Electron and Phonon Properties of Periodic Solids via Quantum Computing

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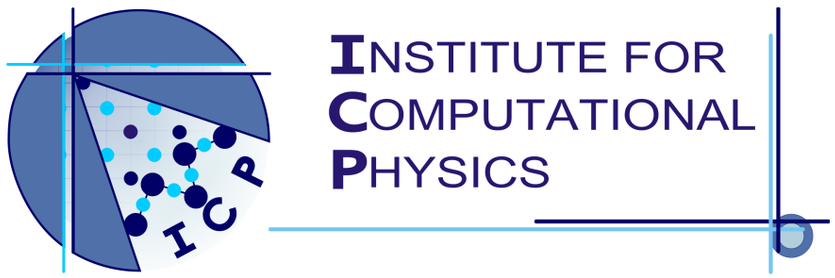
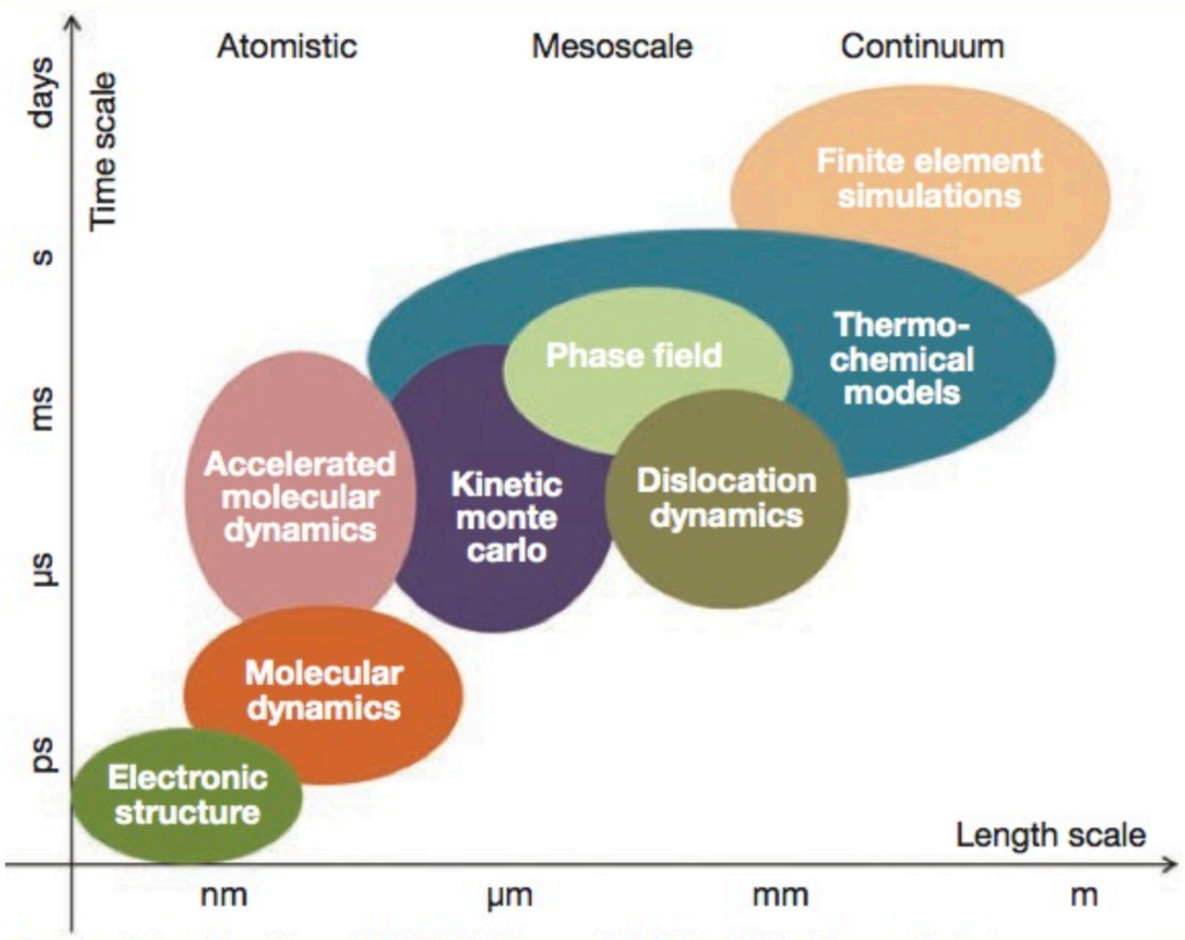
Quantum Computing for Engineers

Winter Semester 21/22

Universität Stuttgart, Germany



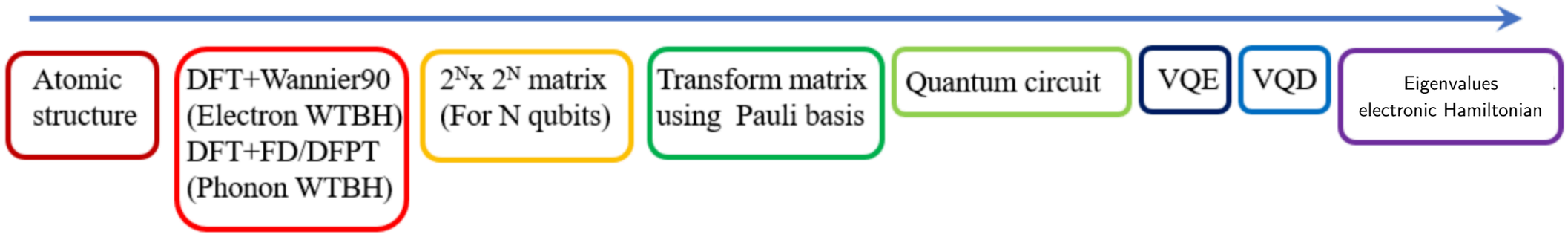
Introduction



Source: http://dx.doi.org/10.1016/j.jallcom.2007.01.102 (with permission)

