MATERIALS PHYSICS IN THE QUANTUM REALM

Challenges in the NISQ Era

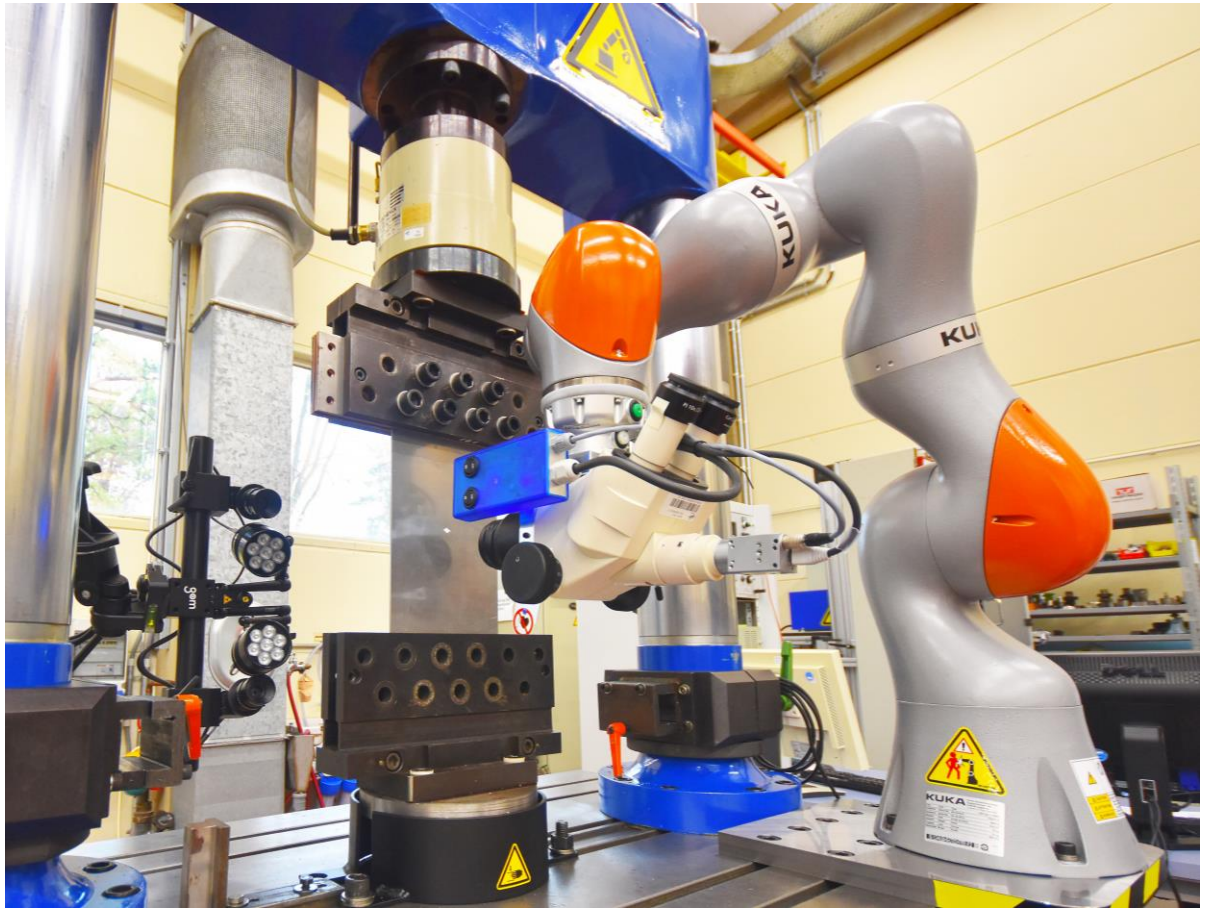
Matthias Sperl, Erik Schultheis, Projekt QuantiCoM, 27.09.2023

