Simulating battery properties using IBM quantum processors

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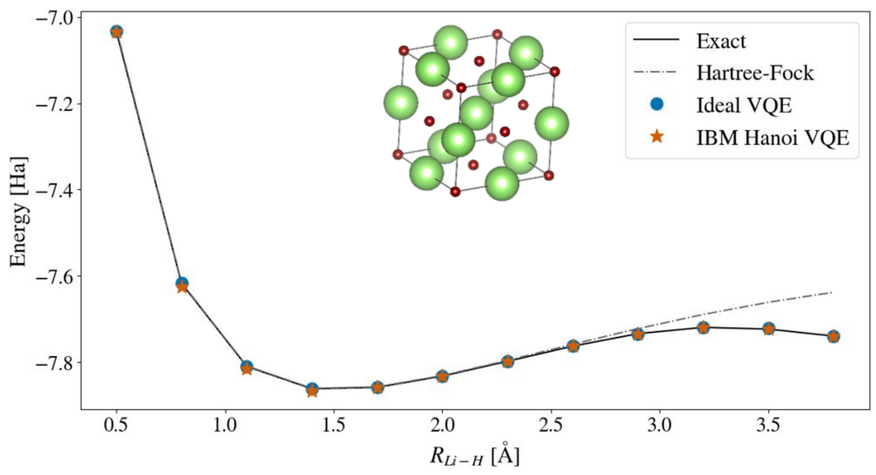
Abstract

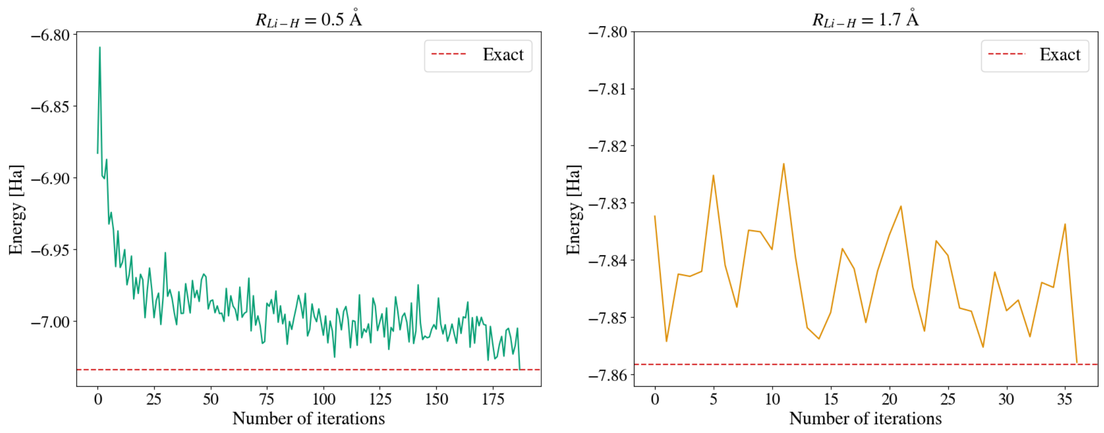
- Developing and implementing improved batteries is a case of particular interest at the present time.
- Quantum computing emerges to potentially outperform classical results.
- Inspired by [1], we investigate **key properties** of **battery-related compounds** for their design and subsequent manufacture.
- We study their energy spectrum using **VQE** on simulators and IBM quantum processors.
- We exploit **point-group symmetries** [2] and **active spaces** to reduce the amount of quantum resources required.