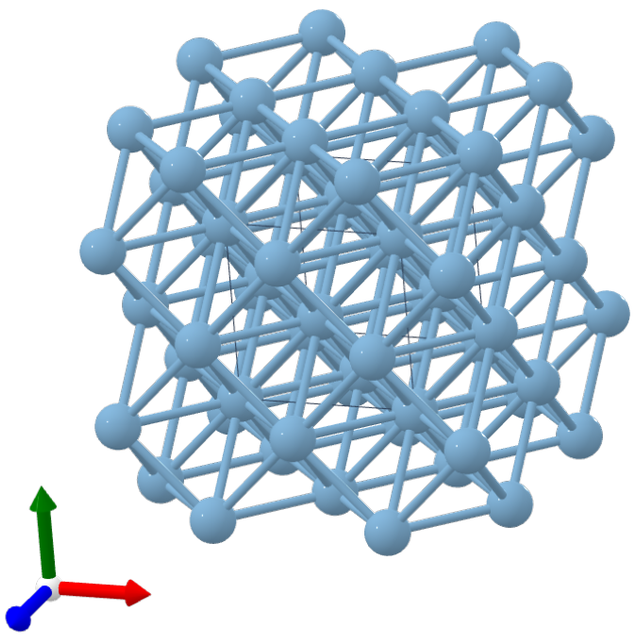
- Goal: solve Schrödinger equation to find the ground state energy
- Hamiltonian increases exponentially
- Classical Computers -> O(exp(n)) -> DFT
- QCs -> O(n) -> VQAs

QC Pipeline

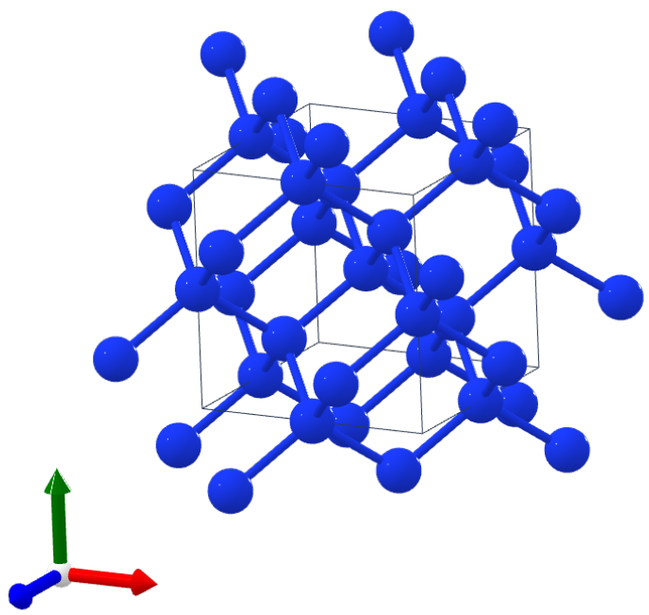


Kamal Choudhary 2021 J. Phys.: Condens. Matter 33 385501

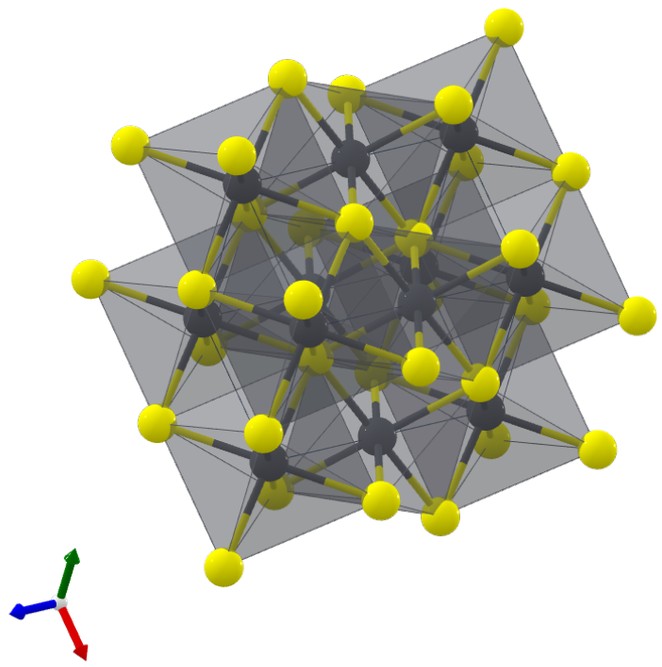
Periodic Structures



fcc Al



cb Si



hex PbS (lead sulphide)

Formula	JARVIS-ID	spg symbol	WTB orbitals
Al	JVASP-816	Fm-3m	8
Si	JVASP-1002	Fd-3m	16
PbS	JVASP-35680	I4/mmm	28

SimTech

INSTITUTE FOR COMPUTATIONAL PHYSICS

University of Stuttgart

JARVIS WTB

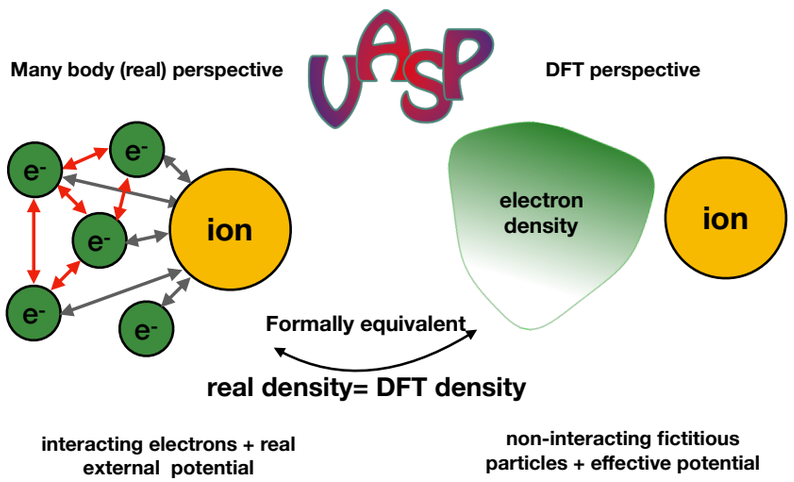
Submit

Select Material*

Si_3D_{Fd-3m}[JVASP-1002]

K-points: Mesh form or High-symmetry line*

Density Functional Theory (DFT)



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WANNIER90

$$|\mathbf{R}n = \frac{V}{(2\pi)^3}\int \mathbf{dk}\, \mathrm{e}^{-\mathrm{i}\mathbf{k}\cdot\mathbf{R}}|\psi_{n\mathbf{k}}|\psi_{n\mathbf{k}}.$$

