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Quantum Computing

for Digital Chemistry at Covestro

NMWP Innovation2Go Web Talk

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Torsten Heinemann, Covestro Deutschland AG

Covestro at a glance

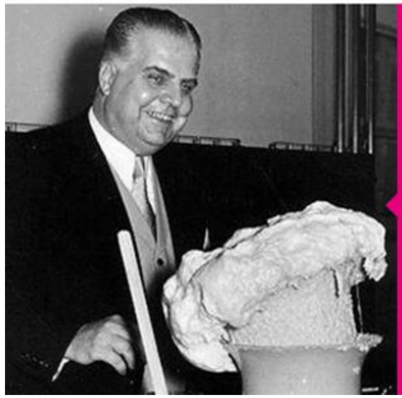
A leading polymer producer

1953

Hermann Schnell discovers polycarbonate

The Bayer chemist, working at the Group's Central Scientific Laboratory in Krefeld-Uerdingen, succeeds in synthesizing polycarbonate.

1937



New perspectives through the discovery of polyurethanes

An invention by the chemist Otto Bayer — who is not related to the family that founded the Bayer Group.

Global player

- 30 sites worldwide
- Close to markets, customers and suppliers

Highly innovative

- Approx. 1100 employees in R&D
- 80 years of ideas and inventions

Automotive and transportation

20%

Construction

16%

Wood and furniture

18%

Electrics and electronics

12%

Chemicals

8%

Sports/leisure, cosmetics, health and others

26%

