NANOSCIENCE COLLOQUIUM

2D-IR spectroscopy of complex molecular systems: Something soft, something sweet, something bright

Prof. Dr. Henrike Müller-Werkmeister

University of Potsdam, Institute of Chemistry - Physical Chemistry,

A B S T R A C T : In my talk, I will discuss examples from our work applying 2D-IR spectroscopy, a femto- to picosecond time-resolved coherent spectroscopy, and ultrafast transient spectroscopy to study structural dynamics in complex molecular systems, including proteins, carbohydrates, and biomimetic soft matter as well as materials. 2D-IR can provide access to electrostatics, H-bonding, and energy transfer processes in all of these systems.

2D-IR can provide insight to secondary structure for proteins and peptides, which can not be analyzed with regular structural biology methods, i.e. crystallography. We have studied intrinsically disordered peptides with a GLFG repeat motif, derived from the nuclear pore complex, and find evidence for different beta-strand geometries in the gel-phases formed via liquid-liquid phase separation.

Carbohydrates are extremely difficult to study by molecular biophysical tools due to the multitude of configurations for the same composition. Using vibrational reporter groups like azide or thiocyanate allowed us to investigate dynamics of carbohydrates by 2D-IR for the first time [1]. In monosaccharides we have studied ring puckering dynamics and can report now a speed limit for the ring pucker, which was not accessible experimentally before. Protein-carbohydrate interactions are highly important in all biochemical processes. The first example we targeted by 2D-IR is mapping the active site of the enzyme hexokinase when bound to glucose. We also now can study enzymatic kinetics, mapping phosphate signatures of ADP-ATP via min to hours [2].

While 2D-IR on its own is accessing the electronic ground state, we are mid-term interested to also study the transient evolution of processes, following a trigger like the uncaging of a substrate or a pH-jump. These tools are generally key for dynamics structural biology studies, i.e. also time-resolved serial crystallography. I will review our work on para-hydroxyphenacyl as photocage [3] and on HTPS as a reversible photoacids.

[1] P. Gasse et al. J. Chem. Phys. 158, 145101, 2023P. Gasse, et al. J. Chem. Phys. 161 195101, 2024.

[2] T. Stensitzki et al., in revision, 10.26434/chemrxiv-2025-j5szt

[3] Y. Pfeifer, et al., Phys. Chem. Chem. Phys. 27, 12899 – 12907, 2025

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