Wannier functions based TBHs

Pauli basis with Qiskit

$$\mathcal{H} = \sum_{a=1}^{N_a} \frac{P_a^2}{2M_a} + \sum_{i=1}^{N_i} \frac{p_i^2}{2m} + \sum_{a<b} \frac{Z_a Z_b e^2}{|R_a - R_b|} + \sum_{i<j} \frac{e^2}{|r_i - r_j|} - \sum_{a,i} \frac{Z_a e^2}{|R_a - r_i|}$$

$$H = \sum_{P \in \{I,X,Y,Z\}^{\otimes n}} h_P P,$$

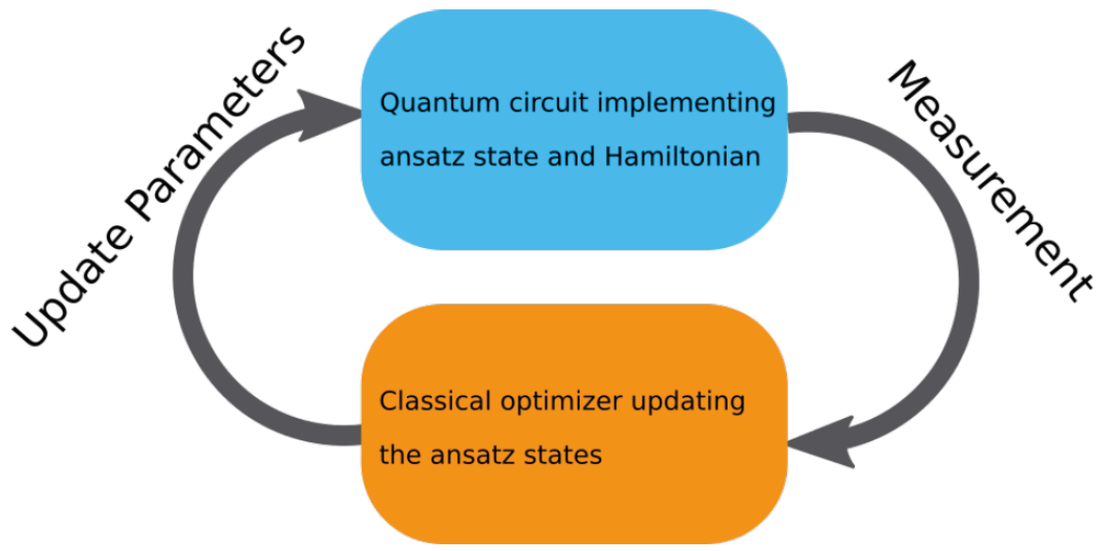
WeightedPauliOperator

class **WeightedPauliOperator(*paulis*, *basis=None*, *z2_symmetries=None*, *atol=1e-12*, *name=None*)** [source]

Weighted Pauli Operator

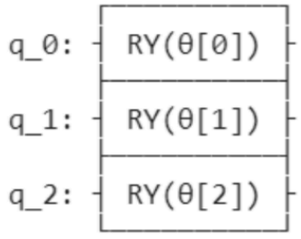
Variational Quantum Algorithms

- VQE improves QPE using Ritz variational principle, wavefunction ansatz and estimates the eigenvalue of the electronic Hamiltonian
- VQD requires the same number of qubits as VQE and uses overlap estimation to deflate eigenstates once they are found, enabling the calculation of the excited states.

