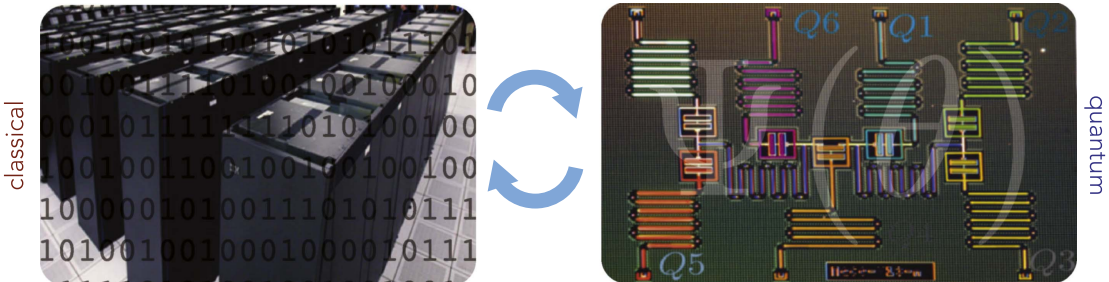

Figure 1. Schematic of a hybrid quantum–classical computing architecture.

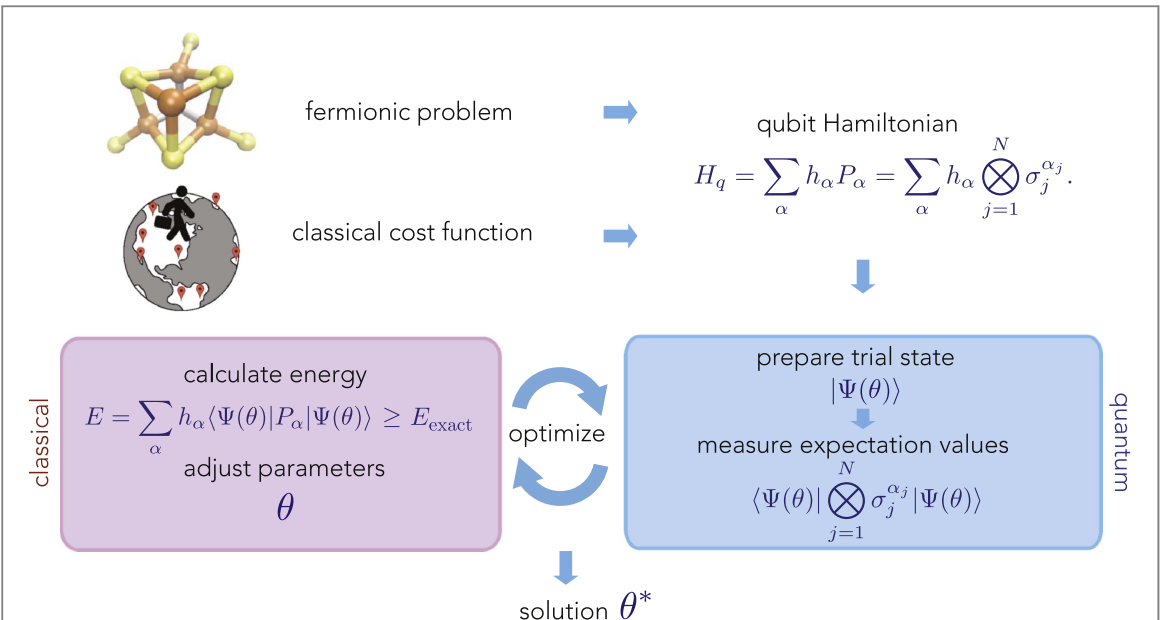

Figure 3. Variational quantum eigensolver method. The trial states, which depend on a few classical parameters $\boldsymbol{\theta}$, are created on the quantum device and used for measuring the expectation values needed. These are combined on a classical computer to calculate the energy $E_q(\boldsymbol{\theta})$, i.e. the cost function, and find new parameters $\boldsymbol{\theta}$ to minimize it. The new $\boldsymbol{\theta}$ parameters are then fed back into the algorithm. The parameters $\boldsymbol{\theta}^*$ of the solution are obtained when the minimal energy is reached.

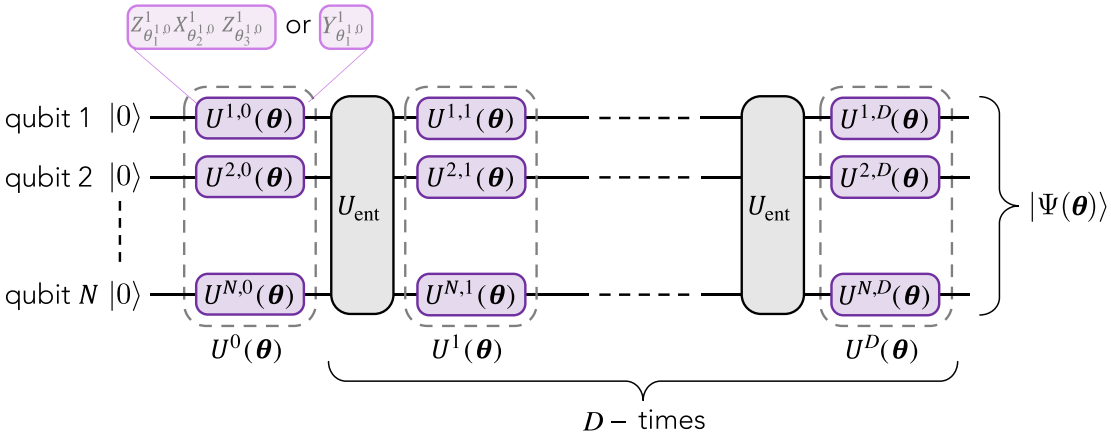

Figure 4. Heuristic preparation of trial states for the variational quantum eigensolver based on single-qubit gates $U(\boldsymbol{\theta})$ interleaved by entangling operations U_{ent} as described in the text.

