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

Towards the all-electrical detection of single nanoparticles at GHz frequencies in fluidic systems - Lucjan Grzegorzewski

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 phototriggered wavepacket dynamics.



Abstract Talk 2: Electrical impedance flow spectroscopy (EIS) enables ultra-fast, electrical, and label-free sensing of single micrometer-sized particles. An open challenge for EIS is to detect particles in sub-500nm regime. That regime includes of a multitude of biological nano-particles like viruses, proteins, or even DNA. State-of-the-art EIS lacks several orders of sensitivity to achieve that goal. In this talk, I will present a novel coupling-based sensor geometry in combination with an interferometric measurement setup. In comparison to our previous setup, major improvements in the sensor design and measurement setup, increased the signal-to-noise ratio (SNR) for cell detection from 15 to 4200. Additionally, I could detect 200nm polystyrene beads with an SNR of 170, to our knowledge the smallest particles ever to be detected with EIS. In conclusion, the improvements pave the way for high-throughput detection of single nanometer-sized biological particles in fluidic systems.



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