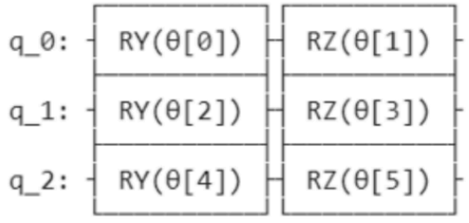


Parametrized circuits VQE-VQD

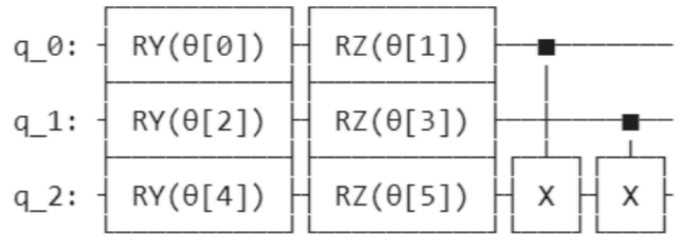
(a) Circuit-1



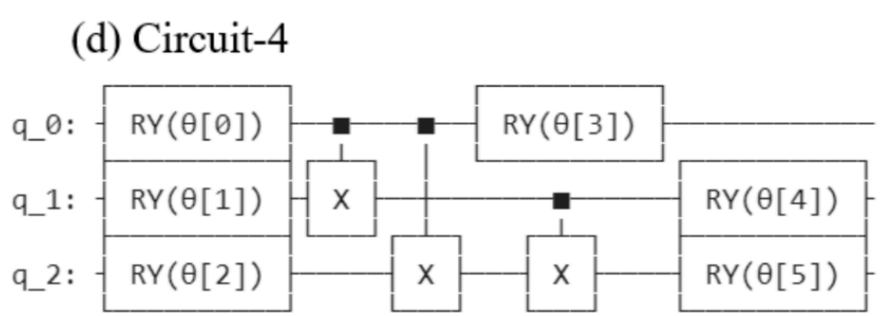
(b) Circuit-2



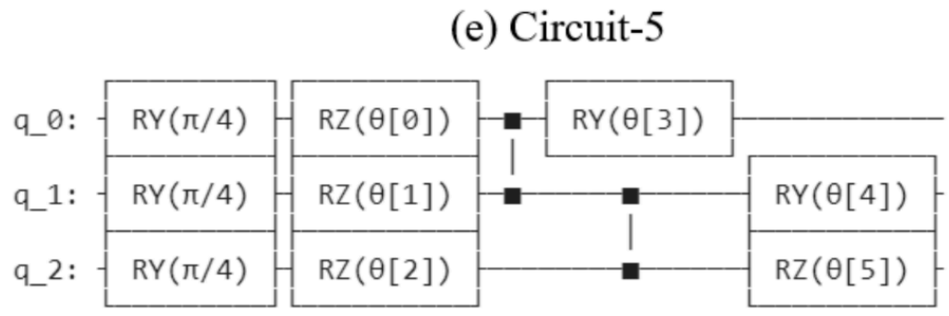
(c) Circuit-3



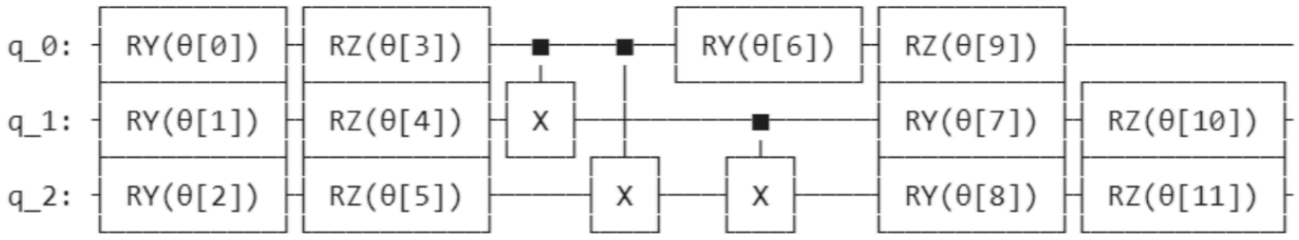
(d) Circuit-4



(e) Circuit-5



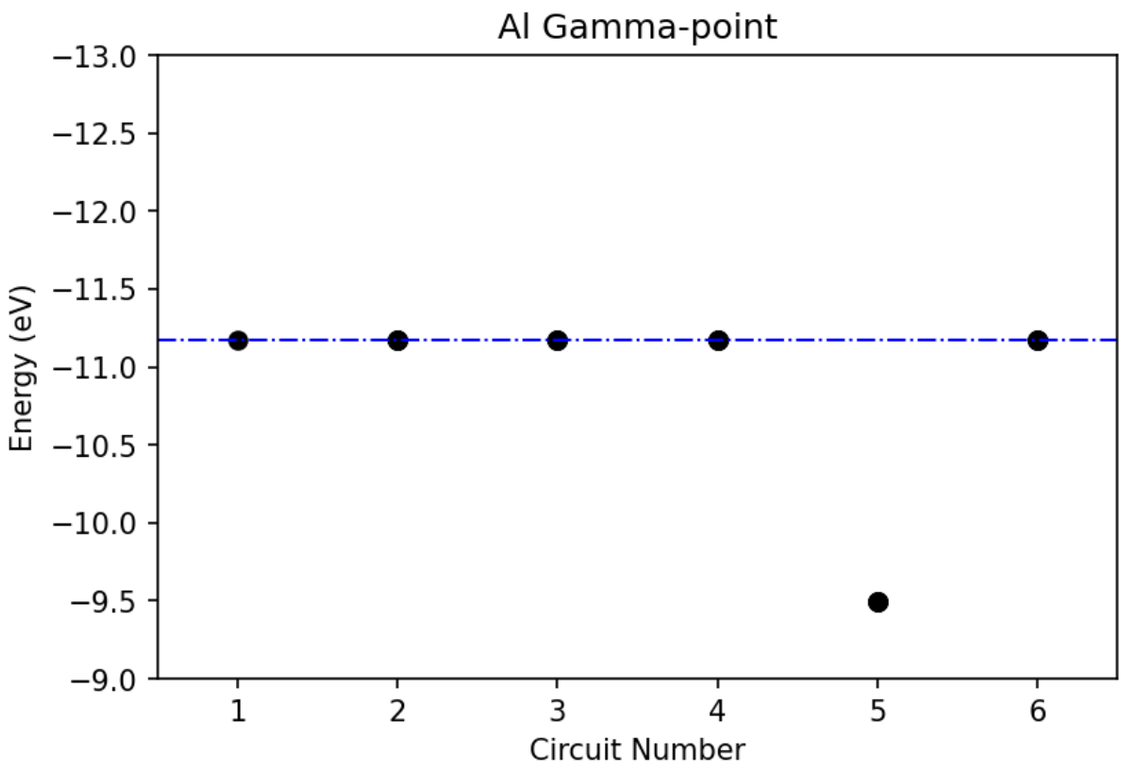
(f) Circuit-6

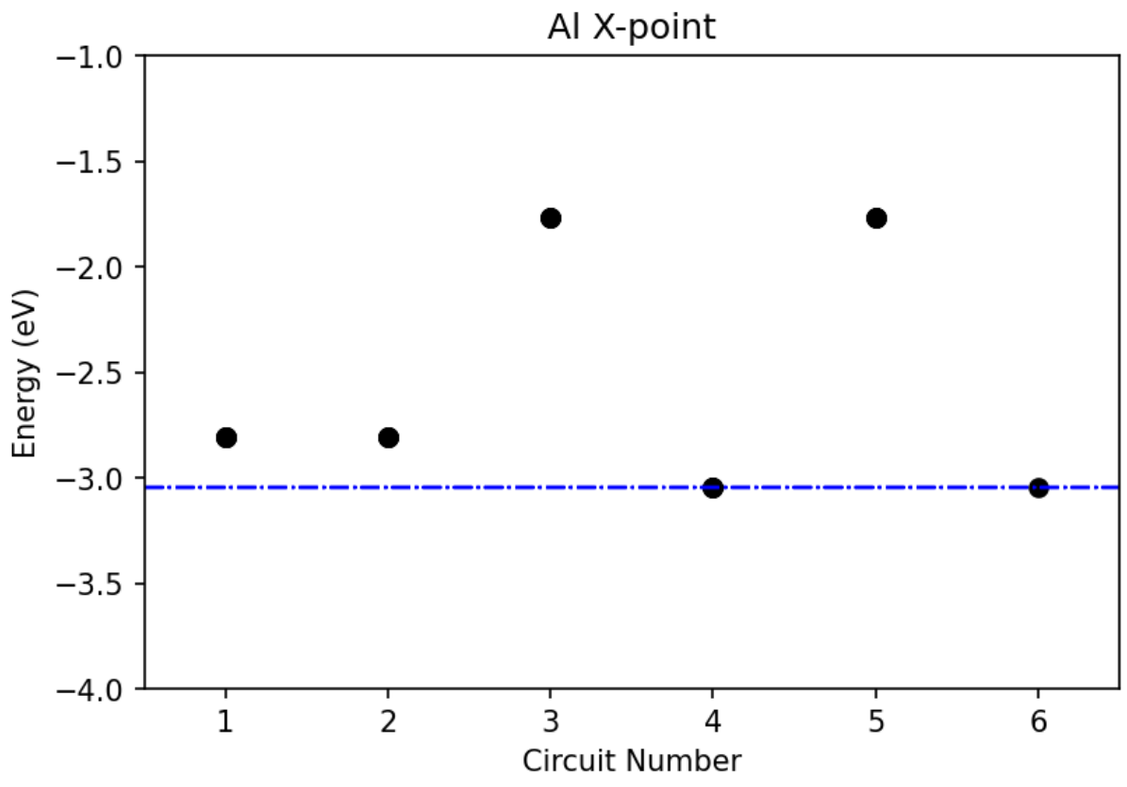


3 qubits case (fcc-AI)