Covestro: Digitalization

Digitization of the core business

R&D, production, supply chain and customer interaction

IT infrastructure

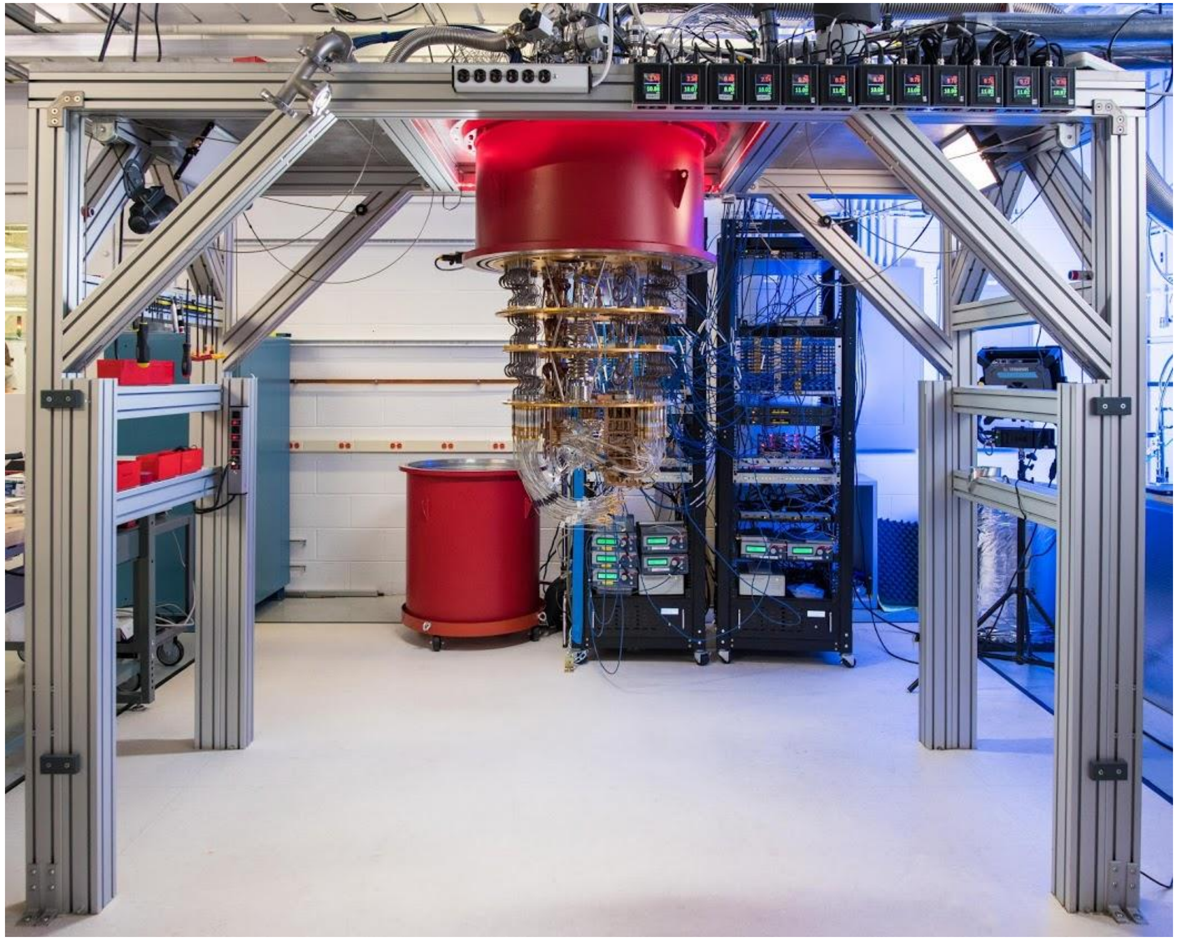
New standards in digital collaboration

Digital business models

Create new value steams

How do quantum computers look like?

A race of multiple hardware platforms



State of the art

- Small scale implementations exist in all platforms
- Small quantum computers already accessible

Engineering challenge

- Scaling to more qubits
- Higher fidelities
- Faster gates and readout

Investments

- From major industries: IBM, Google, Microsoft, Intel, Honeywell, Alibaba, Huawei, VW, BWM, BASF, ...
- From VCs and public sector in US, China, UK, EU

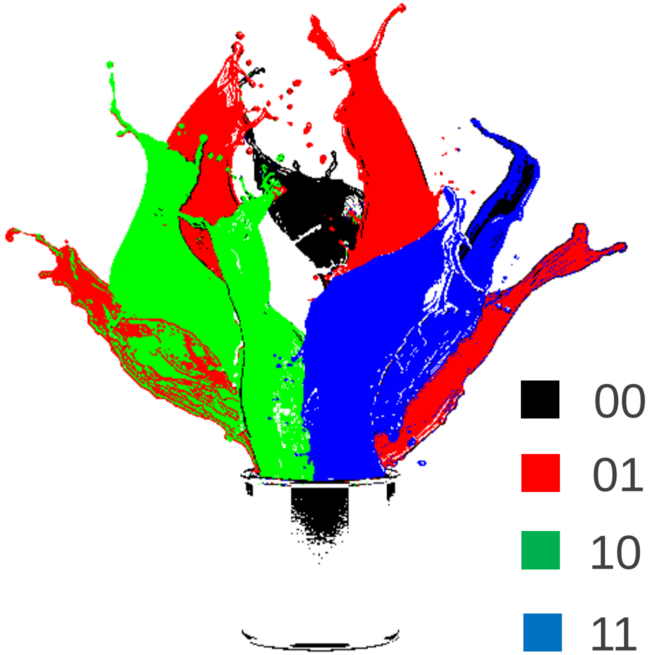
Multiple platforms being developed

- Probability of realization of large-scale machines with disruptive potential is now very high
- Extremely rapid progress on hardware and software

Why are quantum computers more powerful?

Because complexity theory says so...

