Symposium Laboratory Astrophysics (SYLA)

jointly organised by
the Molecular Physics Division (MO),
the Atomic Physics Division (A), and
the Mass Spectrometry Division (MS)

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After the formation of atoms and molecules in the universe they send out their radiation and as such they are ambassadors of distant regions in the universe which are observed from earth. They also act as probes for the physical and chemical conditions in these places and astrophysicists use laboratory spectra not only to identify theses species in their observations but to determine their abundance. Conclusions drawn on their formation and destruction routes give intimate information on the development of stars, molecular clouds, on the atmoshperes of extrasolar planets and other places in the universe. Laboratory astrophysics is providing the necessary microphysics data for this endeavor. The German community is rather active in this field and this symposium addresses some recent technical developments and scientific highlights.

Overview of Invited Talks and Sessions

(Lecture hall Audimax)

Invited Talks

SYLA 1.1	Mon	14:00–14:30	Audimax	**Probing chemistry inside giant planets with laboratory experiments** — •Dominik Kraus
SYLA 1.2	Mon	14:30–15:00	Audimax	**Inner-shell photoabsorption of atomic and molecular ions** — •Stefan Schippers
SYLA 1.3	Mon	15:00–15:30	Audimax	**Molecular Astrophysics at the Cryogenic Storage Ring** — •Holger Kreckel
SYLA 1.4	Mon	15:30–16:00	Audimax	**Observing small molecules in stellar giants - High spectral resolution infrared studies in the laboratory, on a mountain, and high up in the air** — •Guido W. Fuchs
SYLA 2.1	Mon	16:30–17:00	Audimax	**State-to-State Rate Coefficients for NH_3-NH_3 Collisions obtained from Pump-Probe Chirped-Pulse Experiments** — •Christian P. Endres, Paola Caselli, Stephan Schlemmer
SYLA 2.4	Mon	17:30–18:00	Audimax	**A multifaceted approach to investigate the reactivity of PAHs under electrical discharge conditions** — •Donatella Loru, Amanda L. Steber, Johannes M. M. Thunnissen, Daniël B. Rap, Alexander K. Lemmens, Anouk M. Rijs, Melanie Schnell
SYLA 2.5	Mon	18:00–18:30	Audimax	**Exploring the Femtosecond Dynamics of Polycyclic Aromatic Hydrocarbons Using XUV FEL Pulses** — •Jason Lee, Denis Tikhonov, Bastian Manschwetus, Melanie Schnell

Sessions

SYLA 1.1–1.4	Mon	14:00–16:00	Audimax	**Laboratory Astrophysics**
SYLA 2.1–2.5	Mon	16:30–18:30	Audimax	**Laboratory Astrophysics**

SYLA 1: Laboratory Astrophysics

Time: Monday 14:00–16:00 Location: Audimax

Invited Talk SYLA 1.1 Mon 14:00 Audimax
Probing chemistry inside giant planets with laboratory experiments — •Dominik Kraus — Institut für Physik, Universität Rostock — Institut für Strahlenphysik, Helmholtz-Zentrum Dresden-Rossendorf

The interiors of giant planets exhibit extreme conditions: High temperatures and enormous pressures create environments which are not fully understood and hard to encompass for state-of-the-art physics models. Applying the largest and most brilliant laser light sources, it is now possible to investigate such conditions in the laboratory. Recent efforts provide seminal insights into chemistry and phase transitions occurring deep inside giant planets such as carbon-hydrogen phase separation and the formation of superionic water. At the same time, highly interesting materials can be formed via these conditions, such as nanodiamonds or hexagonal diamond, so-called lonsdaleite, which, in its pure form, is predicted to exceed the hardness of cubic diamond. I will present a showcase of recent experiments investigating these topics and provide an outlook for future developments.

