

Quantum Computing: Technology Roadmap, Global, 2012-2032

	Proven Technology	Benchmark Solvers	Quantum Supremacy	Multipurpose Computing
Logical Qubits	5 Logical Qubits	50 Logical Qubits	500 Logical Qubits	5,000 Logical Qubits
Quantum Algorithms	• Quantum Fourier transform • Elementary factorization algorithms (Shor's) • Fundamental search algorithms (Grover's) • Trivial parity learning • Rudimentary quantum machine learning	• Search and optimization (Grover's) • Variational quantum eigensolvers • Quantum genetic algorithms • Quantum chemistry Collective decoding	• Smart optimization algorithms • Advanced machine learning approaches • True fault tolerance methods for error correction • Random numbers generation	• Multipurpose algorithms • Advanced encryption algorithms • Quantum image processing • Quantum algorithms (Dürrand-Hoyer's, Ramesh's, Vinay's)
Main Tasks	• Basic Fourier transform • Basic research, listing • Trivial factorization • Rudimentary fitting • Optical recognition (machine learning)	• DNA microarray analysis • Process engineering optimization • Advanced search • Quantum dynamics • Quantum sampling	• Quantum chemistry • Molecular dynamics • Artificial intelligence for machine learning • Remote sensing • Number random generation	• Large-scale factorization • Operating systems • Smart image recognition • Faster resolution of complex optimization problems

2012 2014 2016 2018 2020 2022 2024 2026 2028 2030 2032

Source: Frost & Sullivan

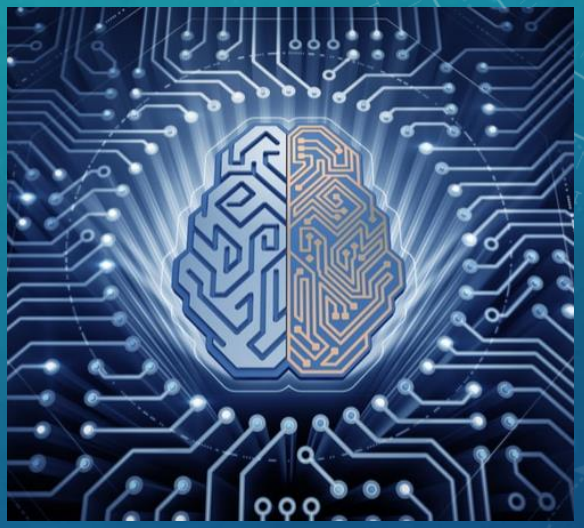
Quantum Computer

IBM Q Lab,
Scientific American (2018)

Current Status:

- **Expensive**
- **Small-Scale**
- **Immature Level**

Quantum Software



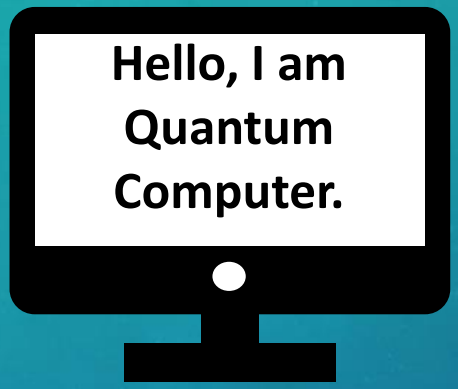
Quantum Computing
MeriTalk (2018)

Current Status:

Heavy & Complex Computation?

Quantum Simulation Platform

➢ using Classical Computers



- ❑ IBM: Quantum Chemistry
- ❑ Huawei: HiQ Cloud Service Platform
- ❑ Google: OpenFermion

