



GESELLSCHAFT DEUTSCHER CHEMIKER
ORTSVERBAND HANNOVER

Einladung zum GDCh-Colloquium des Ortsverbandes Hannover

Das Colloquium findet um 17c.t. im [Dr.-Oetker Hörsaal \(Raum 007, Geb. 2504\)](#) der Leibniz Universität Hannover, [Physikalische Chemie, Callinstraße 3A](#), 30167 Hannover statt.

25.06.2026 Dr. Felipe Menezes, Helmholtz Zentrum München

Beyond Crystal Clarity: Chemical Perspective on Biomolecular Structure, Validation, Interpretation

Being a computational chemist with a background in industry, synthesis, and spectroscopy, we are working at the interface of chemistry, computation, and biomolecular science. This research focuses on the development and implementation of quantum-chemical and artificial intelligence methods, including the design of our own quantum chemistry package, [ULYSSES](#). Developments include AI and ML approaches for drug discovery that integrate quantum-mechanical and molecular dynamics data. The broader goal is to understand the molecular building blocks of life, their behaviour, and their modulation by chemical probes. To this end, we combine atomistic modelling with experimental observables to reproduce and interpret thermodynamic, spectroscopic, and kinetic data.

Coming back to the title of this talk, the conclusion is: Structures without chemistry are still incomplete!

Prof. Dr. Jens-Uwe Grabow
Vorsitz OV Hannover

Vor dem Colloquium findet ab ca. 16 c.t. eine ‚Kaffeerunde‘ mit dem Vortragenden in der [Bibliothek](#) des [Instituts für Physikalische Chemie, Callinstraße 3A](#) statt.