Invited Talk SYLA 1.2 Mon 14:30 Audimax
Inner-shell photoabsorption of atomic and molecular ions — •Stefan Schippers — Justus-Liebig-Universität Gießen

Recent experimental work on the photoabsorption of atomic and molecular ions will be reviewed that has been carried out at the photon-ion merged-beams setup PIPE [1], a permanently installed end station at the XUV beamline P04 of the PETRA III synchrotron radiation source operated by DESY in Hamburg, Germany. Selected results [2] on, e.g., single and multiple L-shell photoionization of low-charged iron ions and on single and multiple K-shell photoionization of negatively and (multiply) positively charged carbon and silicon ions will be discussed in astrophysical contexts as well as inner-shell photoabsorption of molecular ions. These experimental results bear witness of the fact that the implementation of the photon-ion merged-beams method at one of the world's brightest synchrotron light sources has led to a breakthrough for the experimental study of inner-shell photoabsorption processes with ions.

[1] S. Schippers, T. Buhr, A. Borovik Jr., K. Holste, A. Perry-Sassmannshausen, K. Mertens, S. Reinwardt, M. Martins, S. Klumpp, K. Schubert, S. Bari, R. Beerwerth, S. Fritzsche, S. Ricz, J. Hellhund, and A. Müller, X-Ray Spectrometry **49**, 11 (2020) (doi: 10.1002/xrs.3035).
[2] S. Schippers and A. Müller, Atoms **8**, 45 (2020) (doi: 10.3390/atoms8030045).

Invited Talk SYLA 1.3 Mon 15:00 Audimax
Molecular Astrophysics at the Cryogenic Storage Ring — •Holger Kreckel — Max-Planck-Institut für Kernphysik, 69117 Heidelberg, Germany

Ever since the first molecular species were detected in interstellar space, more than 80 years ago, their abundance and formation mechanisms have challenged the curious minds of molecular physicists. Today, the molecular composition of the universe is at the forefront of observational astronomy, as modern telescopes target molecular transitions from infrared to millimeter wavelengths. Besides the observational efforts, reliable laboratory data and comprehensive modeling are required to gain insight into the life cycle of molecules in space. The Cryogenic Storage Ring (CSR) was designed as a versatile test bench to prepare atomic and molecular ion beams for detailed merged beams experiments at cryogenic temperatures and extremely low pressure. We will give an overview of the experimental capabilities of the CSR and present recent results for state-selected reaction studies of molecular ions with free electrons and neutral atoms. These processes are of paramount importance for the chemistry of the interstaller medium and the formation of the first stars in universe.

Invited Talk SYLA 1.4 Mon 15:30 Audimax
Observing small molecules in stellar giants - High spectral resolution infrared studies in the laboratory, on a mountain, and high up in the air — •Guido W. Fuchs — 1Laboratory Astrophysics, University of Kassel (Germany)

Close to the end of their lifetime giant stars lose much of their mass in form of stellar winds and outflows. Opposed to carbon-rich (C-type) stars, the processes of molecule and dust formation in oxygen-rich (M-type) or intermediate-type (S-type) stars is not well understood. Small molecules made of refractory material, like metal, carbon, or silicon, seem to play an important role for the chemistry in these environments. The molecular inventory of circumstellar environments is mostly investigated via radio observations. However, infrared (IR) observations can also be performed as these stellar objects shine brightly in the IR range. In this work, the focus is set on IR observations of prototypical M-type and S-type stars as well as accompanying laboratory investigations on the spectra of small metall bearing molecules. The astrophysical observations were done using high resolution spectrographs like TEXES at the IRTF on Mauna Kea (Hawaii) or EXES onboard the SOFIA airplane. In the laboratory, molecules like TiO, VO, Al2O and other species have been investigated to determine their IR spectra. In this talk, the combined laboratory- and observational approach to identify and analyze small molecules made of refractory materials in circumstellar environments is presented.

