



GESELLSCHAFT DEUTSCHER CHEMIKER
ORTSVERBAND HANNOVER

Einladung zum GDCh-Colloquium des Ortsverbandes Hannover

Das Colloquium findet um 17h c.t. im Dr.-Oetker-HS (Raum 007, Gebäude 2504) der Leibniz Universität Hannover, Institut für Physikalische Chemie und Elektrochemie, Callinstraße 3a, D-30167 Hannover statt.

17.04.2025 Prof. Dr. Konstantinos D. Vogiatzis
Department of Chemistry, University of Tennessee

Topology as a Tool for Molecular Discovery: CO₂-philicity, Ligand Design, and Beyond

The field of chemical sciences has undergone a significant transformation in recent years with the emergence and proliferation of machine learning (ML). Critical elements of ML and modern chemoinformatics include the development of effective molecular representations and chemical descriptors, the systematic collection of precise and standardized data, and the optimization of models for enhanced performance. Our group has developed novel molecular representations based on persistent homology, an applied branch of topology, that can encode the geometric structure and topological information of molecules for chemical applications. In my talk, I will discuss some recent applications of topological features for machine learning related to CO₂ capture, catalyst design, and polymer informatics.

Prof. Dr. Jens-Uwe Grabow
Vorsitz OV Hannover

Vor dem Colloquium findet ab ca. 16h c.t. eine ‚Kaffeerunde‘ mit dem Vortragenden in der Bibliothek des PCI statt.