chemisch physikalische gesellschaft

Gegründet im Jahre 1869 von H. Hlasiwetz, J. Loschmidt, J. Petzval und J. Stefan

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 / Boltzmanngasse 5, 1. Stock
Barrierefreier Zugang: Boltzmanngasse 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.