Classical computers work with discrete states



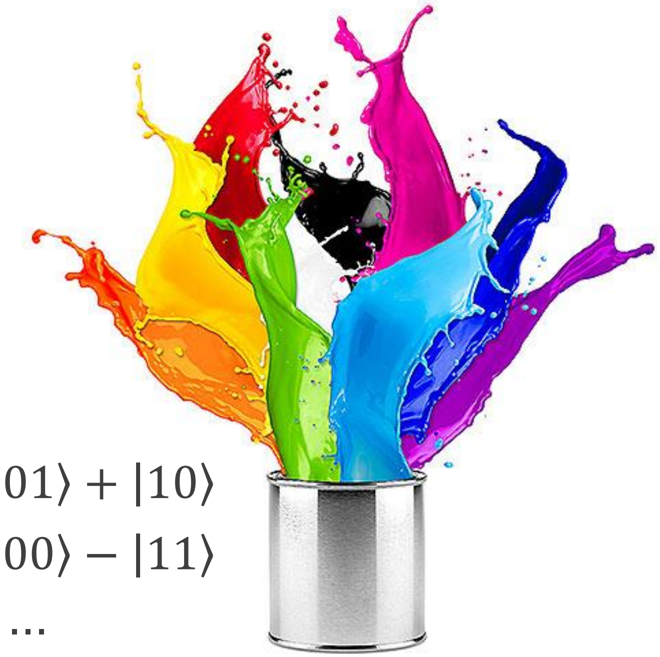
- 00
- 01
- 10
- 11

N bits → 2^N distinct states

Quantum Superposition

- Makes quantum chemistry hard
- Makes quantum computers powerful
- No analogue in the classical world

Quantum computers take shortcuts through superposition states



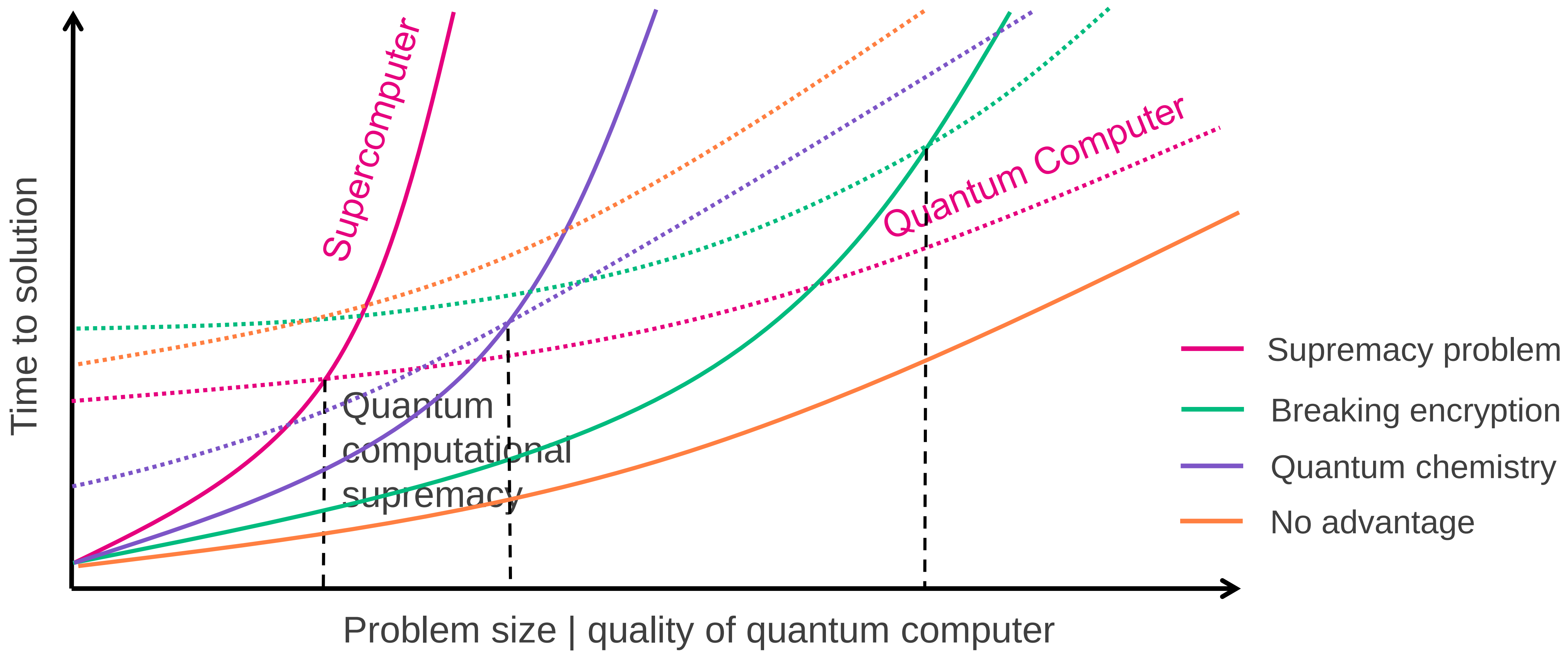
$|\psi\rangle = |01\rangle + |10\rangle$

