CHYN MEETS HARBOR

Simulating time-resolved X-ray absorption spectroscopy of pyrazine at the nitrogen K-edge with a full time-domain approach

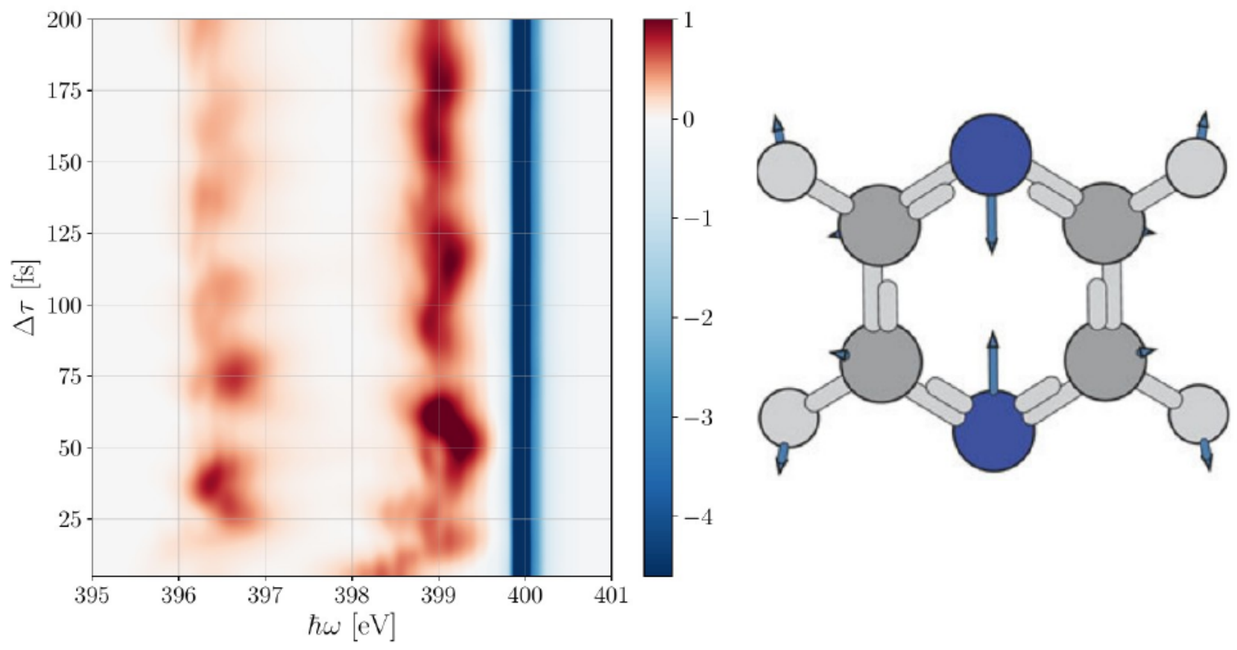
Antonia Freibert
Max Planck Institute for the Structure and Dynamics of Matter, Hamburg