Advanced mechanical testing

Data Generation

High-Throughput

High-Fidelity

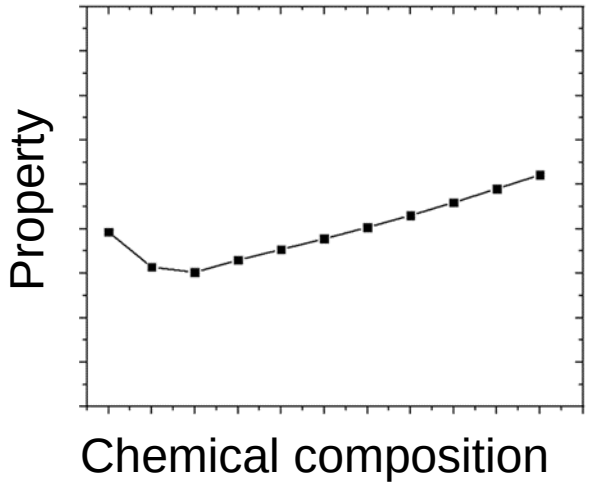


Digital Backbone

QuantiCoM – The Vision

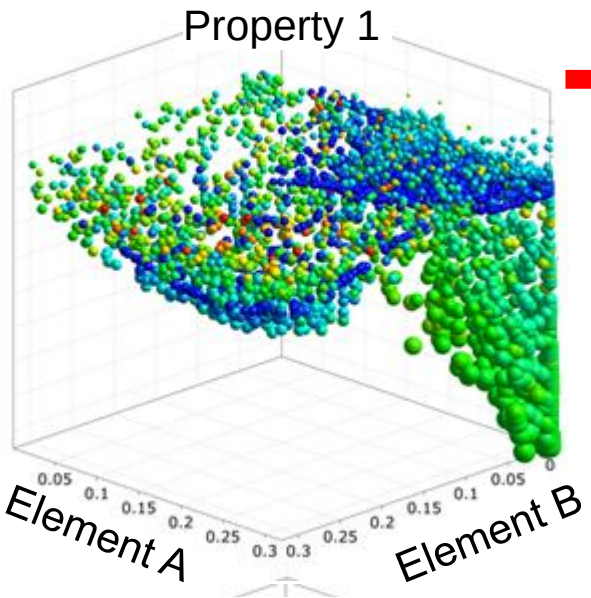
Objective

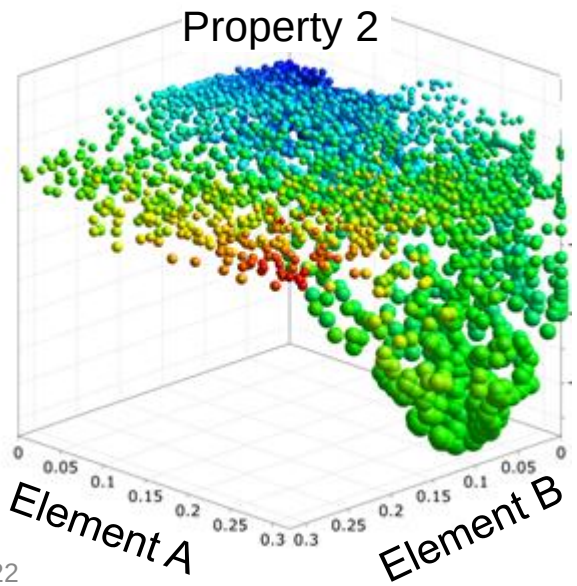
- New alloy with targeted properties

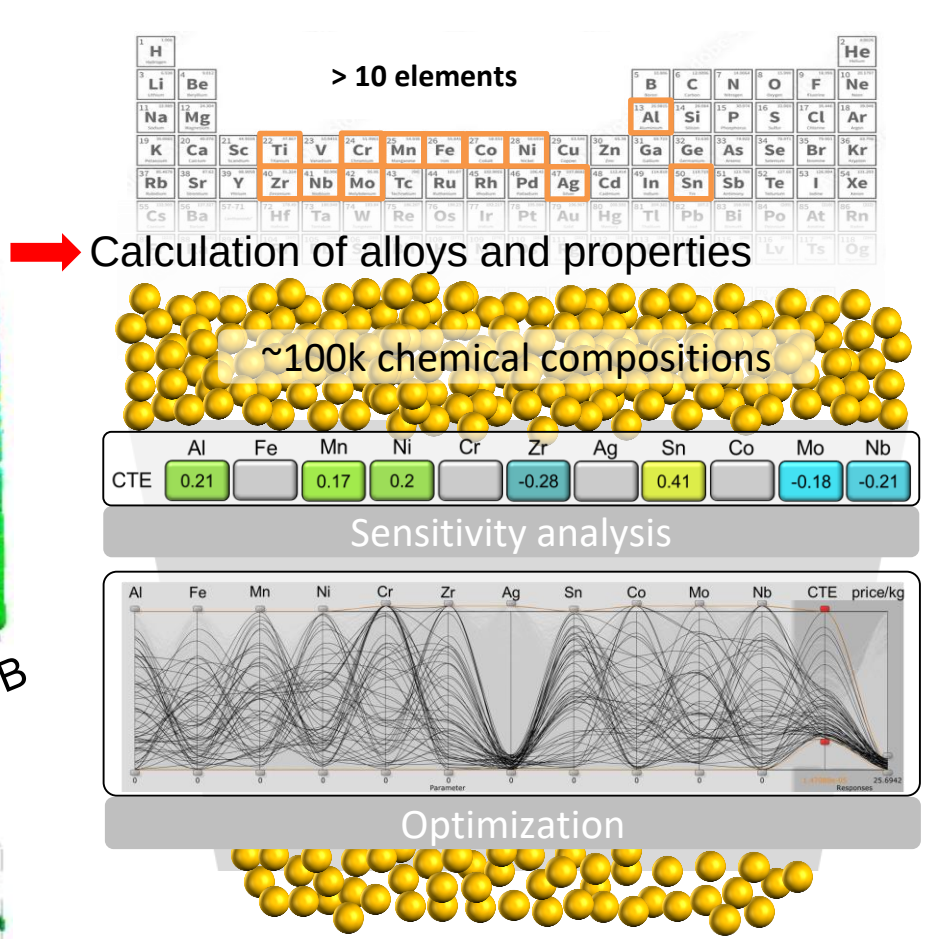


E.g. design criteria

- Property 1: $CTE_{(25 - 500\ °C)}$
- Property 2: cost efficient
- Property 3: strength





