

## MO 1: Chirality

Time: Monday 11:00–13:15

Location: HS XVI

## Invited Talk

MO 1.1 Mon 11:00 HS XVI  
**Tracking and Controlling Chirality** — ●DANIEL REICH — Dahlem Center for Complex Quantum Systems and Fachbereich Physik, Freie Universität Berlin, Berlin, Germany

Chiral observables such as electronic or photoelectron circular dichroism emerge from a complex interplay of the nuclear geometry, the initial state, and the interaction with the driving field. In order to understand and control chiral signatures it is imperative to identify and characterise the key ingredients among this trifecta. In this talk I demonstrate that chirality measures can be used as a tool to track the emergence and predict the strength of chiral observables. Furthermore, I highlight the role of the vibrational degree of freedom on the anisotropy observed for weakly allowed electronic transitions in chiral ketones. I show how the lessons learned from these and related results may serve as important puzzle pieces for quantum control of chiral observables.

MO 1.2 Mon 11:30 HS XVI  
**Robust chiral optical force via electric dipole interactions, inspired by a sea creature** — ●ROBERT P CAMERON<sup>1</sup>, DUNCAN McARTHUR<sup>1</sup>, ALISON M YAO<sup>1</sup>, NICK VOGLEY<sup>2</sup>, and DAQING WANG<sup>2</sup> — <sup>1</sup>SUPA and Department of Physics, University of Strathclyde, Glasgow G4 0NG, United Kingdom — <sup>2</sup>Institute of Applied Physics, University of Bonn, 53115 Bonn, Germany

Inspired by a sea creature, we identify a robust chiral optical force that pushes the opposite enantiomers of a chiral molecule towards regions of orthogonal linear polarization in an optical field via electric dipole interactions. Our chiral optical force can be orders of magnitude stronger than others proposed to date and applies to essentially all chiral molecules, including isotopically chiral varieties which are notoriously difficult to separate using existing methods. We propose a realistic experiment supported by full numerical simulations, potentially enabling optical separation of opposite enantiomers for the first time.

MO 1.3 Mon 11:45 HS XVI  
**Chiral Selector Ion Vibrational Spectroscopy on Amino Acid Enantiomers** — ●FRANCINE HORN<sup>1</sup>, SONJA SCHMAHL<sup>2</sup>, JIAYE JIN<sup>2</sup>, and KNUT R. ASMIS<sup>2</sup> — <sup>1</sup>Leipzig University / Fritz Haber Institute — <sup>2</sup>Leipzig University

The stereochemistry and conformational flexibility of chiral molecules have a strong impact on their biochemical, and pharmacological properties. A central analytical challenge is the generally applicable differentiation of enantiomers, as well as the fast and accurate determination of the enantiomeric excess. Gas phase vibrational action spectroscopy is a highly sensitive, selective, and fast tool for this purpose.

Chiral ionic analytes are transferred into the gas phase, where they interact with volatile chiral selector molecules under the formation of diastereomeric complexes. These are then mass-selected, cryogenically cooled, messenger-tagged and an infrared photodissociation (IRPD) spectrum is measured. The spectra of the vibrationally cold diastereomers exhibit sufficiently different IR fingerprints, such that they can be spectrally distinguished and quantified.

Different intermolecular non-covalent interactions can be present in diastereomers, among them H-bonds,  $\pi$ - $\pi$  interactions and steric hindrance. We study a set of different chiral selector molecules and chiral amino acid analytes with different structural motifs to identify the decisive interactions in the present complexes. We aim at maximizing the differences in the vibrational action spectra of the diastereomers and gain insights into the interactions governing chiral recognition by characterizing the molecular level forces at work.

MO 1.4 Mon 12:00 HS XVI  
**the study of photoelectron circular dichroism in the ionization of (R) - (-) -fenchone by femtosecond laser** — ●WENTAO CHEN<sup>1</sup>, BRENDAN WOUTERLOO<sup>1</sup>, CHIE NAKAYAMA<sup>2</sup>, LUKAS BRUDER<sup>1</sup>, SEBASTIAN HARTWEG<sup>1</sup>, TAKAMASA MOMOSE<sup>2</sup>, and FRANK STIENKEMEIER<sup>1</sup> — <sup>1</sup>Institute of Physics, University of Freiburg, 79104 Freiburg — <sup>2</sup>University of British Columbia, Department of Chemistry, 2036 Main Mall, Vancouver BC, Canada

Photoelectron circular dichroism (PECD) is an intense chiroptical effect when chiral molecules are ionized by circularly-polarized light

(CPL). It would show a forwards/backward asymmetry in photoelectron angular distribution with respect to the CPL propagation direction and be several orders of magnitude more intense than traditional circular dichroism (CD) methods. As it's high sensitivity, PECD could be a fine tool for chirality identification. Here we aim to study the time-resolved PECD effect of (R)-(-)-Fenchone in helium droplets. In the beginning, we used CPL 400nm laser to ionized the Fenchone which is seeded in helium beam and detected the photoelectron by velocity map imaging method. We detected a significant PECD effect after subtracting the signals ionized by CPL lasers at different helicity. Then we will apply linear-polarized 200nm pump laser and CPL 266nm probe laser together with helium droplets method to study the time-resolved PECD effect in (R)-(-)-Fenchone. This will help us to figure out how the helium-droplets environment influences the ultrafast relaxation dynamics in chiral systems.

