Quantum chemistry C12 x Quantinuum x Air Liquide

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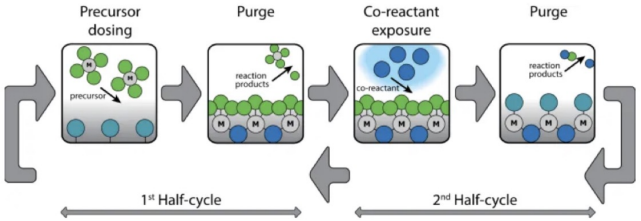
New chemical reactions is key to answer the rapidly evolving needs of the semiconductor industry

Bottom-up nanofabrication by atomic layer deposition (ALD) on precise surfaces (process selectivity) currently gaining momentum

Novel semiconductor nodes progressively requiring more specific reagents and an ever-increasing range of materials

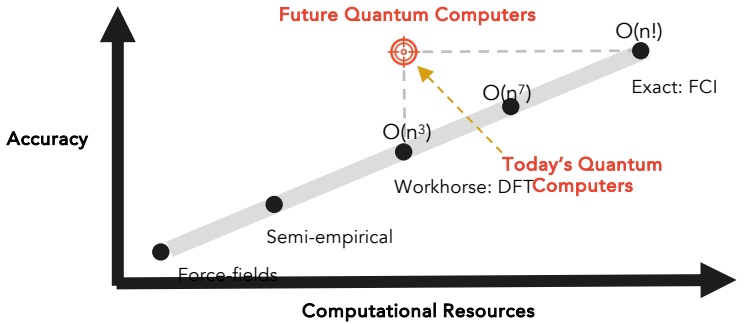
Need to develop selective and stable organometallic precursors



Current computing solutions do not make it possible to answer these new customer needs

Barriers reactions and stability of transition states not correctly estimated by DFT

Challenge of simulating accurately strongly correlated molecules, materials and processes due to the rapid scaling of computational resources with respect to the number of electrons involved



Source: Quantinuum

We started an innovative partnerships to explore how quantum computing supports on a industry-relevant use case

Air Liquide

Use case

World class expertise in quantum chemistry

C12

Quantum hardware

Next-generation quantum computing technology

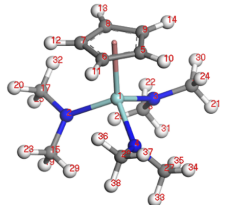
QUANTINUUM

Quantum software

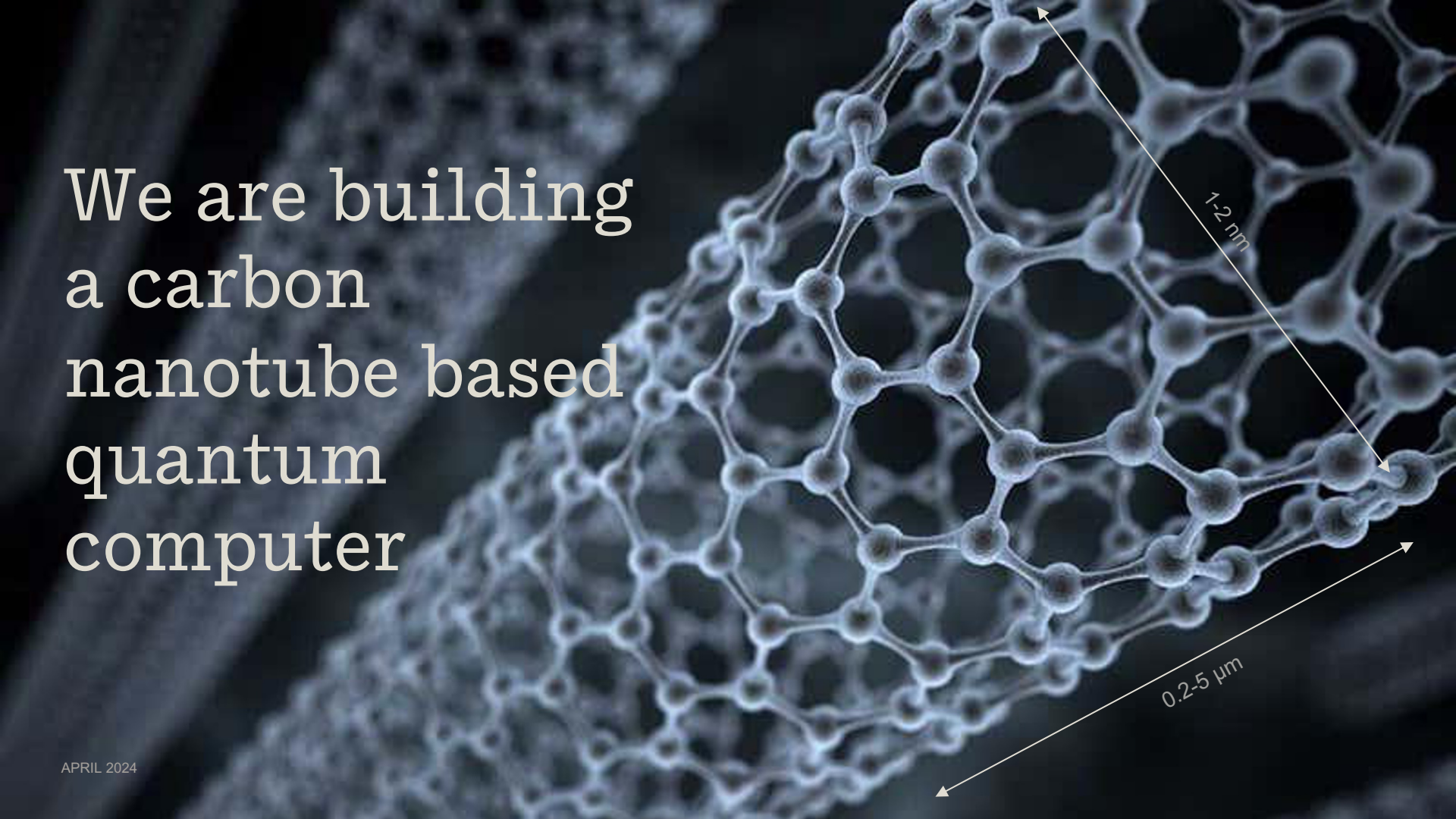
World leader in quantum algorithms for quantum chemistry

