Quantum Computation for Electrochemical Energy Storage: Atomistic and Continuum Models in Battery Research

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The advent of quantum computing in the Noisy Intermediate-Scale Quantum (NISQ) era has brought us the early prototypes of fully-fledged quantum platforms that are capable of executing quantum algorithms for the simulation of chemical systems [1]. Although these NISQ devices are still in their early stages and fault-tolerant architectures are yet to be deployed, hybrid algorithms that delegate some part of the computation to a classical device have been successfully employed in the calculation of the electronic structure of simple molecules.

In this work, we discuss the current challenges of quantum simulations for battery research. On the one hand, we investigate procedures for solving partial differential equations on a quantum computer on our route towards battery cell simulations on quantum computers [2]. On the other hand, we discuss our advances in algorithms to calculate the electronic structure of molecules relevant to energy storage in electrochemistry. We discuss the results of our simulations, executed on Germany's first IBM Quantum System One backend in Ehningen, Baden-Württemberg.

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Literature

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