MO 1.5 Mon 12:15 HS XVI  
**Electron correlation in circular dichroism and chirality-induced spin selectivity** — ●RAOUL M. M. EBELING<sup>1</sup>, MAURICE BÉRINGUIER<sup>1</sup>, VLADIMIRO MUJICA<sup>2</sup>, DANIEL M. REICH<sup>1</sup>, and CHRISTIANE P. KOCH<sup>1</sup> — <sup>1</sup>Freie Universität Berlin, Berlin, Germany — <sup>2</sup>Arizona State University, Arizona, United States of America

We study two phenomena related to the interaction of chiral molecules with circularly polarized light, absorption circular dichroism (CD), and chirality-induced spin selectivity (CISS). We investigate both phenomena in chiral hydrogen and chiral helium, two model systems into which we introduce chirality via an artificial chiral potential. The chiral potential is constructed from a superposition of spherical harmonics and it can be interpreted as a way to mimic the chiral environment of a real molecule. Alternatively, our chiral hydrogen and chiral helium models could even be experimentally realized by placing the atoms in a setup involving several electric fields. By quantifying the chirality of the states with a suitable measure, we study the relationship between the chirality of the states and the CD and CISS. We investigate the influence of the strength of the chiral potential, the strength of the spin-orbit coupling, and the strength of the electron-electron interaction on both CD and CISS.

MO 1.6 Mon 12:30 HS XVI  
**Chirality induced spin polarization in one-photon ionization by circularly polarized light** — ●PHILIP CAESAR FLORES<sup>1</sup>, STEFANOS CARLSTROM<sup>1</sup>, SERGUEI PATCHKOVSKI<sup>1</sup>, ANDRES ORDONEZ<sup>2,3</sup>, and OLGA SMIRNOVA<sup>1,4,5</sup> — <sup>1</sup>Max-Born-Institut, Max-Born-Str. 2A, 12489 Berlin, Germany — <sup>2</sup>Department of Physics, Imperial College London, SW7 2BW London, United Kingdom — <sup>3</sup>Department of Chemistry, Queen Mary University of London, E1 4NS London, United Kingdom — <sup>4</sup>Technische Universität Berlin, 10623 Berlin, Germany — <sup>5</sup>Technion, Israel Institute of Technology, 3200003, Haifa, Israel

Geometric magnetism controls the degree of enantiosensitive response in photoionization of chiral molecules and leads to new extremely efficient enantiosensitive observables (Commun. phys. 6, 2023, 257). Here, we show that the same phenomenon is responsible for: (i) spin-resolved enantiosensitive molecular orientation in photoionization, and (ii) spin-polarization of photoelectrons ejected from atoms and chiral molecules by circularly polarized fields. Our results provide a missing fundamental link between chirality and spin-polarization, and demonstrate that the coupling of geometric field to spin leads to high spin-polarization, which can be achieved even for very small spin-orbit interaction. Our conclusions are illustrated for synthetic chiral matter. We perform *ab initio* simulations of spin dynamics in photoionization of Argon atom using fully coupled spin-orbit code (Phys. Rev. A 106, 2022, 042806), and construct chiral superpositions of electronic states in Argon to quantify the link between chirality and spin-polarization in chiral targets.

MO 1.7 Mon 12:45 HS XVI  
**Models for Predicting Parity Violating Energy Differences in Chiral Molecules** — ●NAMRATA GOHAIN and ROBERT BERGER — Philipps-Universität Marburg, Hans-Meerwein-Straße 4, 35032 Marburg

The weak interaction, unlike the other fundamental forces, violates parity and renders all atoms to be inherently chiral. However, this

effect becomes more pronounced in chiral molecules, leading to a tiny parity violating energy difference[1,2]. As attempts are being made to quantify the influence of parity violation in such molecules experimentally, one can also attempt to develop simplified models that predicts the energy difference between two enantiomers without explicit calculations. This can be advantageous for finding potential candidates that aids the development of high resolution spectroscopic techniques which can detect the parity violation in molecules[3]. In this contribution we will present one such model by focusing on different unsaturated chiral compounds as our candidates.

[1] M. Quack, *Angew. Chem. Int. Ed. Engl.*(1989), 28, 571-586.

[2] R. Berger and J. Stohner, *WIREs Comput Mol Sci.* (2019), 9, e1396.

[3] M. Quack, G. Seyfang and G. Wichmann, *Chem. Sci.* (2022), 13, 10598-10643

MO 1.8 Mon 13:00 HS XVI

**Predicting splittings due to the weak interaction in rotational spectra of chiral clusters containing heavy elements —**

•MIHNEA MLAK-MĂRGINEAN and ROBERT BERGER — Philipps University of Marburg, 35032 Marburg, Germany

Rotational lines of chiral molecules are predicted to be split into those for left- and those for right-handed molecules when the fundamental weak interaction is taken into account. A successful detection of these tiny splittings would demonstrate parity nonconservation in the realms of molecular physics [1]. We aim at the prediction of such splittings in clusters containing heavy elements, which give rise to particularly promising effects. We use an implementation [2] of the zeroth order regular approximation to optimise the ground state electronic wave function of our systems, since relativity and spin-orbit coupling play a major role. Weak interaction contributions are accounted for perturbatively [3], with derivatives of these contributions with respect to atomic coordinates being computed analytically [4]. The latter are crucial for an efficient prediction within a rotation-vibration perturbation theory framework [5]. We will present general trends for the splittings and discuss their origin as well as prospects for the measurements.

[1] Berger, Stohner, *WIREs Comput. Mol. Sci.* 2019, 9, e1396.

[2] van Wüllen, *JCP* 1998, 109, 392, *ZPC* 2010, 224, 413.

[3] Berger, van Wüllen, *JCP* 2005, 122, 134316; Gaul, Berger, *JCP* 2020, 152, 044101.

[4] Brück, Sahu, Gaul, Berger, *JCP* 2023, 158, 194109.

[5] Riley, Raynes, Fowler, *Mol. Phys.* 1979, 38, 877.