# How can quantum computation help improve electrochemical energy storage?

Birger Horstmann

*German Aerospace Center, Wilhelm-Runge-Straße 10, 89081 Ulm*
*Helmholtz Institute Ulm, Helmholtzstraße 11, 89081 Ulm*
*Ulm University, Albert-Einstein-Allee, 89081 Ulm*

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 prospects and challenges of quantum simulations for research on electrochemical energy storage. We introduce the concepts of electrochemical energy storage and the multi-scale approach for theory-based optimization in this field. Simulations on classical computers have developed into an indispensable set of tools for material development. However, several computational challenges remain and (universal) quantum computers could most likely solve many of them.

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.

**Literature**

[1] Cao, Y., Romero, J., Olson, J. P., Degroote, M., Johnson, P. D., Kieferová, M., Kivlichan, I. D., Menke, T., Peropadre, B., Sawaya, N. P. D., Sim, S., Veis, L., & Aspuru-Guzik, A. (2019). Quantum Chemistry in the Age of Quantum Computing. *Chemical Reviews*, *119*(19), 10856–10915.

[2] Pool, A. J., Somoza, A. D., Lubasch, M., & Horstmann, B. (2022). Solving Partial Differential Equations using a Quantum Computer. In *2022 IEEE International Conference on Quantum Computing and Engineering (QCE)*, 864-866.

**Prof Dr. Birger Horstmann** is working on battery modeling with the DLR Institute of Engineering Thermodynamics since finishing his PhD in quantum simulation at the Max-Planck-Institute for Quantum Optics in 2011. He is leader of the group Theory of Electrochemical Materials within the Department of Computational Electrochemistry and senior lecturer at the University of Ulm. His work comprises the theory of interfacial processes in lithium batteries as well as the theory of electrolyte transport through post-lithium battery cells with a focus on zinc batteries. Since a few years, he helps to bring both his experiences, quantum simulations and theoretical electrochemistry, together trying to support the experimental progress in energy storage research at DLR, HIU, and Ulm University.