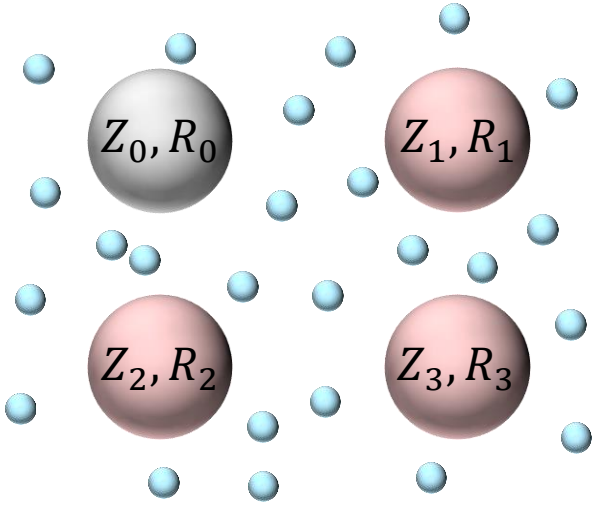


Thermo-dynamic calculations

Optimization steps

High-throughput alloy design enabled by QC/HPC atomistic simulations, experiments and QC-based optimization

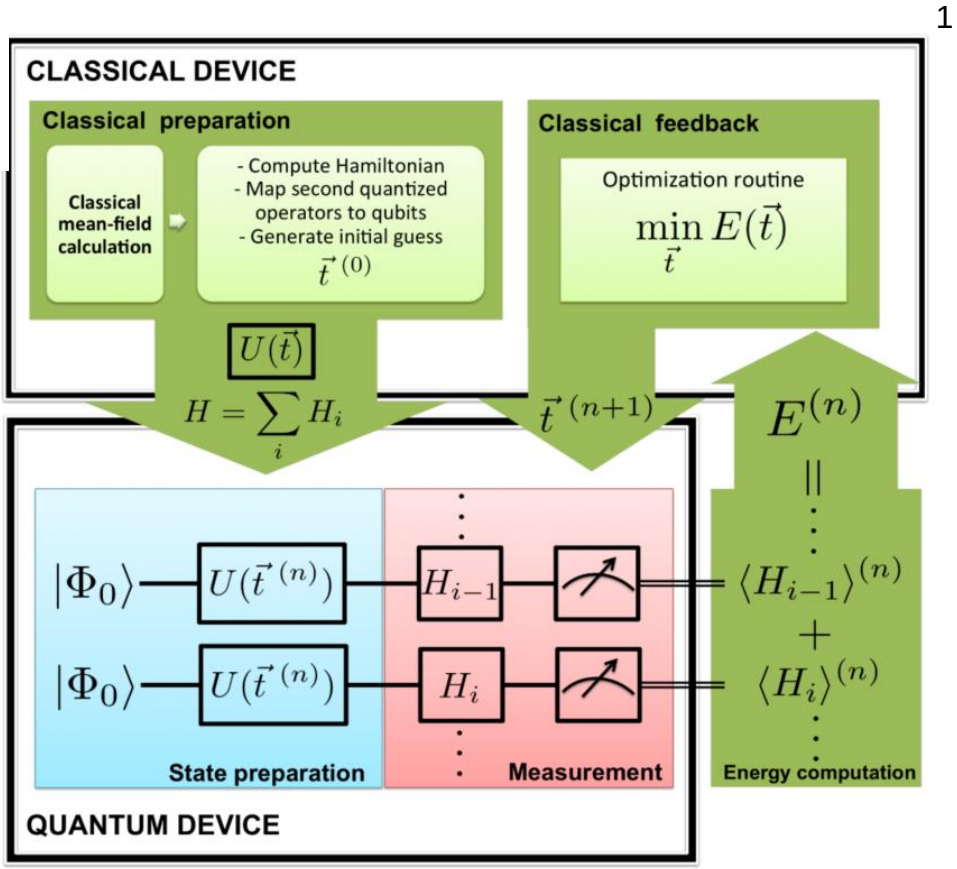
Ab-Initio Electronic Structure on NISQ Devices



$$\hat{H}_{elec} = \sum_{pq} h_{pq} \hat{a}_p^\dagger \hat{a}_q + \frac{1}{2} \sum_{pqrs} h_{pqrs} \hat{a}_p^\dagger \hat{a}_q^\dagger \hat{a}_r \hat{a}_s$$

$$h_{pq} = \int \phi_p^*(r) \left(-\frac{1}{2}\nabla^2 - \sum_I \frac{Z_I}{R_I - r} \right) \phi_q(r) dr$$

$$h_{pqrs} = \int \frac{\phi_p^*(r_1)\phi_q^*(r_2)\phi_r(r_2)\phi_s(r_1)}{|r_1 - r_2|} dr_1 dr_2$$



[1]

- Electronic structure of lattice structures
- Currrent challenges with VQE
  - Basis set
  - Error mitigation
  - Measuring expectation values ($\mathcal{O}(N^4)$ for $\hat{H}_{\text{elec}}$)
  - VQE ansatz circuits
  - Fermion-to-qubit mapping