$|\psi\rangle = |00\rangle - |11\rangle$

…

N qubits → $\sim 2^{2^N}$ distinct states

Which problems can quantum computing solve?
A “bizarre hammer” – Scott Aaronson



NISQ vs. Fault tolerant Quantum computer

Two very different types of quantum computer

NISQ – noisy intermediate scale quantum

- Available today with approx. 50 qubits, soon a few hundred qubits
- One qubit for computing per physical qubit on the device
- Qubits are not perfect, error accumulate during the computation, restricted to running rather short programs, currently usually not restricted by the total number of qubits on the device
- Need to design algorithms that have resilience against noise, need to do error mitigation
- Algorithms are heuristics, need to be tried out, still open question whether quantum advantage can be obtained

FTEC – Fault tolerant error correcting

- Working principle has been demonstrated
- Error correction comes with high overhead: ~1000 physical qubits in the device per logical qubit for computation
- Google and IBM have committed to building such devices (Google 1000 logical qubits before 2030)
- Elementary logic operations are error free, can run arbitrary long programs
- Enables “magic” algorithms, such as virtually exact chemistry simulation in polynomial time; breaking RSA encryption, …
- Algorithms are “deterministic” and can thus be analyzed beforehand, speedups can be proven

Covestro Value Chain and Link to Digital Chemistry

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Value Chain

Product Synthesis → **Formulation** Development → **Processing** Optimization → **Final Part** Performance

