Simulating battery properties using IBM quantum processors

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The need to develop and implement rechargeable batteries with higher capacity, faster charging, and, ideally, lower production costs is a case of particular interest at the present time. While well-established classical computing techniques for simulating batteries already exist, they often struggle to obtain accurate and reliable results. However, quantum computing emerges as a potential framework to outperform them. Inspired by a previous work through the collaboration between Mercedes-Benz and IBM [1], we investigate key properties of battery-related compounds for their design and subsequent manufacture. We study the energy spectrum and the multipolar moments for different molecules using the variational quantum eigensolver (VQE) on simulators and IBM quantum processors. We exploit point-group symmetries [2] and meaningful active spaces to significantly reduce the amount of quantum resources required, which is highly valuable during the NISQ era.

References

[1]   J. E. Rice et al., The Journal of Chemical Physics 154, 134115 (2021)
[2]   D. Picozzi, and J. Tennyson, Quantum Science and Technology 8, 035026 (2023)
[3]   M. Ristol et al. *Simulating battery properties using IBM quantum processors*. (in preparation)
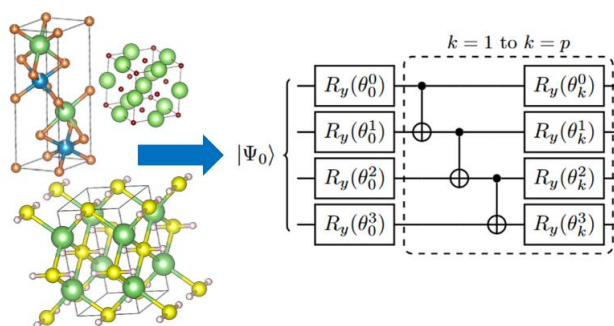
Figures

Figure 1: Diagram illustrating the representation of molecules in their ground state using a parametric quantum circuit, or ansatz, with k layers and 4 qubits. In our study, the initial state $|\Psi_0\rangle$ used is the Hartree-Fock state.
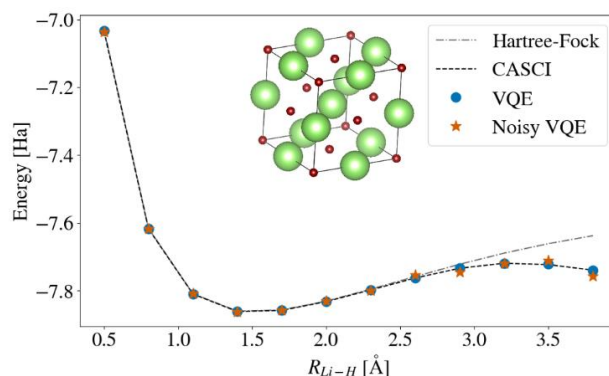

Figure 2: LiH ground state computation for different bond lengths and its unit cell. Results computed simulating the ideal VQE (blue dots) and the noisy VQE (orange stars) are compared against the Hartree-Fock approximation (black line) and the CASCI classical computation (grey line).