SYLA 2: Laboratory Astrophysics

Time: Monday 16:30–18:30 Location: Audimax

Invited Talk SYLA 2.1 Mon 16:30 Audimax
State-to-State Rate Coefficients for NH_3-NH_3 Collisions obtained from Pump-Probe Chirped-Pulse Experiments — •Christian P. Endres[1], Paola Caselli[1], and Stephan Schlemmer[2] — [1]MPI für extraterrestrische Physik, Garching, Germany — [2]Universität zu Köln, Köln, Germany

The kinetics of rotational inelastic NH_3-NH_3 collisions is studied using pump-probe experiments, which are carried out with a Ku-band waveguide chirped pulse Fourier transform microwave spectrometer by observing the ammonia inversion doublets in the ground vibrational state. The population of one ammonia inversion doublet of a single rotational state is altered by a resonant pump pulse. Due to collisions, the resulting deviation from thermal equilibrium propagates to other states and is interrogated by probe pulses as a function of the pump-probe delay time. The bandwidth of the spectrometer allows to probe the intensity of many inversion transitions within a single chirped pulse excitation (probe pulse) on sub-microsecond timescales as a function of the pump pulse conditions. State-to-state rates are obtained by simulations of all coupled states fitted to the temporal behavior of the complete pump probe experiments where many individual (J,K) rotational states are addressed step by step by separate pump pulse sequences.

SYLA 2.2 Mon 17:00 Audimax
Optical Absorption and Photodissociation Properties of Small Silicon-Containing Clusters - $Si_3O_2^+$ — •Taarna Studemund, Marko Förstel, Kai Pollow, Julian Voss, Robert G. Radloff, and Otto Dopfer — Institut für Optik und Atomare Physik, Technische Universität Berlin, Hardenbergstrasse 36, D-10623 Berlin

Interstellar dust consists to a significant fraction of μm-sized silicate particles. Origin and formation mechanisms of such dust, which can form solar systems, are still poorly understood. Si/O-containing molecules may be precursors to the larger silicate particles found. So far, only silicon monoxide (SiO) has been detected in the interstellar medium (ISM) [1]. Larger intermediates remain elusive but should exist if the larger grains are formed from the bottom up.
To understand the photodissociation and optical absorption behavior, structures, and energies of Si/O-containing molecules, we measure optical spectra of mass-selected $Si_nO_m^+$ clusters and compare them to

quantum chemical calculations. Our experimental setup is based on mass spectrometry and resonant laser photodissociation [2]. Initial data show competing fragmentation channels, their appearance energies and branching ratios. In addition, we present the first optical spectrum of $Si_3O_2^+$. The results are discussed in an astrophysical context.

[1] R. Wilson et al, 1971, Astrophys. J. 167, L97.
[2] M. Förstel et al, Rev. Sci. Instrum. 2017, 88, 123110.

SYLA 2.3 Mon 17:15 Audimax

The Optical Spectrum and Astrochemical Relevance of 1-Cyanoadamantane$^+$ — •Parker Crandall, Robert Radloff, Marko Förstel, and Otto Dopfer — Technische Universität Berlin, Berlin, Germany

Astrochemical measurements have demonstrated similarities between the IR spectra of diamondoids and unidentified infrared emission (UIR) bands seen in the spectra of young stars with circumstellar disks.[1,2] Due to their low ionization energy and open-shell character, it is also suggested that the radical cations of these molecules might be responsible for features in the well-known diffuse interstellar bands (DIBs).[3] However, the optical spectra of these cations have not been measured experimentally until recently. Here, we present the first optical spectrum of the 1-cyanoadamantane cation ($C_{11}H_{15}N^+$) and compare it to the recently reported spectrum of the adamantane radical cation.[4] These spectra were recorded in the gas phase at 5 K using a cryogenic 22-pole ion trap. The experimental results are compared to time-dependent DFT calculations for interpretation. Geometric changes due to Jahn-Teller distortion and the astrophysical implications of these ions will also be discussed.

[1] O. Guillois, et al., Astrophys. J., 521, L133 (2009).
[2] O. Pirali, et al., Astrophys. J., 661, 919 (2007).
[3] M. Steglich, et al., Astrophys. J., 729, 91 (2011).
[4] P. B. Crandall et al., ApJL, 900, L20 (2020).