Psi4 OPEN-SOURCE QUANTUM CHEMISTRY

pyscf

QMCPACK Argonne NATIONAL LABORATORY

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Advanced Materials

Quantum Simulation 2.0

All Science

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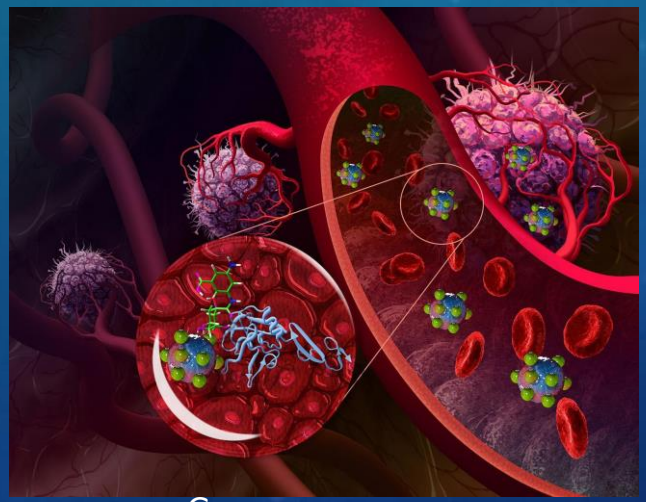
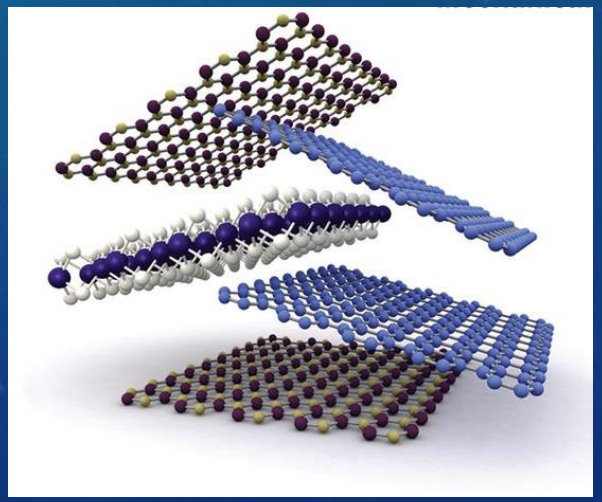
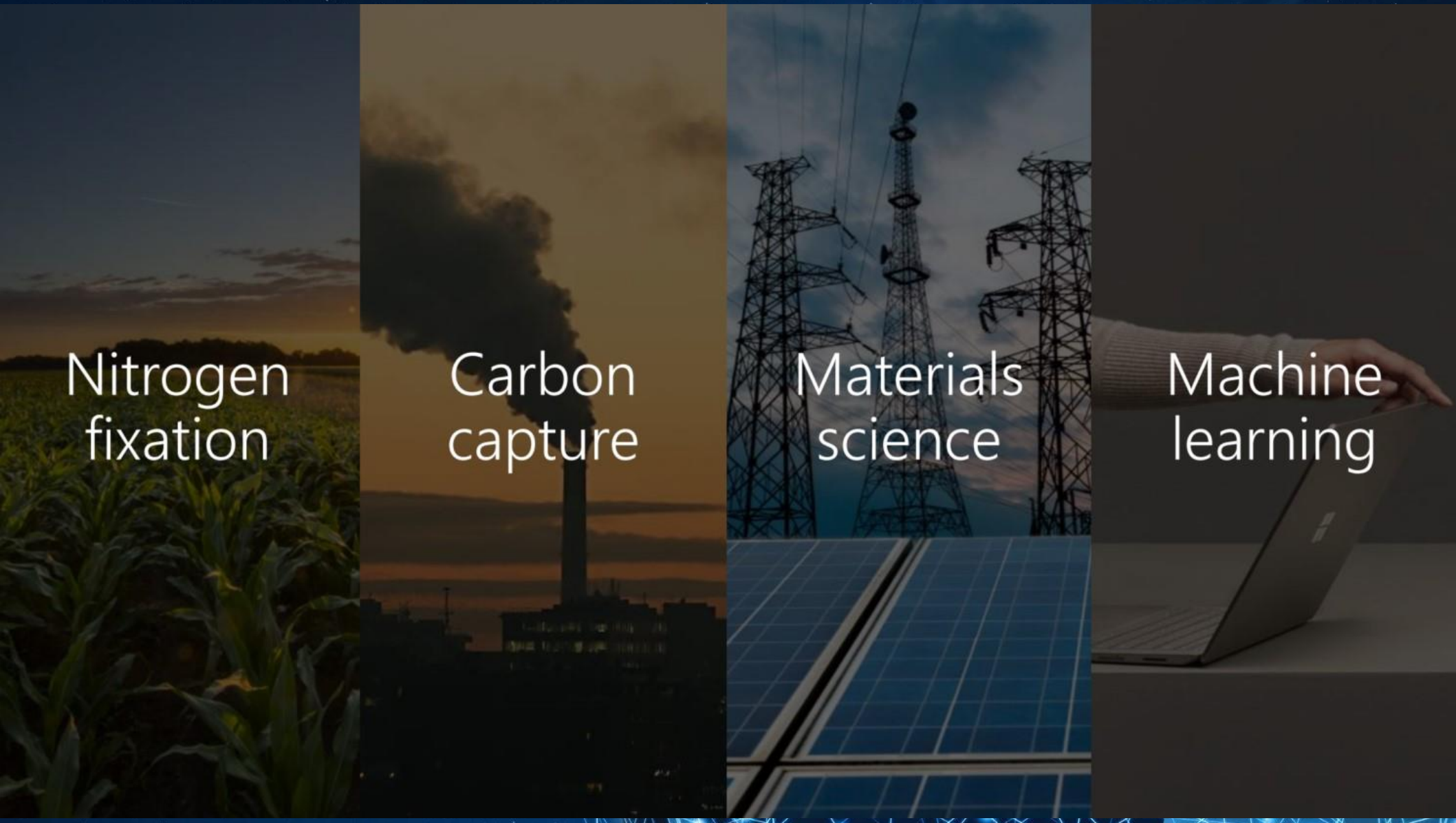


Genengnews.com



Science.com



D. Wecker, Microsoft Quantum

Thank you.