



EINLADUNG

zum Vortrag von

Dr. Mihai Viorel Popescu

Universität Wien, Organische Chemie

Triplet Energy Transfer Catalysis: Insights from Theory and Machine Learning

am Dienstag, 23. Juni 2026, um 17:30 Uhr

Ort: Lise-Meitner-Hörsaal, Fakultät für Physik, Universität Wien,
1090 Wien, Strudlhofgasse 4 / Boltzmannngasse 5, 1. Stock

*Barrierefreier Zugang: Boltzmannngasse 5, Lift, 1. Stock rechts über den
Gang zum Hintereingang des Hörsaals*

Abstract:

Triplet state reactivity has found extensive applications in chemical synthesis, unlocking novel modes of reactivity inaccessible to closed-shell molecules in their ground singlet state. While traditionally UV light has been the primary means of harnessing triplet-state chemistry, developments in modern visible light photocatalysts have reinvigorated interest in this field. Here, we demonstrate how theory can offer deeper understanding of the fundamental processes governing reactivity through mechanistic analysis. A dynamics-based theoretical framework is introduced that moves beyond the prevailing thermodynamic picture of triplet energy predictions, revealing the role of molecular motion in governing reactivity. We then show how machine learning strategies may leverage these ideas to enable rapid prediction and interpretable chemical insight, opening new avenues for the rational design of triplet-state synthetic systems amenable to visible light sensitisation.

CHEMISCH-PHYSIKALISCHE GESELLSCHAFT

c/o Universität Wien, Fakultät für Physik, 1090 Wien, Boltzmannngasse 5, Austria

Generalsekretär: Christl Langstadlinger

Tel.: +43-(0)1-4277/51108 - Mobil: 0664-60277 51108

E-Mail: christl.langstadlinger@univie.ac.at - <http://www.cpg.univie.ac.at>

ZVR-Zahl: 513907440

Konto: Bank Austria - IBAN: AT22 1100 0086 4440 8000 - BIC: BKAUATWW