

GDCh-Vortragsreihe Wintersemester 2026/27

Antrittsvorlesung - Inauguration Lecture

Prof. Robert Mayer

Physikalische Organische Chemie, TUM

mit dem Thema

Physical Organic Chemistry in the Age of Big Data: Predicting Reactivity and Catalysis in Water

Dienstag, 03. November 2026, 17 Uhr c.t.
TUM-Department Chemie, Lichtenbergstr. 4, Garching,
Science Cinema (Hörsaal CH26411)

gez. Prof. Dr. Roland A. Fischer
2. Vorsitzender MChG

Physical Organic Chemistry in the Age of Big Data: Predicting Reactivity and Catalysis in Water

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Abstract:

Water is the solvent of life and an increasingly important medium for sustainable chemistry. However, predicting which molecules will react with one another in water, how fast, and by which mechanism remains challenging. This is because reactions in water proceed through multiple competing pathways of acid/base catalysis, making reactivity in water a multiparameter problem that manual experiments can hardly sample. In this lecture, I will describe how my group addresses this challenge by combining high-throughput experimentation and data science with the kinetic and mechanistic toolbox of physical organic chemistry. Using carbonyl additions and phosphoryl transfer reactions as examples, I will show how datasets of tens of thousands of rate constants allow us to predict reaction rates, disentangle competing mechanisms, and identify optimal catalysts. Finally, I will outline our future efforts to rationalize and predict catalysis in reaction networks, in water and beyond.