Physikalisches Kolloquium — Physics Colloquium

Einladung — **Invitation**

Monday, 20 November 2023

Lecture Hall N24/H13, at 16:15
Coffee and cookies will be served in front of the lecture hall from 16:00

Towards Multi-Scale Battery Simulations with Quantum Computers

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https://hiu-batteries.de/en/researches/research-groups/research-group-prof-birger-horstmann/

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.

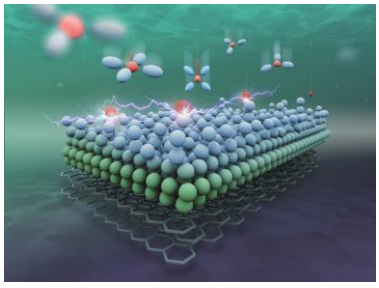
Electrochemical energy storage, for example in batteries, offers high energy efficiency and suitable energy density for relevant applications. In this work, we discuss the prospects and challenges of quantum simulations for research on electrochemistry. We introduce the concepts of batteries and the 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: How can quantum computers help?

On the one hand, we investigate procedures for solving partial differential equations on a quantum computer on our route towards battery cell simulations [2]. On the other hand, we discuss our advances in algorithms to address the quantum chemistry of molecules. Our simulations are executed on current NISQ devices.

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.



Host: Prof. Dr. Jens Michaelis, Institute of Biophysics

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