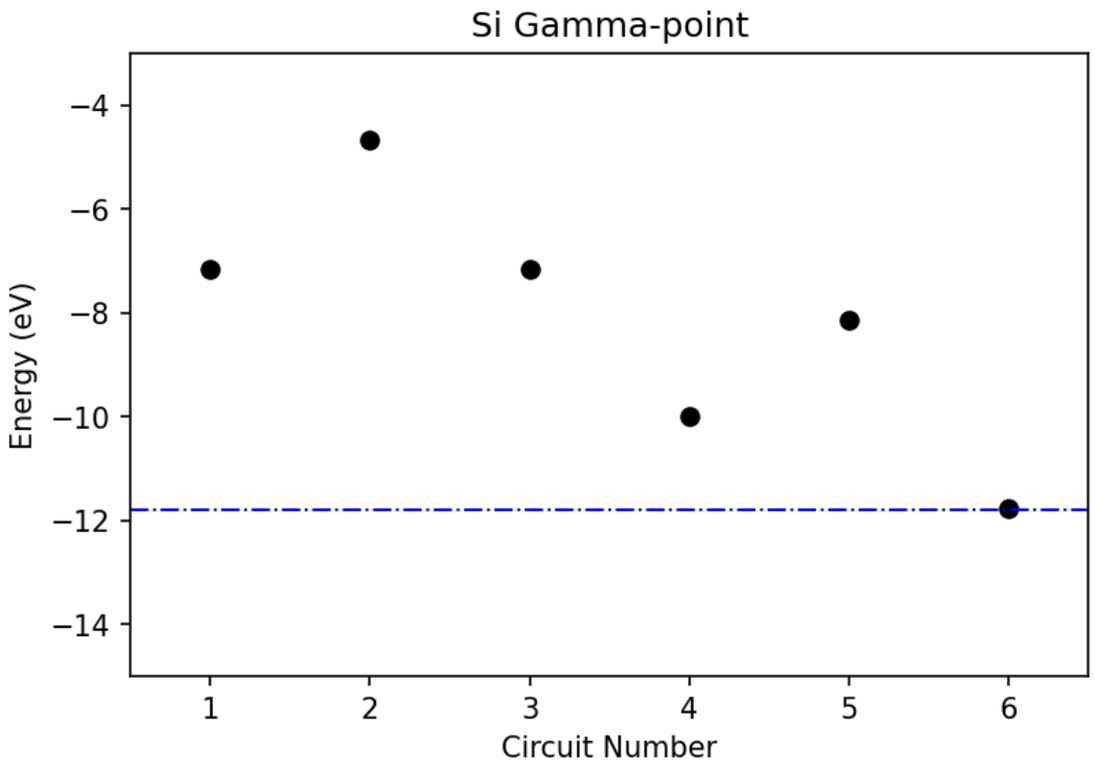
RESULTS

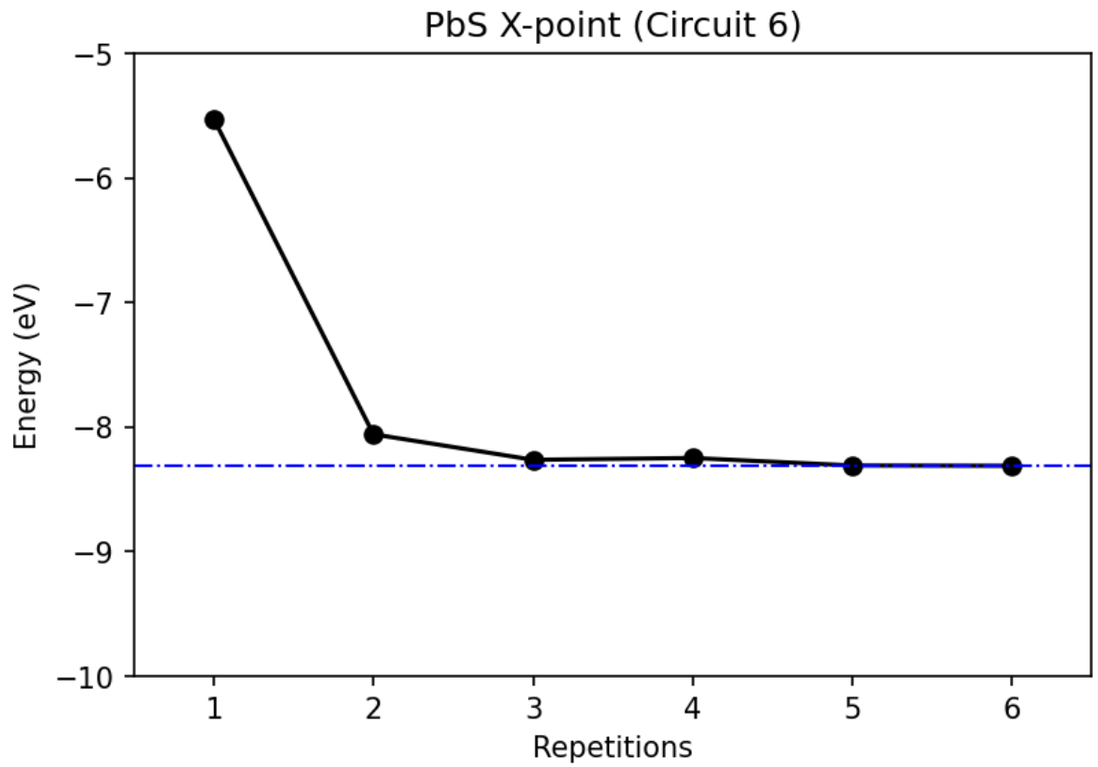
Circuit selection





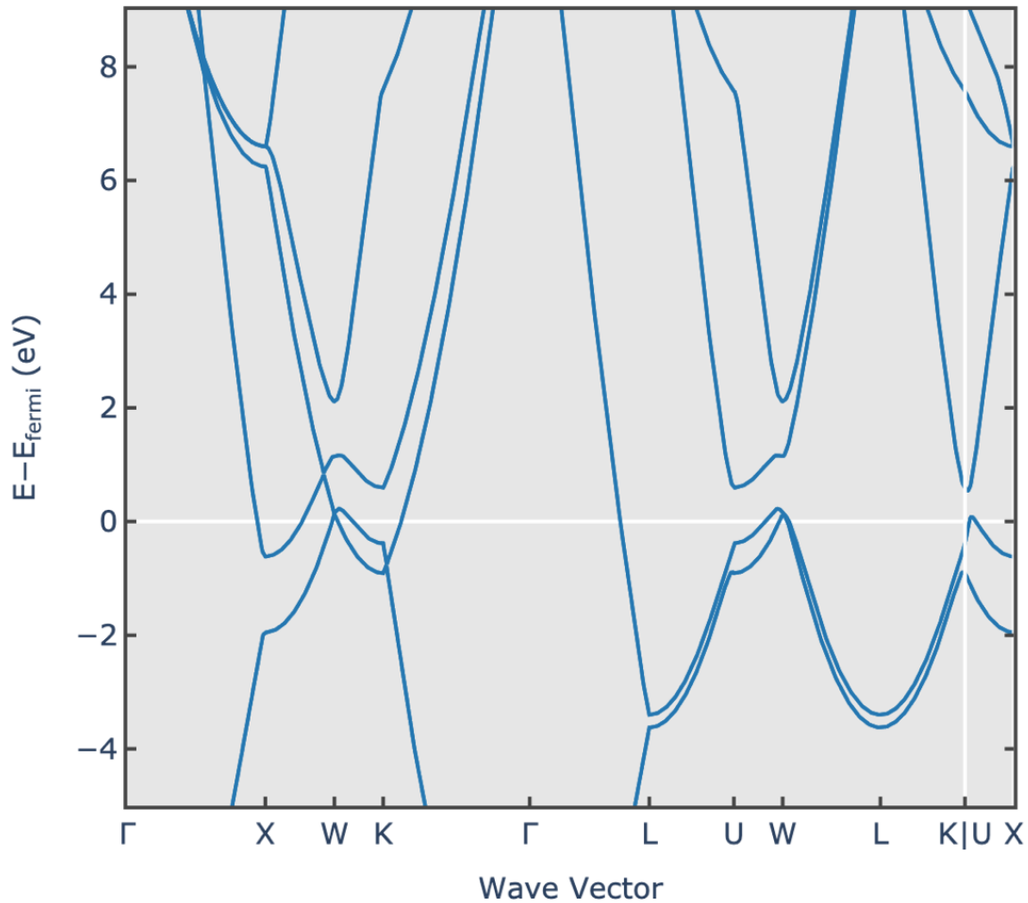
Circuit selection