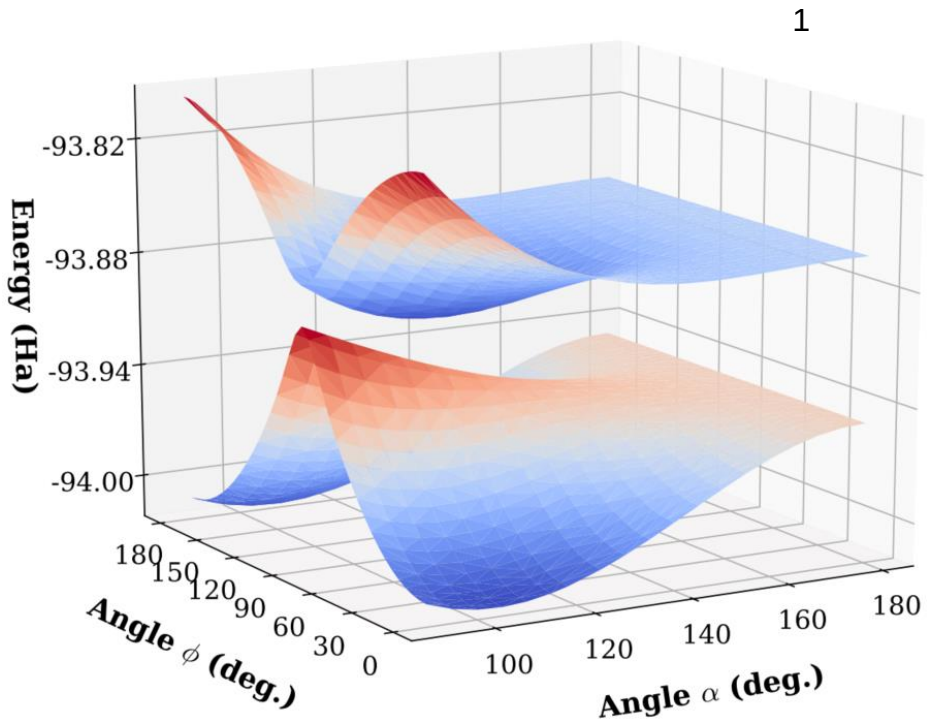
[1] Romero et al. 2017 „Strategies for quantum computing molecular energies using the unitary coupled cluster ansatz“

Excited States with VQE

- Excited states are important for
  - Photochemistry
  - Chemical reactions
  - Defects
  - Quantum applications

- Quantum Subspace Expansion[2]
- Subspace-Search VQE[3]

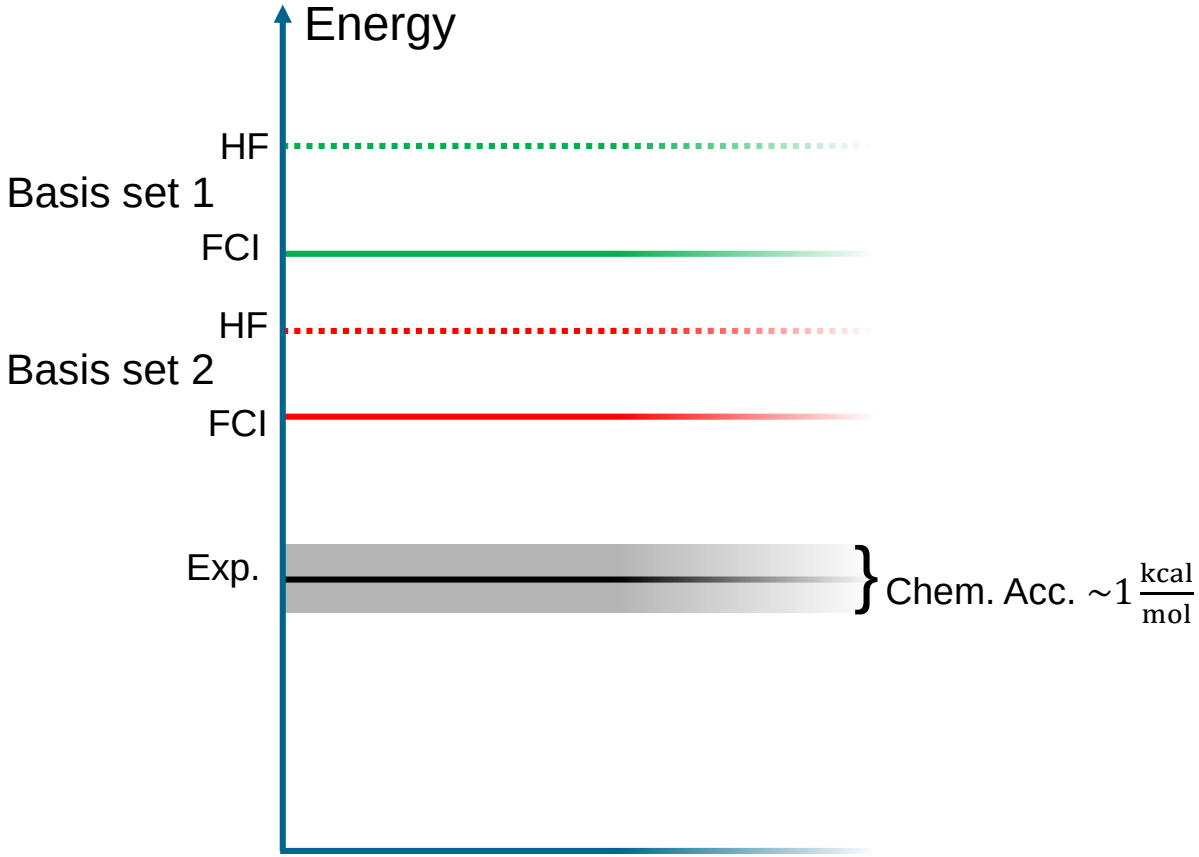
- Ground state gives information about equilibrium geometries

