

Illuminating Biomolecular Complexity: X-ray Free Electron Lasers and Vibrational Spectroscopies for Protein, Aggregates, and Cellular Architectures



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Multidimensional IR Spectroscopy (2D-IR) as tool to study protein dynamics

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Ultrafast multidimensional IR spectroscopy (2D-IR) can provide detailed information on local structural dynamics in peptide, proteins or complex systems like models of protein condensates. 2D-IR is a femtosecond laser spectroscopy with its intrinsic time-resolution on par with the fundamental timescale of chemical dynamics, fs to ps. For biological systems the capability to directly probe H-bonding dynamics, changes of electrostatics and conformational dynamics are important. In particular for intrinsically disordered systems or beta-sheet rich structures, 2D-IR has benefits over FTIR spectroscopy, as weak signals (i.e. shoulders) are much sharper in the 2D-IR spectra. The information obtained from 2D-IR spectra is thus complementary to insights from X-Ray diffraction experiments. In this contribution, the basics of 2D-IR and applications to biomolecular systems shall be reviewed and prospects for future integration between 2D-IR and XFEL experiments will be addressed. To this end, we have already performed initial 2D-IR experiments on protein crystals with fixed target sample delivery similar as for TR-SFX experiments.

Scholarship eligibility

no

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