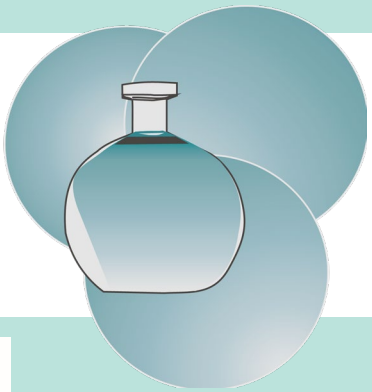
Fakultät für Naturwissenschaften

Institut für Chemie



lädt ein

gemeinsam mit der Gesellschaft Deutscher Chemiker zum

GDCh
GESELLSCHAFT DEUTSCHER CHEMIKER

Vortrag

von Herrn

Prof. Steven A. Lopez

Department of Chemistry & Chamical Biology
Norheastern University

"Machine-learning-accelerated photodynamics simulations in complex environments towards new photomedicines"

am: 16. Mai 2024

um: 16:00 Uhr

wo: im Raum 1/232

Die kleine Kaffeerunde vor dem Vortrag beginnt um 15:30 Uhr im Raum 1/232.
Das Mitbringen von eigenen Trinkgefäßen ist erwünscht.

Gäste sind herzlich willkommen!

TECHNISCHE UNIVERSITÄT
IN DER KULTURHAUPTSTADT EUROPAS
CHEMNITZ

Prof. Dr. Michael Sommer
Telefon: 0371 / 531 32507
E-Mail: michael.sommer@chemie.tu-chemnitz.de

Fakultät für Naturwissenschaften

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Department of Chemistry & Chamical Biology
Norheastern University

GDCh
Gesellschaft Deutscher Chemiker

Machine-learning-accelerated photodynamics simulations in complex environments towards new photomedicines

Photochemical reactions are increasingly important for constructing value-added, strained organic architectures. Direct excitation and photoredox reactions typically require mild conditions to access therapeutic gases (e.g., carbon monoxide) and new synthetic methodologies. *A priori* design of photochemical reactions is challenging because degenerate excited states often result in competing reaction mechanisms to undesired products. Further, a lack of experimental techniques that provide atomistic structural information on ultrafast timescales (10^{-15} – 10^{-12} s) has limited general rules about these reactions. Computations, however, provide a path forward. I will discuss how my group has leveraged multiconfigurational complete active space self consistent field (CASSCF) calculations, non-adiabatic molecular dynamics, and machine learning (ML) techniques to understand reaction mechanisms and enumerate new reaction pathways. I will introduce our new open-access machine learning tool, Python Rapid Artificial Intelligence *Ab Initio* Molecular Dynamics (PyRAI^{2}MD), which enables 100,000-fold longer simulations than current NAMD simulations with multiconfigurational quantum chemical methods. I will describe how PyRAI^{2}MD has enabled the first ML-NAMD simulations with QM/QM (CAS/HF) training data. The presentation will explain the origins of the reactivities and selectivities of photochemical pericyclic reactions and CO-evolving reactions in aqueous environments.

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Prof. Dr. Michael Sommer
Telefon: 0371 / 531 32507
E-Mail: michael.sommer@chemie.tu-chemnitz.de