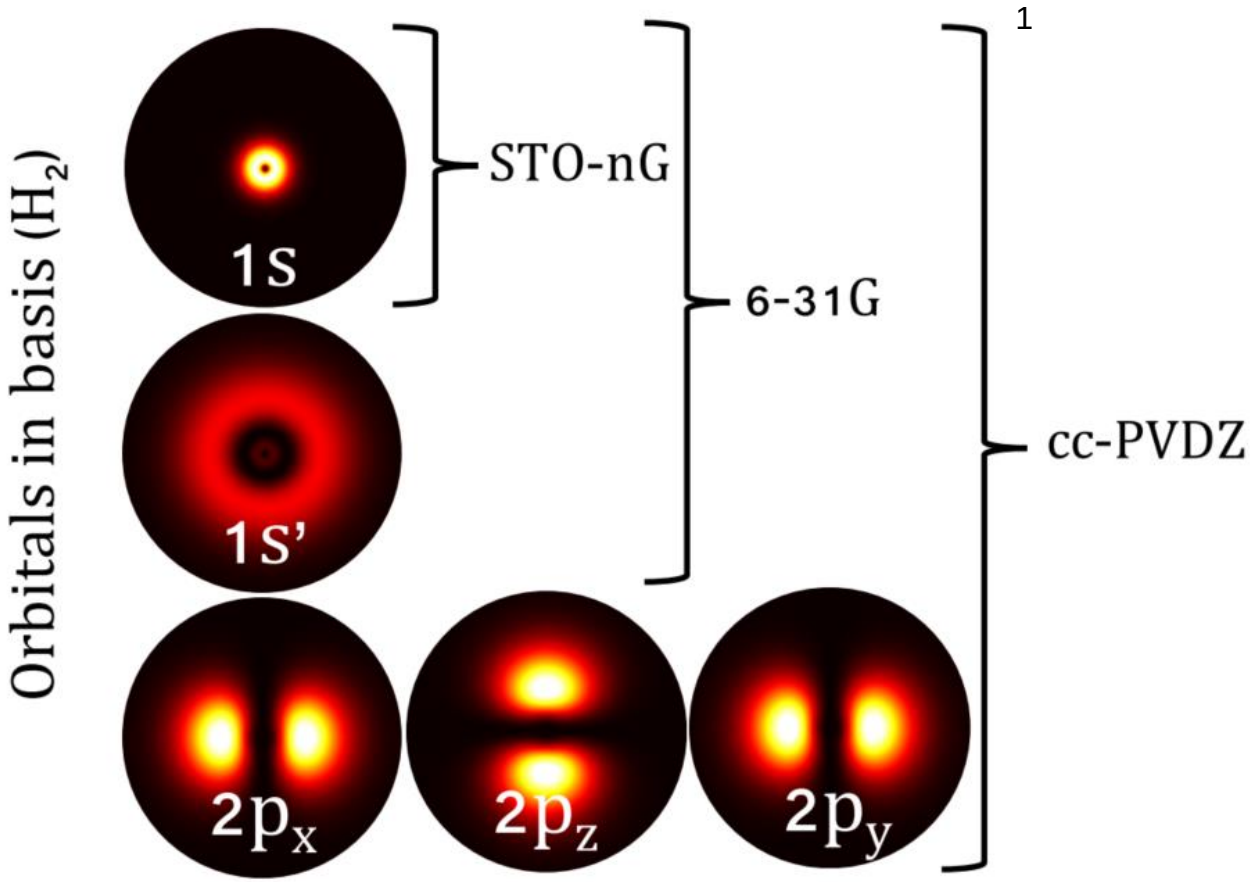


[1] Yalouz et al. 2021 „A state-averaged orbital-optimized hybrid quantum–classical algorithm for a democratic description of ground and excited states“
[2] McClean et al., 2017, „Hybrid quantum-classical hierarchy for mitigation of decoherence and determination of excited states“
[3] Nakanishi et al., 2019, „Subspace-search variational quantum eigensolver for excited states“