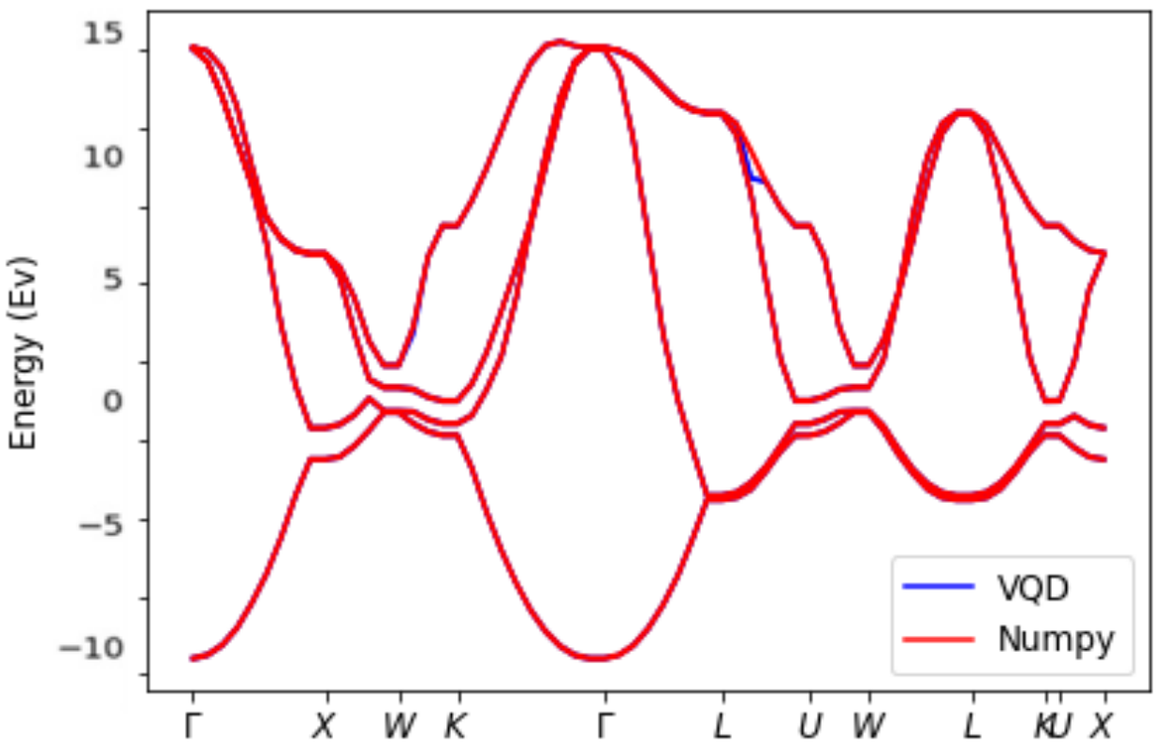




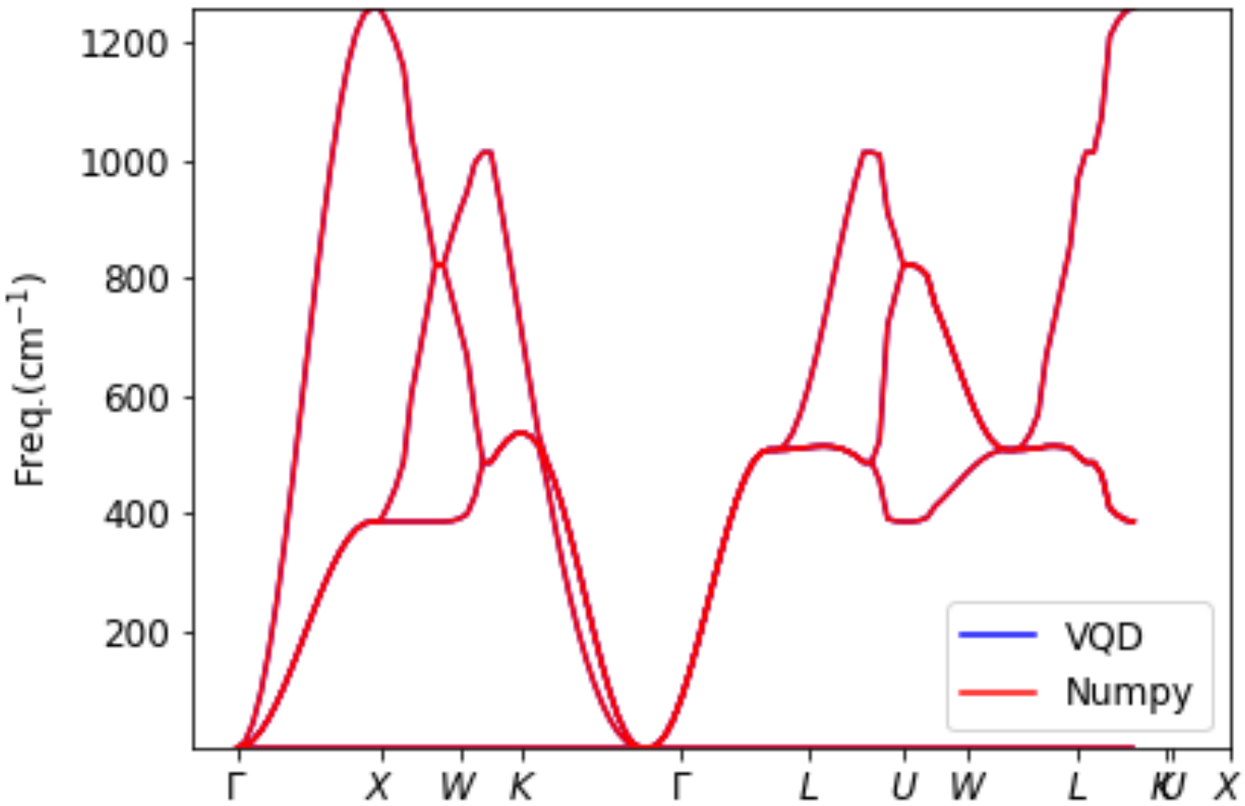
fcc-Al bandsctructure

- Circuit 6: EfficientSU2
- n. reps. = 2
- backend = statevector_simulator





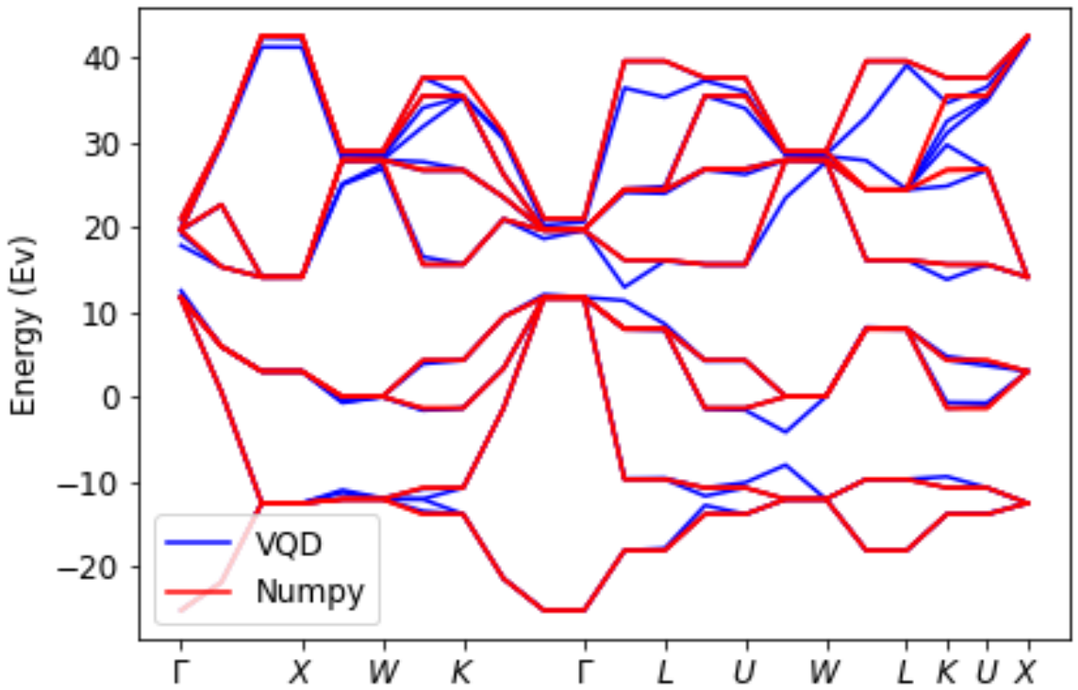
