Session of "Fokus Materialchemie" – Wednesday, **17.12.2025** 14:00
@ Seminarraum BA 05 (TU-Wien, Getreidemarkt 9, BA, OG. 05, BA05G02)
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Optoelectronics of Photoactive Molecules: Match of Experiment and Modeling

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In the talk, the physical principles behind optical spectroscopy are briefly explained, and the connection between theoretical physics and molecular spectroscopy is elucidated. Further, the design principles for UV/VIS absorpbent molecules are laid down based on the theoretical principles. The application to flavin molecules used for publishing is discussed.

Optical spectroscopy is a central experimental tool in chemistry, yet the physical principles that determine spectroscopic observables are often treated implicitly. In this talk, I will give a concise and intuitive overview of the fundamentals of optical spectroscopy, focusing on the essential aspects of light–matter interaction and their connection to molecular electronic structure. The link between theoretical physics and molecular spectroscopy is highlighted by discussing how electronic transitions, transition dipole moments, and symmetry considerations give rise to characteristic UV/Vis absorption spectra.

Based on these concepts, practical design principles for UV/Vis-absorbing molecules are formulated, emphasizing how conjugation, substituent effects, and molecular environment influence absorption wavelengths and intensities. These ideas are illustrated through their application to flavin molecules, which serve as versatile chromophores in publishing-related technologies. The talk aims to provide experimental chemists with physical intuition that supports both spectral interpretation and the rational design of functional light-absorbing molecules.