Basis Sets and Chemical Accuracy

- Basis set is first approximation we make

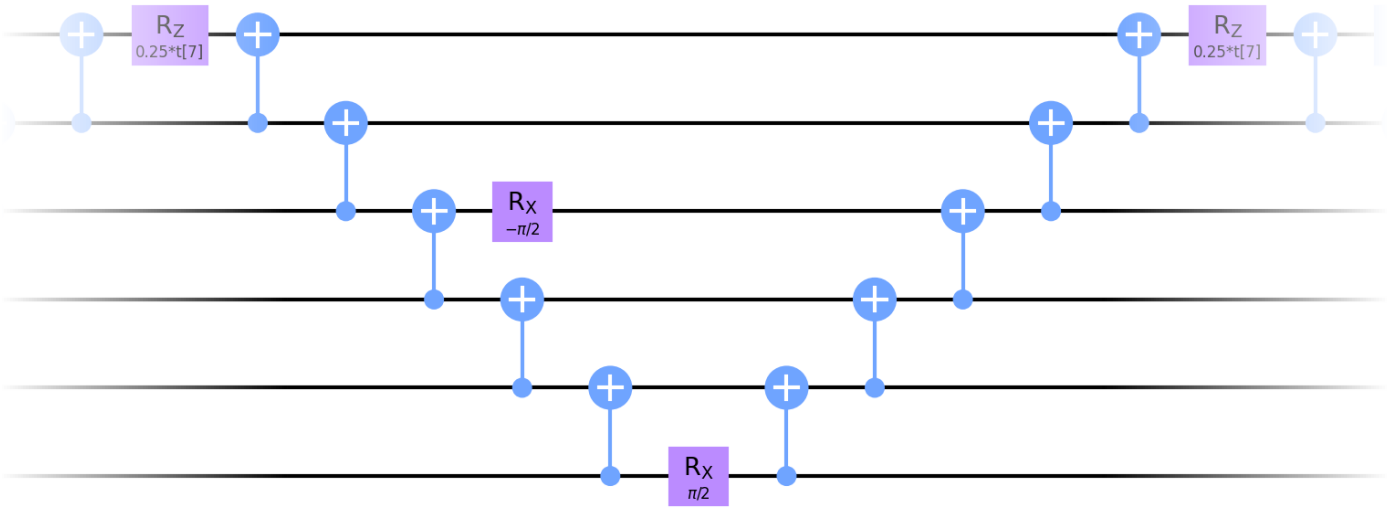




[1] McArdle et al. 2020 „Quantum computational chemistry“

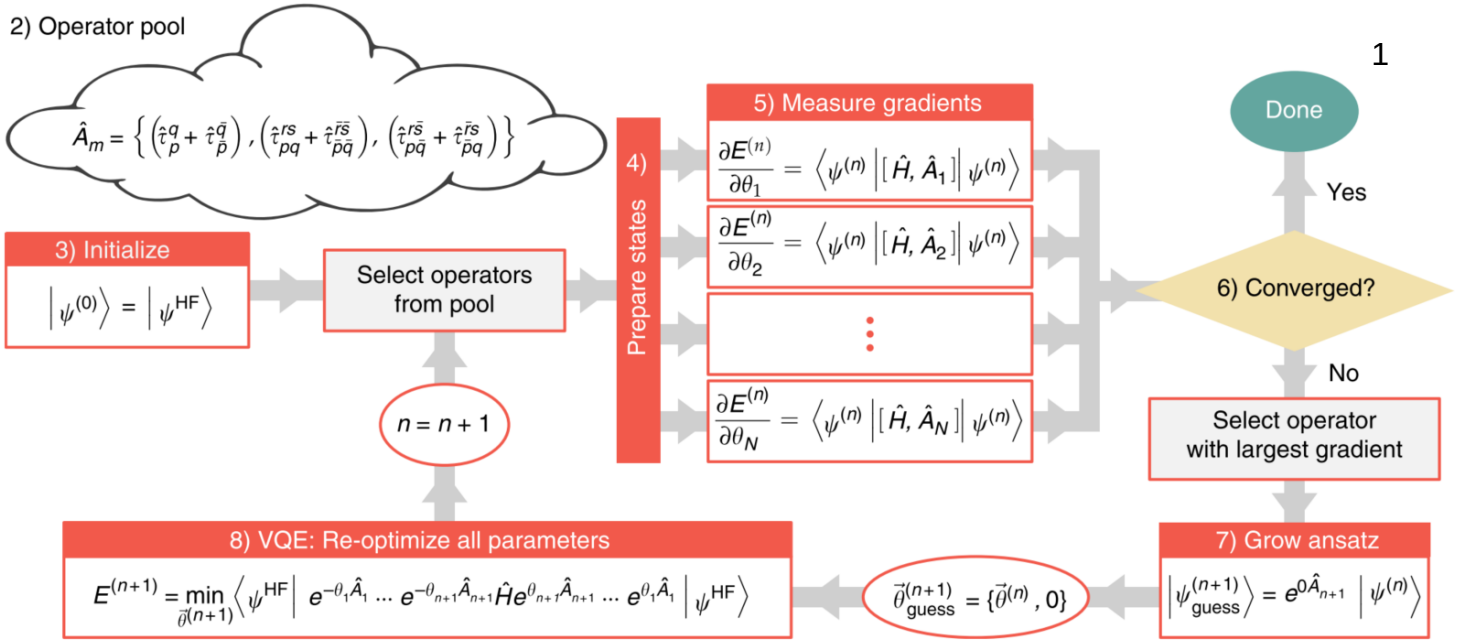
VQE State Preparation on NISQ Devices

- Prepare electronic ground state with parameterized quantum circuit
- Chemically inspired ansätze:
  - Unitary coupled cluster with single and double excitations (UCCSD)
- Numerous CNOT layers and deep ansatz circuit
- Small hardware connectivity and coherence times

