



# Kolloquium des Wilhelm-Ostwald-Instituts

**Prof. Dr. Sergey I. Bokarev**

*Technische Universität München*

**Montag, 23.01.2023, 16:15 Uhr**

*Wislicenus-Hörsaal, Johannisallee 29, 04103 Leipzig*

## **Spectroscopy and Dynamics of Transition Metal Complexes**

### **Abstract**

The past decade heralds the gradual change of the ultrafast paradigm in physics and chemistry from the femtosecond to subfemtosecond and even a few tens of attoseconds domain. The fascinating growth in the number of ultrafast phenomena studies is due to establishment of new sources such as X-ray free-electron lasers and high harmonic generation setups that give access to dynamics at electronic time scales. To keep pace with experiments, accurate and efficient theoretical methods need to be developed. In my talk, I will discuss several computational protocols: First, I will describe efficient approaches to compute valence and core photoionization and Auger decay in molecules employing different flavors of the central-potential method and beyond it. Second, I will present our recent developments of the density-matrix-based time-dependent restricted active space configuration interaction method ( $\rho$ -TD-RASCI) to compute the ultrafast electron dynamics. The applications of these theoretical protocols will be exemplified by the simulations of the linear X-ray spectra, high harmonic generation, ultrafast charge migration, and spin-flip dynamics in molecules and transition metal complexes.

*Ab 15:30 Uhr findet ein gemeinsames Kaffeetrinken in Raum 410 (TA) statt.*