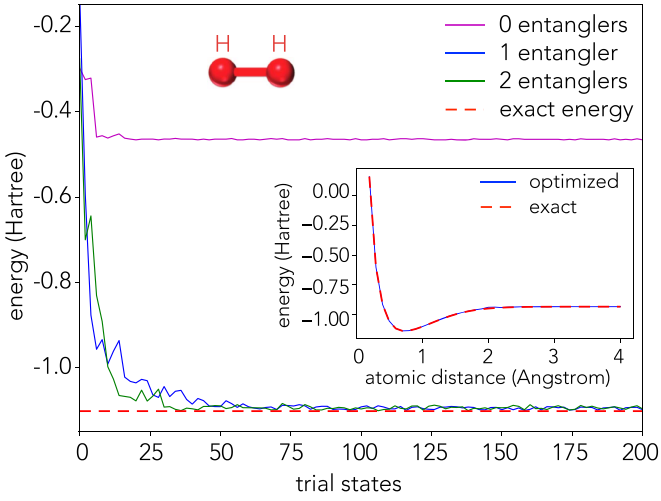

Figure 5. Quantum simulation of the hydrogen molecule on an ideal quantum simulator. At the equilibrium geometry and no entangler block in the circuit, the energy converges to a state with an energy that is about 50% too high. With two or more entanglers, the exact energy is obtained. The inset shows the entire dissociation profile for a hydrogen molecule calculated with four entangling steps.

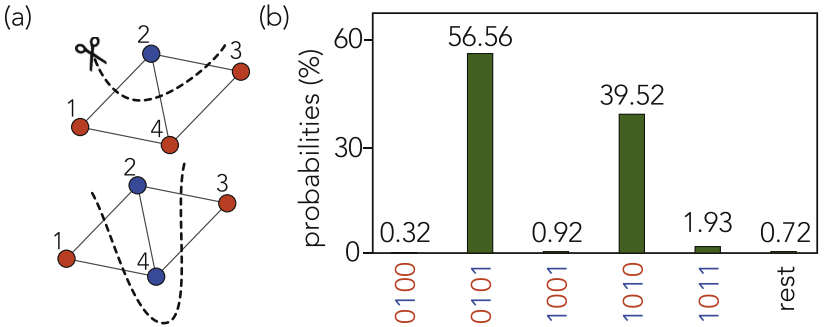

Figure 6. (a) Two different cuts for a MaxCut instance with four vertices. The lower cut has a larger cumulated weight and represents the partitioning that solves the problem. (b) Solution of the problem using the VQE with heuristic trial-states and a depth $D = 3$ circuit.

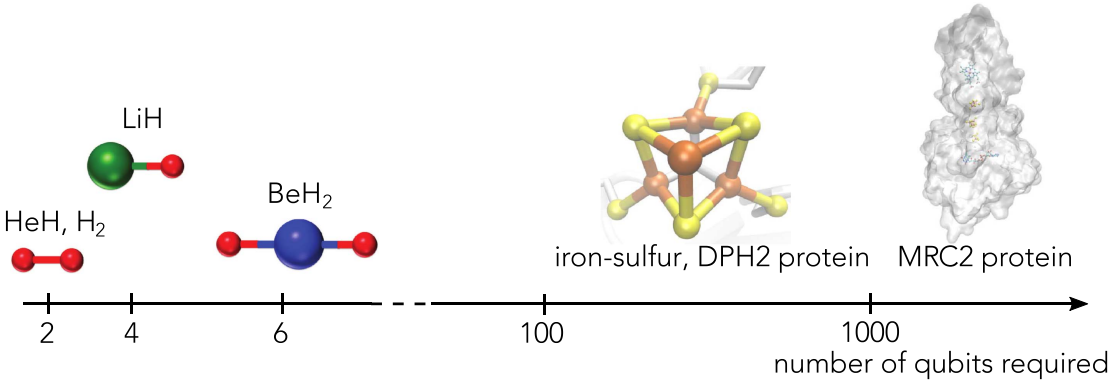

Figure 7. Qubit resources needed for quantum chemistry. Qubit numbers up to ten are based on existing experiments, whereas the resources for larger molecules are estimates. From left to right: hydrogen molecule, lithium hydride, beryllium hydride, iron sulphor (Fe–S) cluster in DPH2 complex of Pyrococcus Horikoshii (PDB entry code 3LZD), and Fe–S clusters sequence in cytochrome B560 subunit of mitochondria (PDB entry code 3SFD).