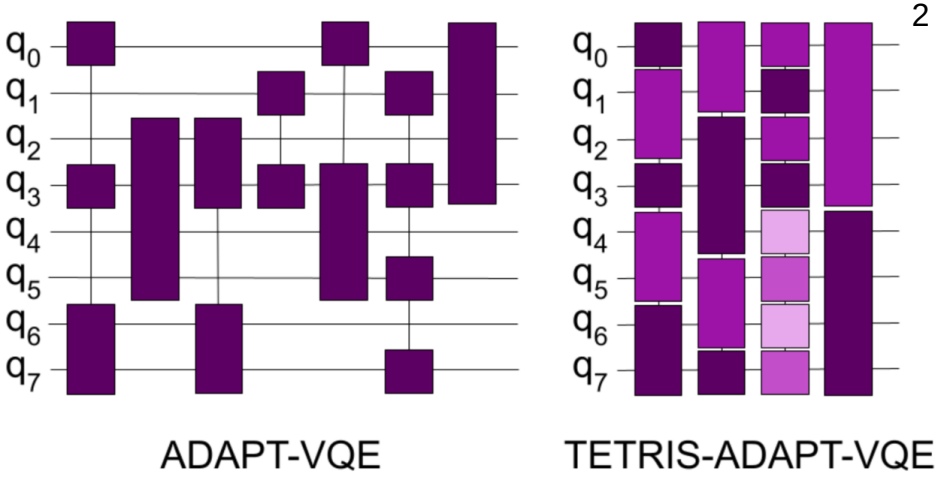


VQE State Preparation on NISQ Devices

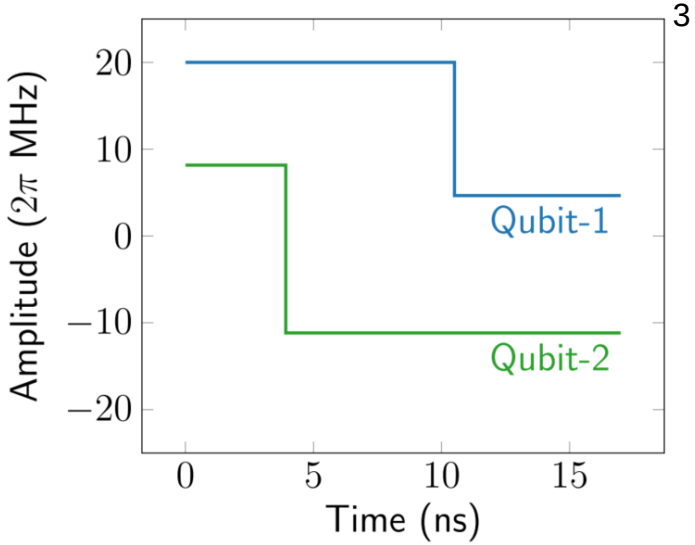
- Prepare ground/excited state with shallow circuit



1



2

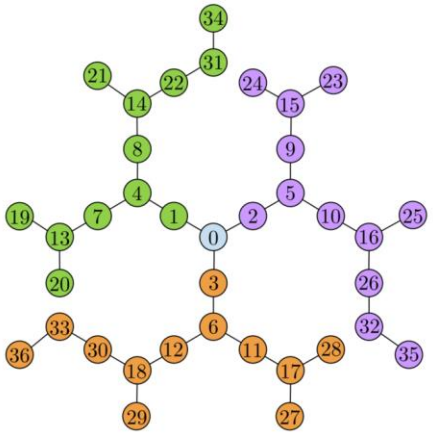


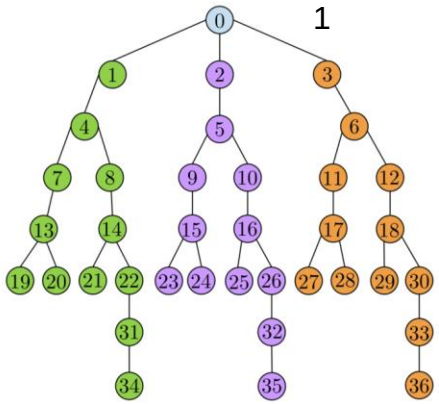
3

- Conserve quantum numbers with symmetries

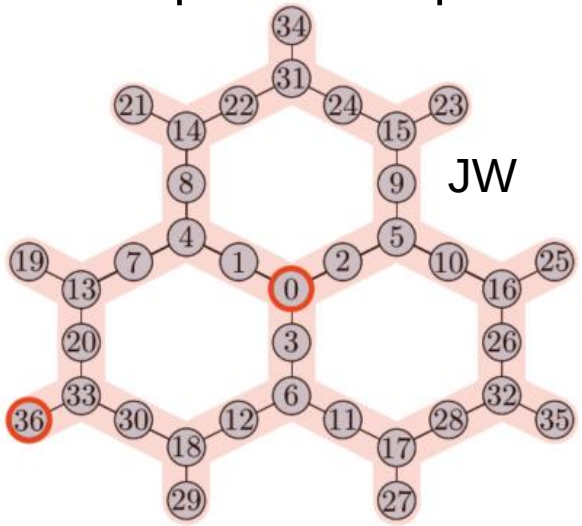
[1] Grimsley et al. 2019 „An adaptive variational algorithm for exact molecular simulations on a quantum computer“
[2] Anastasiou et al. 2022 „TETRIS-ADAPT-VQE: An adaptive algorithm that yields shallower, denser circuit ansätze“
[3] Meitei et al. 2020 „Gate-free state preparation for fast variational quantum eigensolver simulations: ctrl-VQE“