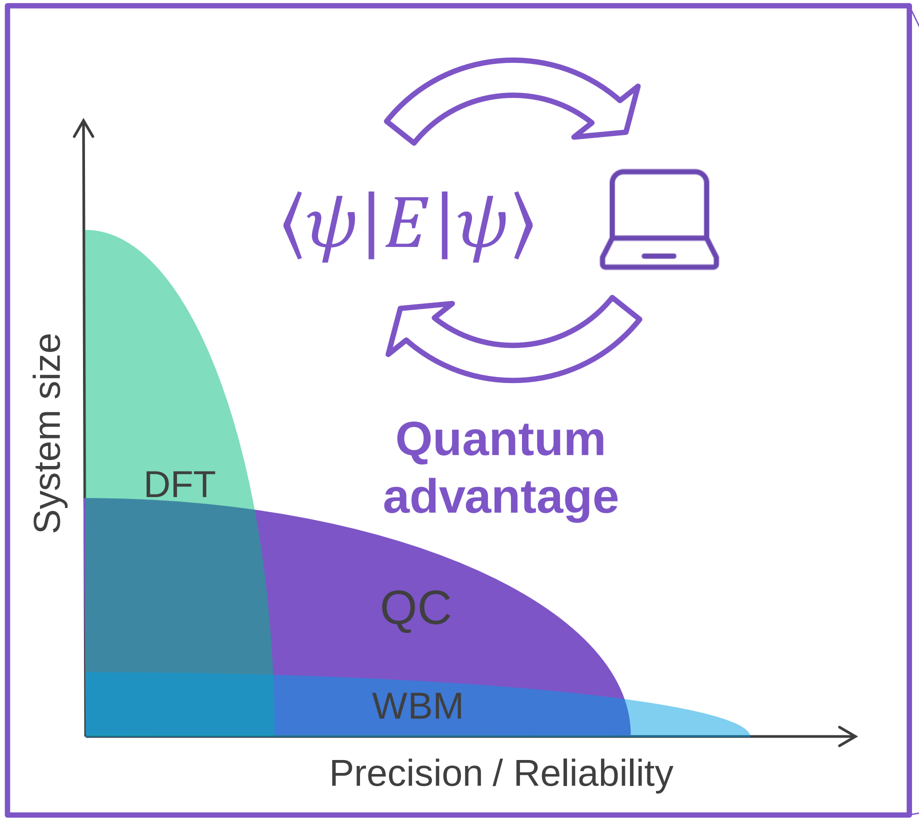
ONE CIRCULAR VISION

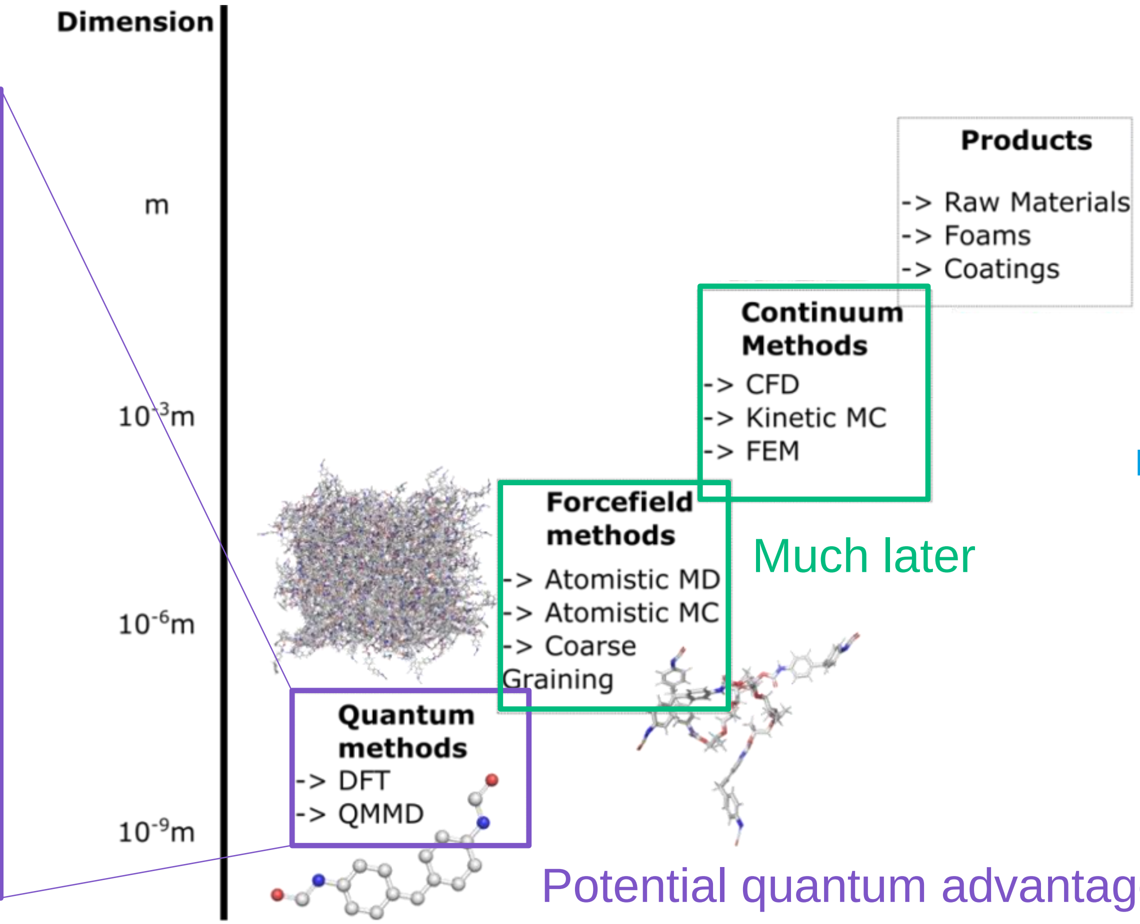
"Computational Chemistry" Methods

Quantum Methods → Forcefield Methods → Continuum Methods

Quantum computing in digital R&D

From solving the Schrödinger equation to products





Potential quantum advantage soon

New products

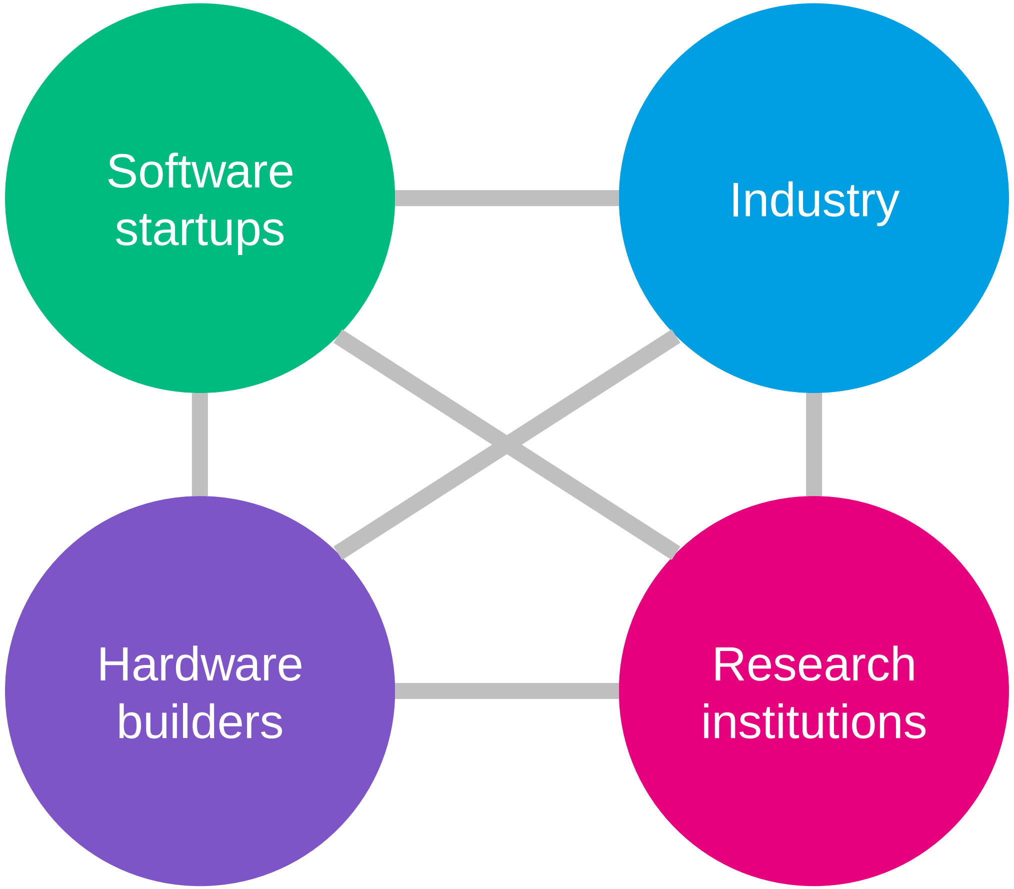
New production technology

Increase R&D efficiency and widen scope

DFT: Density Functional Theory, WBM: Wave function Based Methods, MD: Molecular Dynamics, MC: Monte Carlo, CFD: Continuum Fluid Dynamics

Covestro approach to quantum computing

A global network enabling industrial use cases



Take home

- Quantum Computing technologies rapidly progressing
- Chemical industry likely among the first to profit from a quantum advantage
- Range of promising applications
- Beware the hype

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