

## A 4: Electron Dynamics in Chiral Systems SYCS 1 (with MO)

Time: Monday 10:30–12:30

Location: Audimax

### Invited Talk

A 4.1 Mon 10:30 Audimax

**Electron dynamics in chiral systems: From structure determination to violation of fundamental symmetries** — ●ROBERT BERGER — Technische Universität Darmstadt, Darmstadt, Germany

Chiral systems serve as versatile laboratories for detailed studies on the intriguing interplay between handed objects, be they circularly polarised light, polarised electrons, neutrinos or chiral nuclear arrangements. The study of electron dynamics in such systems allows for instance to determine the specific handedness of a chiral system or even to unravel underlying symmetry principles of the fundamental laws of nature.

In this contribution, the diverse role of electron dynamics in chiral systems will be outlined and recent applications in determination of molecular structure, namely absolute configuration of handed molecules, will be presented. Additionally, fundamental symmetries and detection of their violations in chiral systems will be discussed, ranging from nuclear spin-dependent parity violation in diatomic and polyatomic molecules to parity and time-reversal violating features like the electron electric dipole moment.

### Invited Talk

A 4.2 Mon 11:00 Audimax

**Electron Scattering in Chiral Photoionization: probing fundamental electron-molecule interactions to chiral molecular recognition** — ●IVAN POWIS — University of Nottingham, Nottingham, UK

The photoionization of chiral species by circularly polarized light produces an asymmetric angular distribution of photoelectrons. The forward-backward asymmetries are typically 3-30%, perhaps three orders of magnitude greater than in other chiroptical phenomena. A peculiarity of this phenomenon is a much enhanced sensitivity to scattering phase shifts, and photoelectron Circular Dichroism (PECD) experiments measuring these asymmetries offer fresh generic insights into electronnuclear interactions.

The magnitude of the PECD effect offers a unique sensitivity to probe, in dilute environments, static and dynamic aspects of molecular chirality per se. Absolute molecular configuration (handedness)-relevant for pharmaceutical, odour, and pesticide production - can be reliably determined by eliminating the common liquid phase interference from induced chiral structure in a solvation shell. More subtle features of molecular conformation (shape) are similarly exposed in this manner. The concept of "shape" is important in many approaches to molecular recognition in e.g. understanding enzyme interaction at receptor sites. Weak, non-bonding molecular interactions drive this recognition. We will conclude by showing how the structure of a prototype self-assembling complex, built by H-bond chiral-recognition between smaller chiral molecules, can be probed in cold molecular beam environments by PECD.

### Invited Talk

A 4.3 Mon 11:30 Audimax

**Enantiomer Identification of Chiral Molecules in Mixtures using Microwave Three-Wave Mixing** — ●MELANIE SCHNELL — Max-Planck-Institut für Struktur und Dynamik der Materie, Hamburg, Germany

Chiral molecules are fascinating chemists for more than 150 years. The two enantiomers of a chiral molecule can have completely different biological effects. For example, the right-handed enantiomer of carvone smells like spearmint while the left-handed one smells like caraway. In nature, chiral molecules often exist in mixtures with other chiral molecules. Their analysis aiming at identifying the molecular components, determining which enantiomers are present, and measuring the enantiomeric excesses (ee) is still one of the challenging tasks of analytical chemistry, despite its importance for modern drug development.

We present here a new method of differentiating enantiomeric pairs of chiral molecules in the gas phase [1,2] based on broadband rotational spectroscopy. The phase of the acquired signal bares the signature of the enantiomer, as it depends upon the combined quantity of their dipole-moment components, which is of opposite sign for the two enantiomers. The signal amplitude is proportional to the ee. A significant advantage of our technique is its inherent mixture compatibility, and we also present absolute configuration determination.

[1] D. Patterson, M. Schnell, J.M. Doyle, *Nature* 497 (2013) 475-477.  
[2] V.A. Shubert, D. Schmitz, D. Patterson, J.M. Doyle, M. Schnell, *Angew. Chem. Int. Ed.* (2013) DOI: 10.1002/anie.201306271

### Invited Talk

A 4.4 Mon 12:00 Audimax

**Mass-selective circular dichroism spectroscopy of chiral molecules** — ●ULRICH BOESL — Technische Universität München, Garching, Germany

The combination of circular dichroism (CD) and mass spectrometry is a young developing research field which promises to become a new analytical tool for mass selective probing of chirality. Such a chiral sensor opens new applications e.g. for studies of chiral catalysis or for analysis of chiral biomolecules brought into the gas phase by laser desorption techniques. This paper deals with a special type of mass selective circular dichroism called REMPI-CD (resonance enhanced multiphoton ionization circular dichroism). REMPI, on the one-hand side, combines optical spectroscopy (first absorption step) with ionization (second absorption step) and thus with mass spectrometry. It has a two-dimensional selectivity with the parameters UV-wavelength and molecular mass. CD, on the other hand, is a frequently used effect to discriminate between the two enantiomers of chiral substances. REMPI-CD then is the small relative difference of ion current induced by left and right circularly polarized laser light. In this paper, measures are presented to enhance the accuracy for these small differences. In addition, REMPI allows for new special effects such as cumulative CD and molecular-ion-CD which are unknown in conventional CD. Finally a strong enhancement of the CD-effect has been observed for cold molecules in supersonic gas beams.