Zr precursor for ZrO_2, proposed by Air Liquide

Zirconium amido cyclopentadienyl complex [CpZr(N(CH3)2)3]



We are building a carbon nanotube based quantum computer



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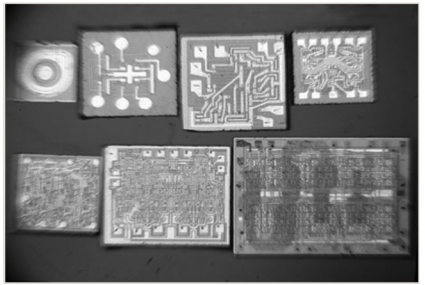
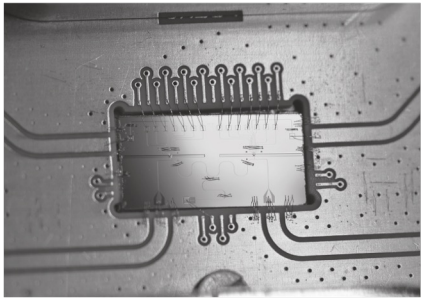
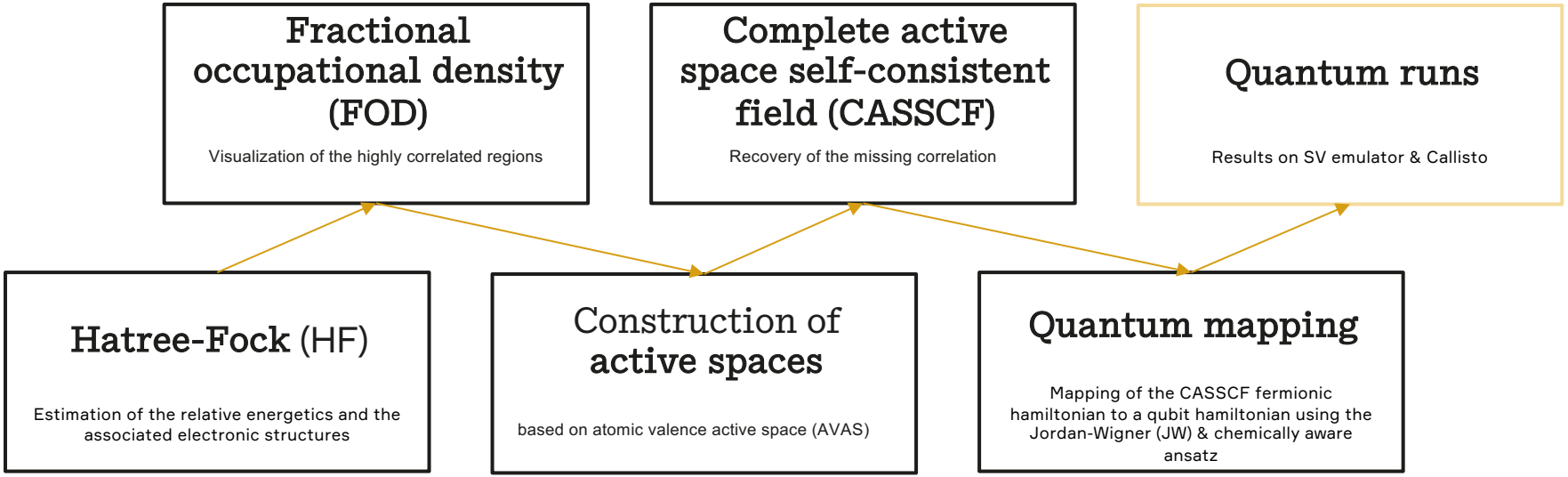
Carbon nanotubes will be what silicon was for classical transistors: the enabling material