Invited Talk SYLA 2.4 Mon 17:30 Audimax

A multifaceted approach to investigate the reactivity of PAHs under electrical discharge conditions — •Donatella Loru[1], Amanda L. Steber[1,2], Johannes M. M. Thunnissen[3], Daniël B. Rap[3], Alexander K. Lemmens[3,4], Anouk M. Rijs[5], and Melanie Schnell[1,6] — [1]Deutsches Elektronen-Synchrotron DESY, Notkestrasse 85, 22607 Hamburg, Germany — [2]Departamento de Química Física y Química Inorgánica, Facultad de Ciencias, Universidad de Valladolid, 47011 Valladolid, Spain — [3]Radboud University, Institute of Molecules and Materials, FELIX Laboratory, Toernooiveld 7c, 6525 ED, Nijmegen, The Netherlands. — [4]Van't Hoff Institute for Molecular Sciences, University of Amsterdam, Science Park 904, 1098 XH, Amsterdam, The Netherlands — [5]Division of BioAnalytical Chemistry, AIMMS Amsterdam Institute of Molecular and Life Sciences, Vrije Universiteit Amsterdam, De Boelelaan 1108, 1081 HV Amsterdam, The Netherlands — [6]Institute of Physical Chemistry, Christian-Albrechts-Universität zu Kiel, Max-Eyth-Straße 1, 24118 Kiel, Germany

Polycyclic aromatic hydrocarbons (PAHs) are a class of molecules whose presence in the interstellar medium (ISM) has been established via the aromatic infrared bands (AIBs), mid-IR emissions ($3 - 20\ \mu$m) detected in several interstellar objects. The ubiquitous nature of the AIBs suggests that PAHs are widely spread in the ISM and, as such, they are expected to play an important role in interstellar physics and chemistry. Despite their importance, little is known about the reactivity of PAHs under the harsh energetic conditions of the ISM. To explore the reactivity of PAHs under laboratory conditions, we coupled an electrical discharge nozzle with spectroscopic techniques. Under plasma conditions, PAHs are expected to undergo fragmentation processes and/or recombination chemistry. The species formed are then detected via their mass and their IR signature by IR-UV ion dip spectroscopy, and via their microwave signature by broadband rotational spectroscopy.

Here, we present our results obtained from the electrical discharge experiments on the PAHs naphthalene ($C_{10}H_8$) and phenanthrene ($C_{14}H_{10}$) with acetonitrile (CH_3CN). The different sensitivity of the two spectroscopic techniques revealed an interesting diversity in the resulting species from the electrical discharge experiments of the two investigated PAHs.

Invited Talk SYLA 2.5 Mon 18:00 Audimax

Exploring the Femtosecond Dynamics of Polycyclic Aromatic Hydrocarbons Using XUV FEL Pulses — •Jason Lee[1,2], Denis Tikhonov[1,3], Bastian Manschwetus[1], and Melanie Schnell[1,3] — [1]Deutsches Elektronen-Synchrotron DESY, Hamburg, Germany. — [2]The Chemistry Research Laboratory, University of Oxford, Oxford, United Kingdom. — [3]Institute of Physical Chemistry, Christian-Albrechts-Universität zu Kiel, Kiel, Germany.

Satellite infrared measurements show signatures of aromatic vibrations in practically every corner of the universe, attributed to polycyclic aromatic hydrocarbons (PAHs) in the interstellar medium (ISM). These PAHs account for up to 20% of carbon in space and have long been proposed as carriers of the Diffuse Interstellar Bands and Unidentified Infrared Bands.

Given their abundance, PAHs have been the subject of laboratory experiments for many decades, exploring their interaction with a wide range of photon energies. Our experiments utilise XUV pulses at 30.3 nm (40.9 eV) from the Free-Electron-Laser FLASH at DESY, Hamburg to replicate some of the harsh radiation of the ISM. The femtosecond laser pulses allow us to investigate the ultrafast relaxation and fragmentation of PAHs. Combining the ion time-of-flight data, ion imaging data and electron imaging data provides a detailed insight into the various molecular processes occurring after the initial photoionisation.