Bonn 2025 – SYAD Overview

Symposium SAMOP Dissertation Prize 2025 (SYAD)

jointly organised by all divisions of the section AMOP

Gereon Niedner-Schatteburg Chair of Physical Chemistry RPTU Kaiserslautern-Landau Erwin Schrödinger Strasse 52 67663 Kaiserslautern gns@rptu.de

The topical divisions within SAMOP jointly award a PhD prize 2025. The prize acknowledges outstanding research from a PhD work and its excellent written and oral presentation. Eligible for nomination were outstanding PhD theses from the research fields of SAMOP completed in 2023 or 2024. Based on the nominations and independent reviewing, a jury of SAMOP representatives selected four finalists for presentation of their research in the framework of this dissertation prize symposium. Right after the symposium, the awardee will be selected by the prize committee. The winner will be announced in the course of the DPG Ceremonial Session (Festsitzung) on Tuesday afternoon.

Overview of Invited Talks and Sessions

(Lecture hall HS 1+2)

Invited Talks

SYAD 1.1	Mon	14:30-15:00	${\rm HS}\ 1{+}2$	A simple method to separate single- from multi-particle dynamics
				in time-resolved spectroscopy — •Julian Lüttig
SYAD 1.2	Mon	15:00-15:30	${\rm HS}\ 1{+}2$	Time-resolving quantum dynamics in atoms and molecules with
				intense x-ray lasers and neural networks — •Alexander Magunia
SYAD 1.3	Mon	15:30-16:00	${\rm HS}\ 1{+}2$	How rotation shapes the decay of diatomic carbon anions —
				•Viviane C. Schmidt
SYAD 1.4	Mon	16:00-16:30	$_{ m HS}$ 1 $+2$	Interstellar stardust from stellar explosions recorded in a deep-
				ocean ferromanganese crust within the last 10 million years —
				•Dominik Koll

Sessions

 ${\rm SYAD}\ 1.1-1.4\quad {\rm Mon}\quad 14:30-16:30\quad \ {\rm HS}\ 1+2\quad \ {\bf SAMOP\ Dissertation\ Prize\ Symposium}$

Bonn 2025 – SYAD Monday

SYAD 1: SAMOP Dissertation Prize Symposium

Time: Monday 14:30-16:30 Location: HS 1+2

The interpretation of time-resolved spectroscopy such as transient absorption (TA) relies on the isolation of a specific nonlinear order, typically the third order, of the sample response. Usually the excitation power is chosen low enough to suppress unwanted higher orders such as exciton-exciton annihilation. However, measurements at low excitation power often exhibit poor signal-to-noise ratio and the contamination by higher-order contributions cannot be quantified. In the opposite case of too high powers, higher-order signals connected to multi-particle dynamics are present and have to be considered in the analysis. We developed a technique using linear combinations of TA spectra at selective powers to extract uncontaminated nonlinear signal contributions. Thus, we access single-particle signals with high signalto-noise ratio and obtain separate multi-particle dynamics [1,2]. Our technique can be easily implemented in any TA experiment and is applicable to any type of quantum system. We measured a broad variety of samples such as quantum dots, photosynthetic complexes, silicon nanocrystals, and polymers. The method provides direct access to the various terms of the perturbative expansion of light-matter interaction allowing one to systematically increase the number of interacting particles, infer their interaction energies and reconstruct their dynamics. [1] P. Malý et al., Nature **2023**, 616, 280.

[2] J. Lüttig et al., J. Phys. Chem. Lett. **2023**, 14, 7556–7573.

Invited Talk SYAD 1.2 Mon 15:00 HS 1+2 Time-resolving quantum dynamics in atoms and molecules with intense x-ray lasers and neural networks — ◆ALEXANDER MAGUNIA — Max-Planck-Institut für Kernphysik

The dynamics of electrons in atoms and nuclei in molecules are essential to the properties of matter. While the electronic processes can be incredibly fast, on the order of a femtosecond or faster, laser pulses even shorter in time allow to resolve them nevertheless. The two main avenues for achieving such short pulses, High-order Harmonic Generation (HHG) and Free-Electron Lasers (FELs), typically imply going to the extreme-ultraviolet (XUV) and x-ray spectral regimes as well.

In this talk, the very first experiment combining FEL and HHG pulses is presented. A prototypical photochemical reaction, the coupling of nuclear and electronic responses during state-selective photodissociation of molecular oxygen, is time resolved. In addition, ultrafast electronic-population transfer mechanisms in the XUV/x-ray regime, in particular Rabi oscillations studied with absorption spectroscopy, will be addressed. This further enables machine-learning applications for reconstructing time-dependent quantum properties, such as the electronic-state populations.

Invited Talk SYAD 1.3 Mon 15:30 HS 1+2

How rotation shapes the decay of diatomic carbon anions — •VIVIANE C. SCHMIDT — Max-Planck-Institut für Kernphysik, Heidelberg, Germany

Molecules that are internally highly excited play an important role in a range of fields from atmospheric to plasma physics. Modelling such systems requires a detailed understanding of the molecules' behaviour under these extreme conditions. However, this is a non-trivial task due to the high density of excited states as well as the variety of competing decay mechanisms available. The diatomic carbon anion C₂ presents an excellent benchmark to understand the interplay of different decay channels at high internal excitation. The system is arguably the most extensively studied molecular anion in history. Yet, its decay behaviour at high internal excitation has long remained a puzzle for physicists. When produced in a hot ion source, a subset of the resulting anions spontaneously eject their excess electron with a very narrow lifetime span of about 3 ms. While this autodetachment phenomenon has been known since the 1990s, the responsible anionic excited states and their decay mechanism have long remained elusive. Based on our measurements of autodecay of highly excited C_2^- at the Cryogenic Storage Ring (CSR) facility in Heidelberg, we carried out detailed calculations of the excited states and their decay behaviour. Here, we were able to uncover the profound effect rotational excitation has on the system's electronic landscape. This in turn alters the available decay channels at high excitations and enabled the discovery of a new autodetachment mechanism, which explains the measured feature.

Stars are the element factories in the universe. Stellar explosions eject freshly synthesized radionuclides into interstellar space which subsequently can be accreted by Earth. These radionuclides are the finger-prints of stellar nucleosynthesis.

In this work, I characterized a 10-million year old ferromanganese crust from the bottom of the Central Pacific and chemically extracted single atoms of live interstellar radionuclides $^{60}\mathrm{Fe},~^{244}\mathrm{Pu}$ and $^{247}\mathrm{Cm}$ for accelerator mass spectrometry. The dating of the crust with cosmogenic $^{10}\mathrm{Be}$ led to the discovery of an unexpected anomaly during the late Miocene, which has the potential to be used as a new dating anchor on the Myr timescale for deep-ocean archives.

Highly time-resolved profiles of supernova 60 Fe and r-process 244 Pu and 247 Cm revealed two influxes of supernova-produced interstellar stardust within the last 10 Myr. The influx profile of 244 Pu and 247 Cm constrain the last r-process event in the Milky Way.