fcc-Al phonon DOS

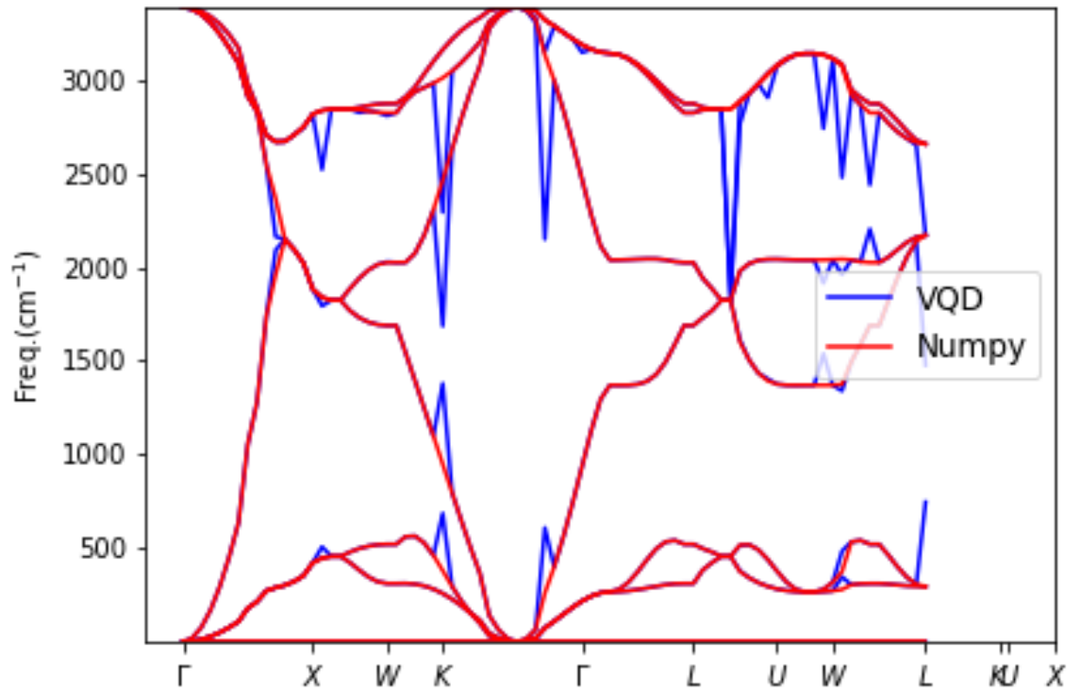


- Only “positive” frequencies: stable material
- Phonon filter helps to assess if a material is relaxed and stable.

