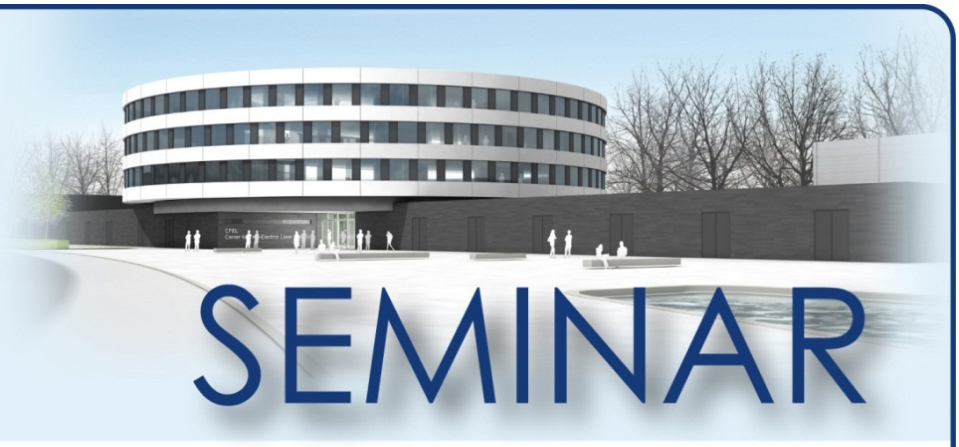
CFEL SCIENCE



SEMINAR

10th April 2024 - 2:00 p.m.

CFEL-bldg. 99, seminar room IV

Maurits W. Haverkort

Institut für Theoretische Physik, Universität Heidelberg, Germany

Theoretical pump-probe spectroscopy in quantum solids using non-linear response functions: The example of NiO

The theoretical prediction of dynamics in correlated quantum materials is challenging. Many competing interactions, including local correlations, multiplets, charge-transfer, covalence, and band-formation all need to be considered. As a result new low energy quasi-particles with long lifetimes can emerge. Despite the possibility for low lying excitations to decay in multiple ways, long lived excitations with well defined energy momentum dispersions can exist in correlated quantum materials. A theoretical prediction of the dynamics in this case needs to extend over time scales that are several orders of magnitude larger than the reciprocal of the leading energy scales in the problem. This is a true numerical challenge.

Using non-linear response theory we present a theoretical method to tackle this challenge. The method is suited to describe pump–probe spectroscopy from THz to x-ray frequencies including the electronic dynamics of the material in various spectroscopy forms. We will show examples of this method using NiO. We can get a quantitative prediction of the optically pump–optically probed photo-electron spectra and its long lived coherent dynamics.

Host: Robin Santra – CFEL-DESY Theory Division