Synthesis of crystalline plasmonic superstructures

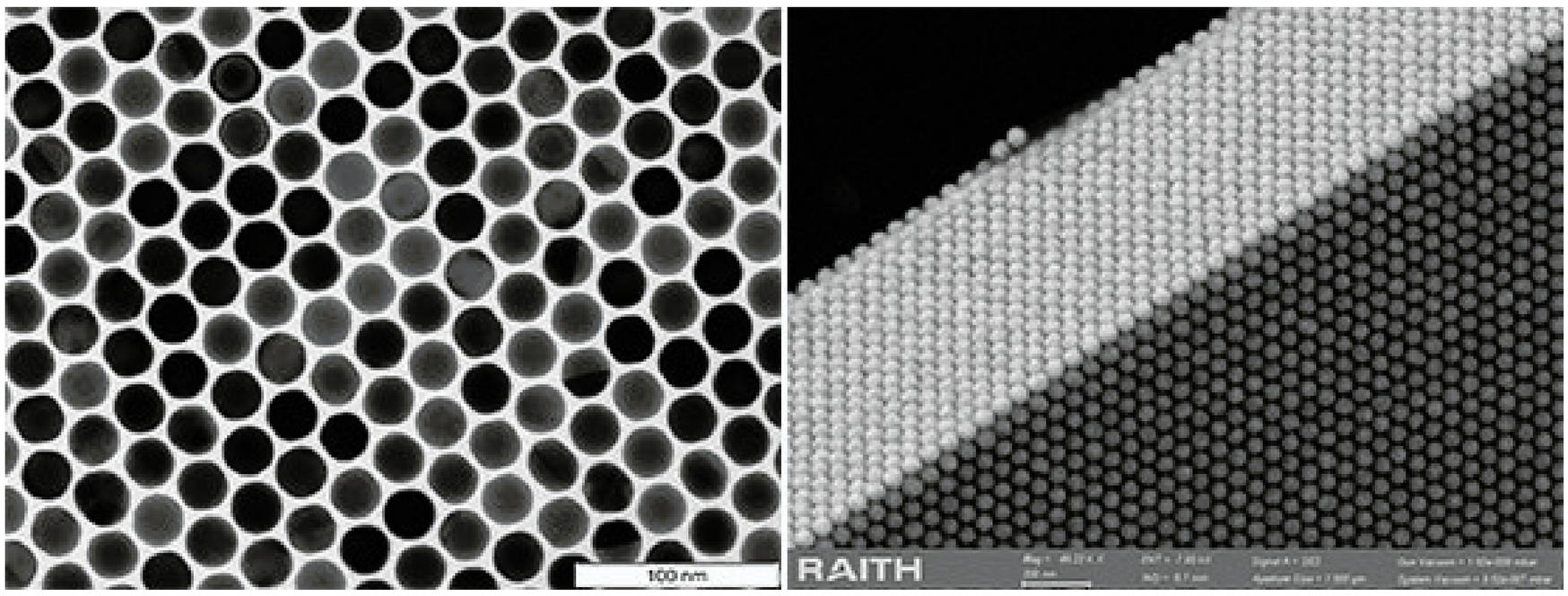
Dr. Florian Schulz
Institute for Nanostructure and Solid State Physics, University of Hamburg

Abstract Talk 1: Ultrafast X-ray absorption spectroscopy offers elemental specificity and in principle access to the natural time evolution of valence excitations when studying electronic and structural configurations of molecules and materials. Due to the complex nature of probing structural dynamics on the femtosecond timescale, detailed theoretical studies are required to link the spectroscopic observables to the underlying dynamics and thereby access the high information content contained in this experimental method. A large influence of nuclear dynamics can be expected in nonlinear spectroscopy which requires a time-dependent framework that is able to describe non-adiabatic phenomena.

I will present time-resolved X-ray absorption spectroscopy simulations of pyrazine at the nitrogen K-edge including wavepacket dynamics in both the valence- and core-excited state manifolds. We discuss the validity of the widely used short-time (or Lorentzian) approximation which neglects the nuclear dynamics following the X-ray probe transition. We further demonstrate the impact of an explicit description of the external electric field and explicitly calculate the effect of an increasingly longer excitation pulse on the observed photo-triggered wavepacket dynamics.



Abstract Talk 2: The self-assembly of nanoparticles can be utilized to synthesize crystalline superstructures. The synthesis of crystalline superstructures of gold nanoparticles (AuNP) will be presented and how these structures can be characterized with electron microscopy and small-angle X-ray scattering. Not only structural features as lattice constants are of interest but also the degree of order: how could it be quantified and how does it affect the properties of the superstructures? The optical properties of AuNP are dominated by plasmons and in well-defined AuNP superstructures the coupling of plasmonic dipoles can lead to new emergent properties, in particular extreme light-matter interactions. It will be discussed how these emergent properties are tuned via the structure and why they are interesting for applications like surface-enhanced Raman- and IR-spectroscopy.



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