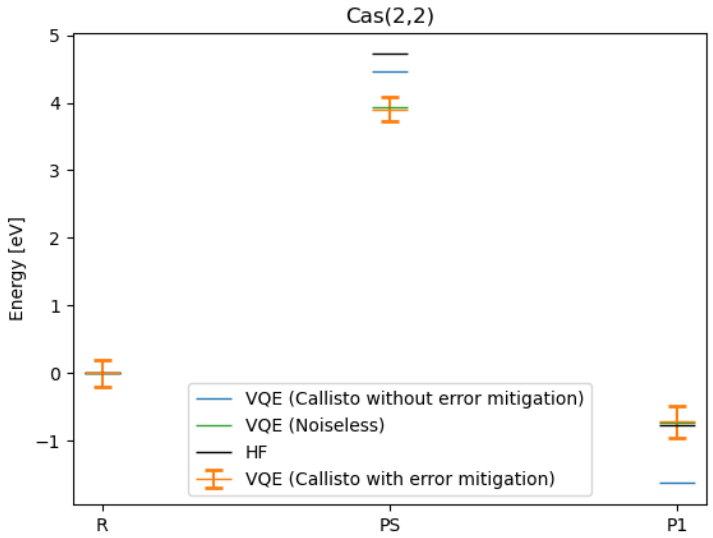
Classical computing **[From 1960s]**	Silicon	
Quantum computing **[From 2020s]**	Carbon nanotubes	

We built a unique hybrid quantum/classical workflow on a specific problem

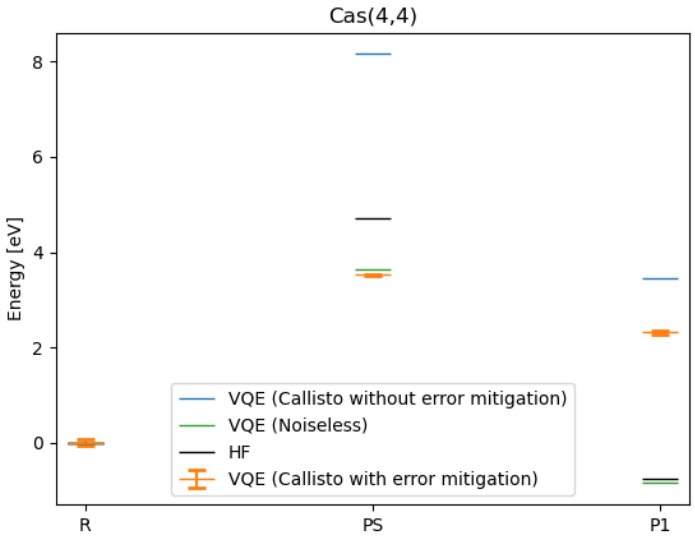


When running on Callisto, the error is at chemical accuracy for CAS(2,2) and c. 90 mHatree for CAS(4,4)

Relative energies of TS and P1 states



Relative energies of TS and P1 states



Main achievements & take-aways

Construction of models for the three states of the reaction

Interface of Callisto with `TKET` and `InQuanto`

VQE simulations using a statevector simulator as well as Callisto

It is possible to simulate a reduced version of an industry-relevant problem on a (even noisy) quantum computer

The tested algorithm (VQE) cannot be scaled

Leading the next materials leap in quantum computing

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