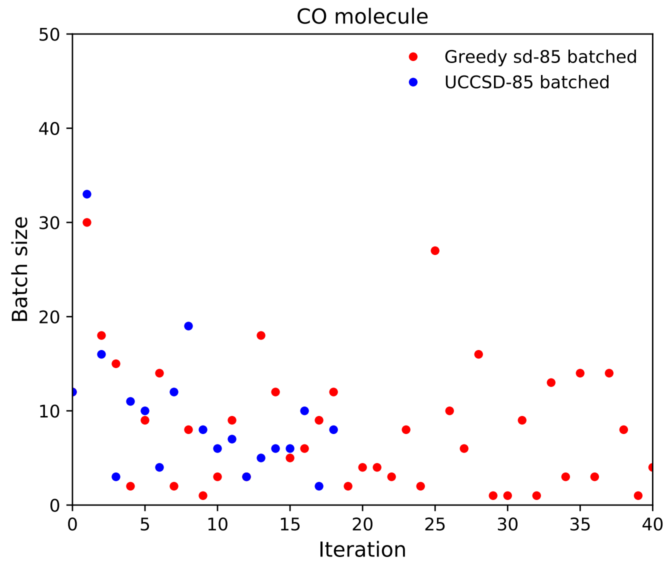
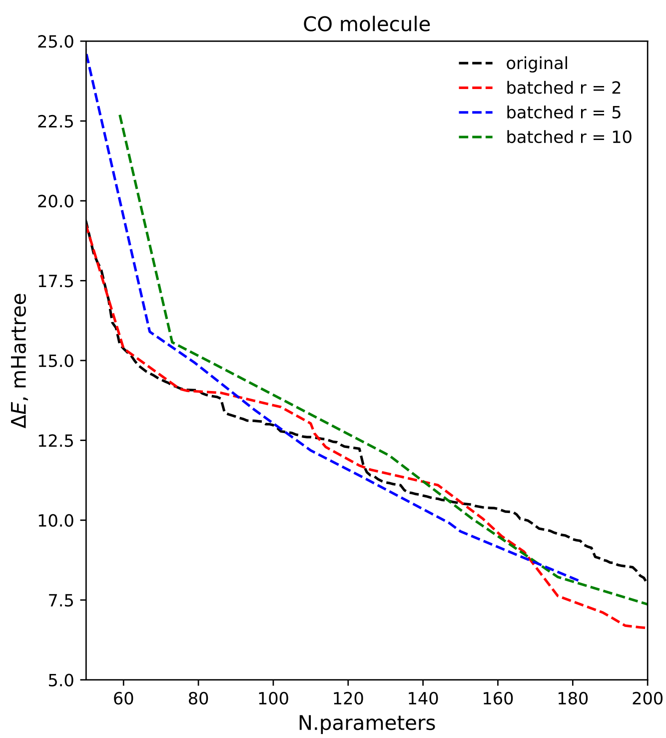
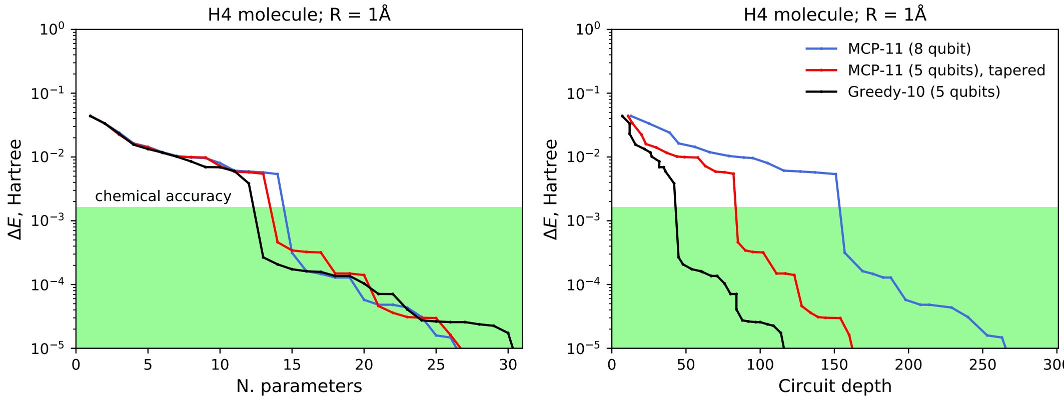
**SUPPLEMENTARY INFORMATION**