cb-Si analysis

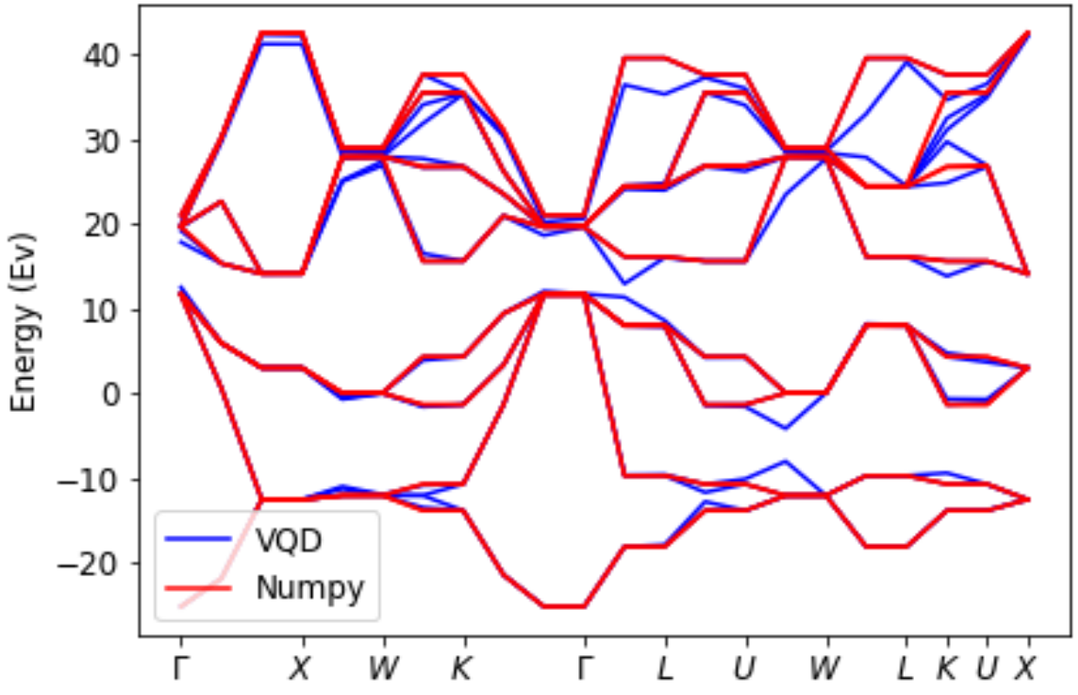
- Circuit 6: EfficientSU2
- n. reps. = 2
- backend = statevector_simulator



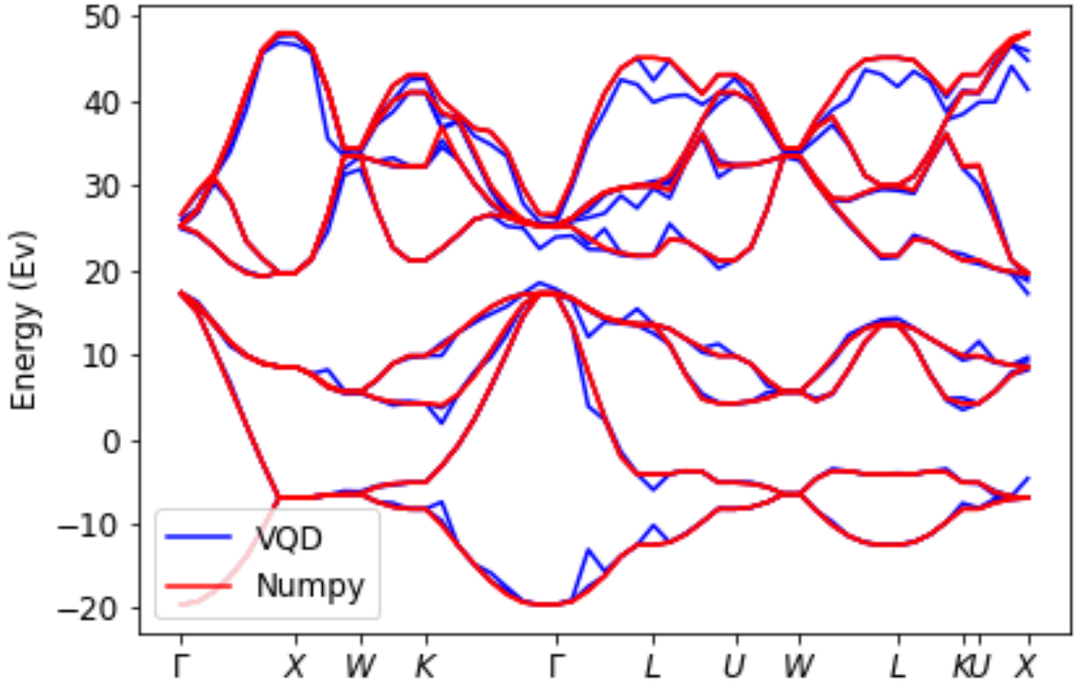


band structure vs reps: cb-Si

- Circuit 6: EfficientSU2
- n. reps. = 2
- backend = statevector_simulator



- Circuit 6: EfficientSU2
- n. reps. = 6
- backend = statevector_simulator



Conclusions

- Wannier + VQE good approach for NISQ QCs and eHs
- For small number of Wannier orbitals very accurate
- Faster than classical approach for small unit cells

Future Steps

- Structure optimisation via QC: Represent the molecular hamiltonian as a pauli basis (EUMEN, Cambridge, PBC-adapted VQE).
- QC-accurated MLIPs: From DFT accuracy to QC to feed potentials for MD simulations.

Thank you!