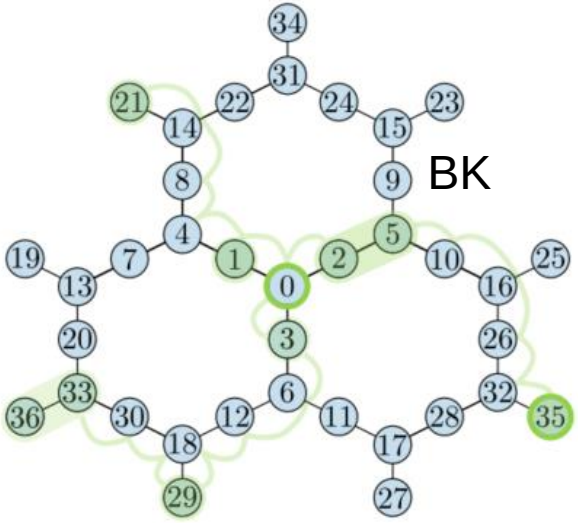
Fermion-to-Qubit Mappings

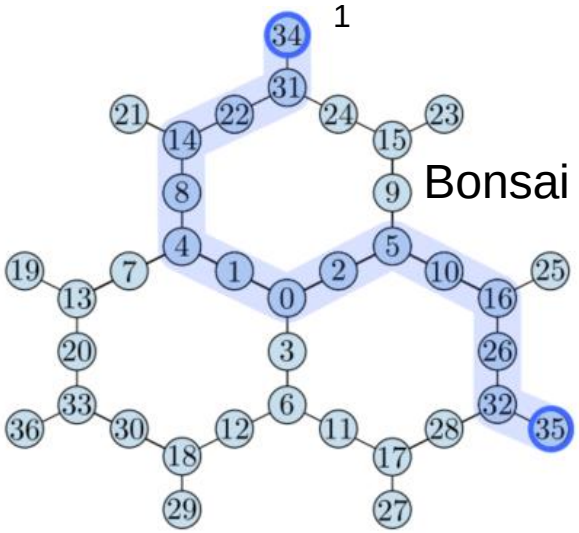




- Jordan-Wigner – $\mathcal{O}(N)$
  - Store occupations in qubits, large Pauli Z strings
- Parity – $\mathcal{O}(N)$
  - Store parity in qubits, large Pauli X strings
- Bravyi-Kitaev – $\mathcal{O}(\log_2 N)$
  - Store partial sums of occupations in qubits
- Bonsai – $\mathcal{O}(\sqrt{N})$
  - Hardware-specific mappings with lower SWAP overhead





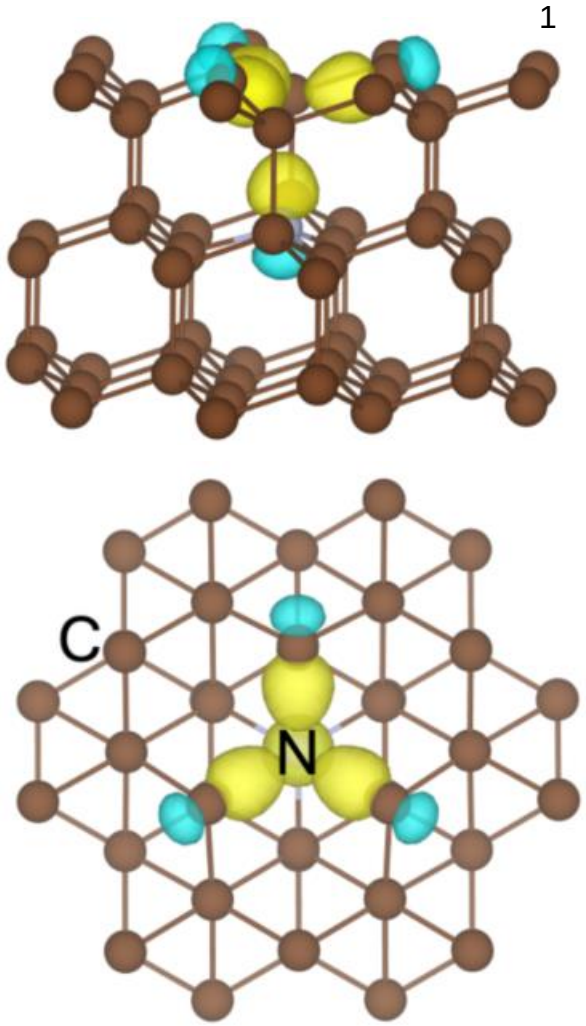


[1] Miller et al. 2023 „Bonsai Algorithm: Grow Your Own Fermion-to-Qubit Mappings“

Defects and Embedding

- Defects are critical for material properties
- Rare defects require large supercells
  - Quantum computing
  - Embedding theories

- Concentrate on localized sub-space (active space)
  - Spatially or energetically localized around defect
- Describe environment with mean-field approach



[1]

[1] Muechler et al. 2022 „Quantum embedding methods for correlated excited states of point defects: Case studies and challenges“