Max-Planck-Institut für Struktur und Dynamik der Materie

Max Planck Institute for the Structure and Dynamics of Matter

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CFEL Seminar room IV (Bldg. 99)

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Transient Chirality in Chemistry and Biology: Capturing the Structural Evolution of Molecules in Solution

Most biological functions and many chemical processes are driven by chiral nanoscale molecular machines in solution, whose structures evolve on multiple time and length scales: from the ultrafast rotations of photo-driven synthetic molecular motors to the global conformational changes of proteins on the microsecond time scale. Yet capturing the associated conformational transitions in real-time continues to be a formidable experimental challenge, as prominent established methods come with their own limitations: solution nuclear magnetic resonance is limited to millisecond real-time resolution, whilst solution X-Ray scattering requires large-scale X-Ray facilities. A promising laboratory-based alternative is circular dichroism (CD), the absorption difference of left- and right-handed circularly polarized light, which is sensitive to the chiral geometrical arrangement of light-absorbing chemical groups within a molecular system. Steady-state CD is already a well-established tool in the far and middle ultraviolet (UV) < 300 nm, where equilibrium structures of proteins, DNA and functional chiral organic complexes are routinely characterized. However, pushing this technique into the time-domain has remained a challenge for over three decades, with only few isolated reports with sub-nanosecond resolution [1].

In this talk, I will present a technological breakthrough with the first time-resolved CD (TRCD) spectrometer that combines highly sensitive broadband UV-detection (250-370 nm) with pulsed laser sources and sub-picosecond time-resolution [2]. With this instrument, it is now possible to extract broadband CD spectra of photo-excited molecular states and follow their transient chirality changes with femtosecond resolution. This is opening a new avenue for capturing solution-phase structural dynamics in chemical and biological systems that I will illustrate with two examples: the coupling of electronic and structural dynamics in a chiral supramolecular metal-complex [3], and the application of a site-specific CD-label to track conformational changes of the peptide backbone [4]. On this basis I will present future developments that will establish TRCD as a complementary method for research in protein dynamics and chiral photochemistry, where the chirality of excited electronic states is the key design feature of chiral organic light-emitting diode materials and unidirectional molecular motors, for example.

[1] J. Meyer-Ilse et al., Laser Photon. Rev. **7**, 495 (2013)
[2] M. Oppermann et al., Optica **6**, 56 (2019)
[3] J. Lacour et al., Angew. Chem. Int. Ed. **37**, 2379 (1998)
[4] M. Oppermann & J. Spekowius et al., J. Phys. Chem. Lett. **10**, 2700 (2019)

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