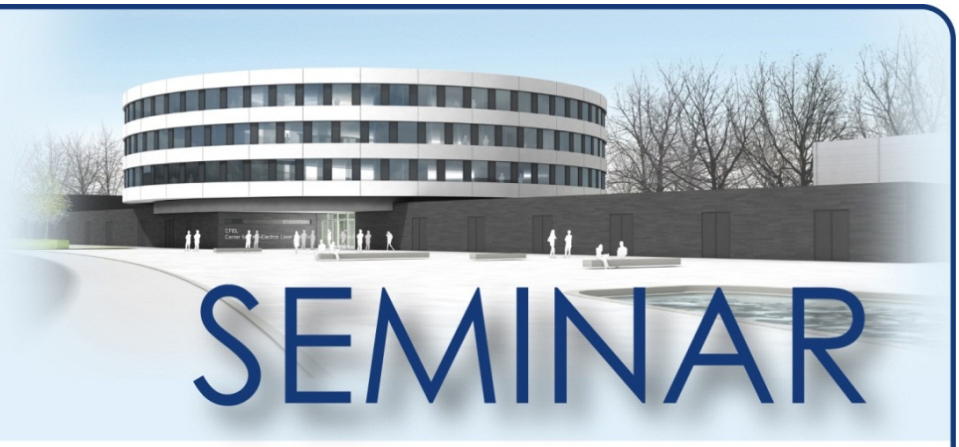
CFEL SCIENCE



SEMINAR

29th January 2025 - 2:00 p.m.

CFEL-bldg. 99, seminar room IV

Mayank Vashistha

Center for Free-Electron Laser Science, DESY, and
Department of Physics, University of Hamburg, Germany

Theoretical insights into serial femtosecond crystallography under non-Born-Oppenheimer dynamics

Serial femtosecond crystallography (SFX) has revolutionized the ability to observe ultrafast structural dynamics, particularly in biomolecules such as proteins, yet its theoretical foundations remain an area of active investigation—especially for systems experiencing strong non-Born-Oppenheimer effects or traversing conical intersections. In this talk, I will present a quantum-electrodynamics-based framework for SFX, which provides a rigorous validation of the standard assumptions commonly applied in time-resolved diffraction experiments. By employing a modal decomposition of diffraction signals in reciprocal space, the electron density in real space can be equivalently decomposed in cases of low pump excitation probability, consistent with assumptions used in recent studies [1]. One key result is that near conical intersections, the number of structural modes contributing to the SFX signal is determined solely by the number of electronic states involved, irrespective of the number of nuclear degrees of freedom [2]. This finding not only accelerates structural determination in time-resolved SFX but also offers a robust theoretical foundation for analyzing ultrafast processes in biologically significant systems such as proteins undergoing functional changes. The talk will highlight the theoretical implications and potential extensions of this framework for experimental and computational studies.

[1] A. Hosseinizadeh *et al.*, *Nature* **599**, 697 (2021).

[2] M. Vashistha *et al.*, *Phys. Rev. Res.* **6**, 043198 (2024).

Host: Robin Santra – CFEL-DESY Theory Division