Results

LiH

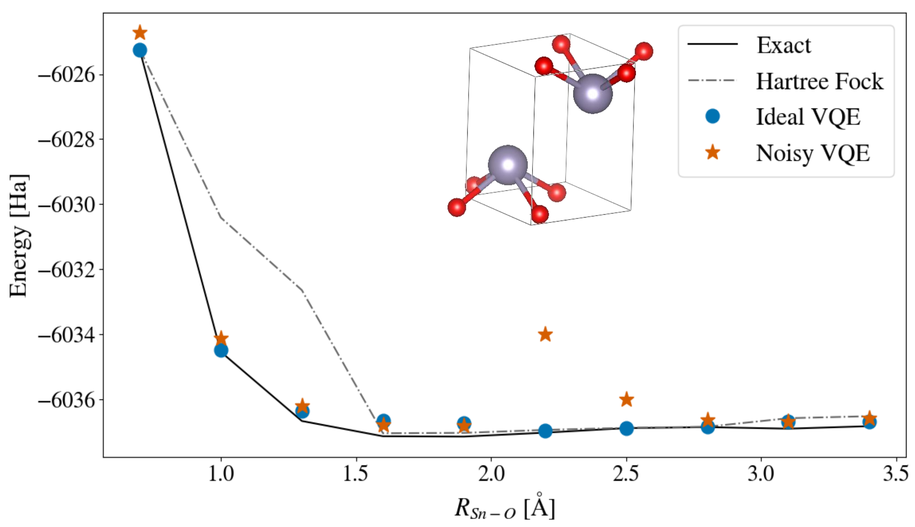
Parameters	
MO	3
AE	2
Qubits	3
Layers	1





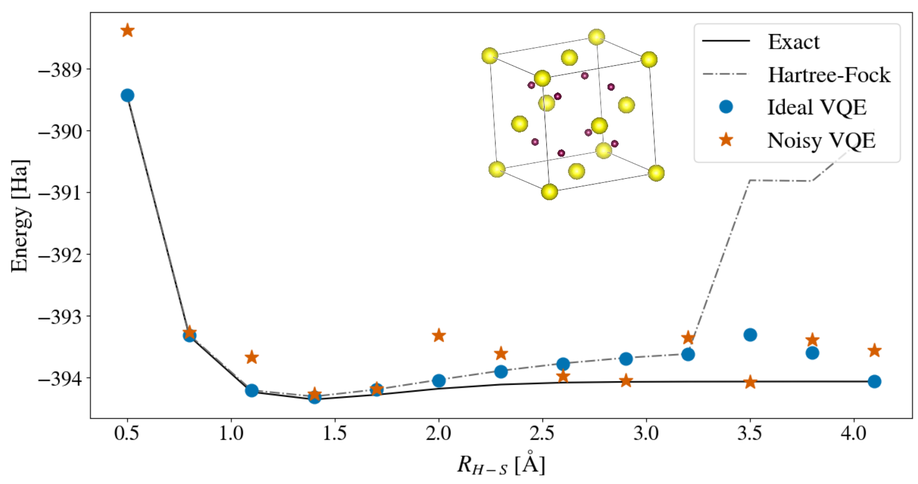
SnO

Parameters	
MO	5
AE	6
Qubits	6
Layers	1



H_2S

Parameters	
MO	6
AE	8
Qubits	8
Layers	1



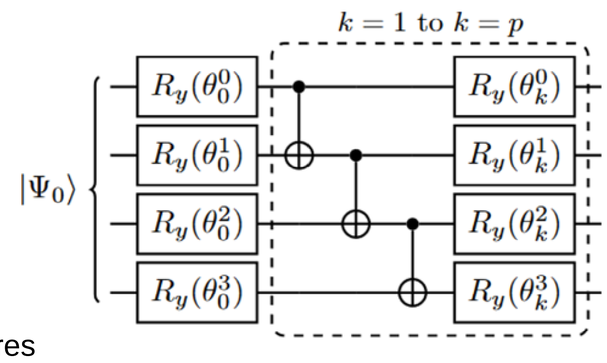
Methodology

Quantum problem

- Molecule definition
  - Initial geometry, active space with PySCF library and STO-3G basis
- Reduced hamiltonian
  - Exploiting point-group and $\mathbb{Z}_2$symmetries (Quantum Symmetry [2])

Tools

- Ansatz
  - $|\Psi_0\rangle \rightarrow$ Hartree Fock



- Classical optimizers
  - Sequential Least SQuares Programming optimizer (SLSQP)
  - Simultaneous Perturbation Stochastic Approximation optimizer (SPSA)
- Variational Quantum Eigensolver (VQE) algorithm

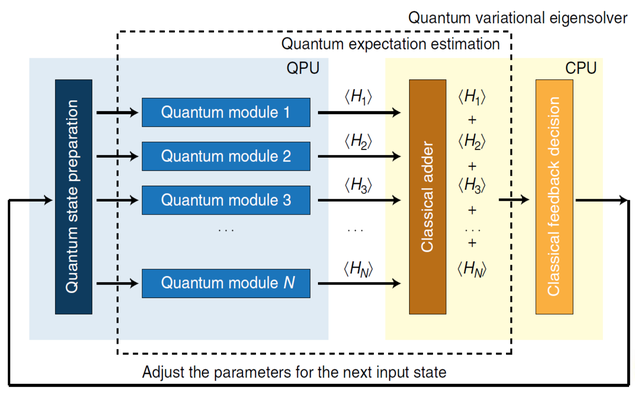
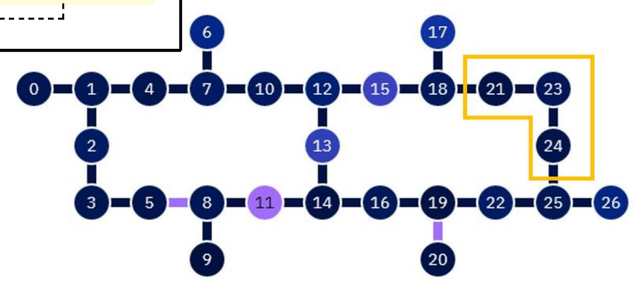


Image extracted from [4]



IBM processors

- QASM simulator with noise model
- IBM Hanoi

Outlook

- Computation of the **energy spectrum** for different molecules using IBM processors and classical simulators.
- Good results with a significantly **low number** of optimizer **iterations** after the first computation, and using low quantum resources, particularly beneficial in the NISQ era.
- Next step: computing **dipole moments** based on the obtained ground states and studying more complex molecules such LiHS, LiCoO2 and Li2S.

References

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Acknowledgements

We thank Dario Picozzi for the helpful discussions. We acknowledge the use of IBM Quantum services for this work. The views expressed are those of the authors and do not reflect the official policy or position of IBM or the IBM Quantum team. Authors thank the support of the Basque Government through HAZITEK program (Q4Real project, ZE-2022/00033), the Government of Biscay (Bizkaiko Foru Aldundia–Diputación Foral de Bizkaia) through Lantik and its Industry Focused Quantum Ecosystem initiative which provided access to the IBM quantum computers.