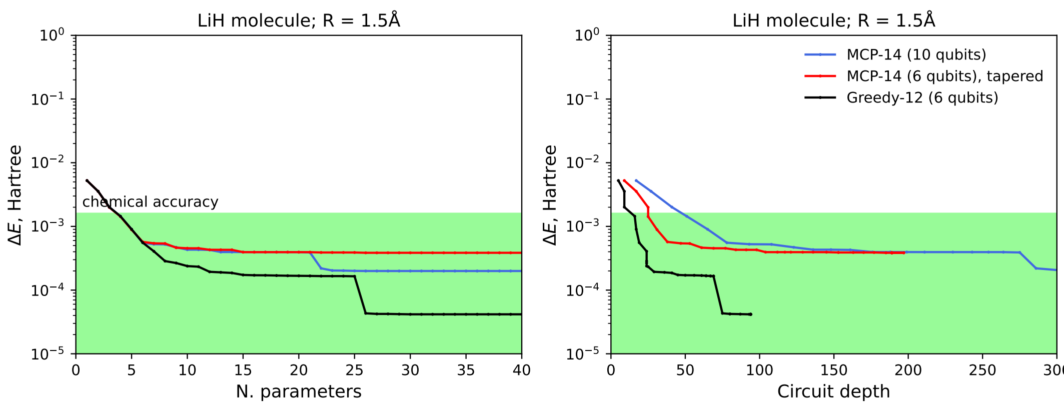

Supplementary Figure 1: **Batch size at different iterations of batched ADAPT-VQE for CO molecule computed with fermionic and qubit pool.** Fermionic ADAPT-VQE results (blue) are marked as “UCCSD-N ”, where N indicates the size of the fermionic pool with single and double excitations. Qubit ADAPT-VQE results (red) are referred to as Greedy sd-N (qubit polynomial complete pool with Pauli strings originated from each single and double fermionic excitation), where N is the qubit pool size.




Supplementary Figure 2: **Energy convergence for CO molecule for batched and original qubit ADAPT-VQE**. Batched implementation was tested with gradient ratio $r = 2, 5, 10$. We selected $r = 2$ for impelementation of batched ADAPT-VQE for all the considered molecules.




Supplementary Figure 3: **Qubit ADAPT-VQE convergence of energy with respect to the number of parameters and the circuit depth for $H_4$ molecule**. The results are provided at molecular radius $R$ equal 1.0 angstrom (Å). $\Delta E$ is the energy difference with the exact ground state energy in Hartree. MCP-11 is the minimal complete pool acting in the original qubit space of 8 qubits suggested in Ref. [1]. 'MCP-11, tapered' is built from MCP-11 by applying tapering procedure. Greedy-10 pool is a qubit linear complete pool constructed using the computational scheme proposed in this work and acts in a 5-qubit space.




Supplementary Figure 4: **Qubit ADAPT-VQE convergence of energy with respect to the number of parameters and the circuit depth for LiH molecule**. The results are provided at molecular radius $R$ equal 1.5 angstrom (Å). $\Delta E$ is the energy difference with the exact ground state energy in Hartree. MCP-14 is the minimal complete pool acting in the original qubit space of 10 qubits suggested in previous work [1]. 'MCP-14, tapered' is built from MCP-14 by applying tapering procedure. Greedy-12 pool is a qubit linear complete pool constructed using the computational scheme proposed in this work and acts in a 6-qubit space.

[1] Shkolnikov, V. O., Mayhall, N. J., Economou, S. E. & Barnes, E. Avoiding symmetry roadblocks and minimizing the measurement overhead of adaptive variational quantum eigensolvers (2021). 2109.05340.