



GESELLSCHAFT
DEUTSCHER CHEMIKER

KOLLOQUIUM

Sommersemester 2025

Titel

**“After 100 years of quantum mechanics, do
theoreticians still need experiments?”**

Vortragender

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Abstract

In 2025 we are celebrating the International Year of Quantum Science and Technology, as 100 years ago a series of papers started shaping a completely new field in physics and ultimately in chemistry. Formally, all of the equations that we need to describe molecules and chemical reactions were provided around that time. Since then we have been mostly building approximations to make the problem computationally amenable. We have also profited enormously from advancements in hardware, transforming theoretical chemistry from a niche subject to one of the most impactful fields of research. But even now we must ask the question, how reliable are our quantum chemical calculations? Where did we land after these 100 years?

In this talk I would like to revisit why theoreticians in general do not work with error bars, how we could possibly change our ways and will also detail the efforts made at Göttingen to revitalise experiment-based benchmarking in theoretical chemistry. This involves not only making experimental data more accessible to theoreticians, but also working together with different labs to design critical experiments, cross-validation of spectroscopic measurements and how the data gathered can be used to design new computational protocols. I will also share some insights into the blind challenges we have organised over the last few years and the impact of these community efforts.

Ort

Chemie, HS3 – Campus Nord, Otto-Hahn-Straße 6
Anfahrt: <http://www.ewit.ccb.tu-dortmund.de/gdch/anfahrt.html>

Zeit

Dienstag, 13.05.2025, 14:00 Uhr Beginn Seminar, 14.30 Uhr Vortrag

gez. Professor Dr. Andreas Steffen

Gesellschaft Deutscher Chemiker Ortsverband Dortmund