

## Symposium Molecules in Helium Droplets (SYHD)

jointly organised by  
the Molecular Physics Division (MO) and  
the Atomic Physics Division (A)

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With 4 invited talks, SYHD reports on helium considering dimers up to nano-sized droplets, the latter empty, singly doped with molecules, with clusters via multiple particle doping, and ionized droplets, addressing quantum features such as vortices, quantum halos and Efimov states. Thereby, techniques such as coulomb explosion imaging, coherent diffractive imaging with X-FEL pulses, messenger spectroscopy of ions, and mass selected ion spectroscopy are applied as well as time dependent helium density functional theory.

### Overview of Invited Talks and Sessions

(Lecture hall E415)

#### Invited Talks

SYHD 1.1	Wed	11:00–11:30	E415	<b>Structure and field-induced dynamics of small helium clusters</b> — •MAKSIM KUNITSKI, JAN KRUSE, QINGZE GUAN, DÖRTE BLUME, REINHARD DÖRNER
SYHD 1.2	Wed	11:30–12:00	E415	<b>Coherent Diffraction Imaging of isolated helium nanodroplets and their ultrafast dynamics</b> — •DANIELA RUPP
SYHD 1.3	Wed	12:00–12:30	E415	<b>Clustering dynamics in superfluid helium nanodroplets: A theoretical study</b> — •NADINE HALBERSTADT, ERNESTO GARCÍA ALFONSO, MARTÍ PI, MANUEL BARRANCO
SYHD 1.4	Wed	12:30–13:00	E415	<b>Messenger spectroscopy of molecular ions – Development of a new experimental setup</b> — •ELISABETH GRUBER

#### Sessions

SYHD 1.1–1.4	Wed	11:00–13:00	E415	<b>Molecules in Helium Droplets</b>
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## SYHD 1: Molecules in Helium Droplets

Time: Wednesday 11:00–13:00

Location: E415

**Invited Talk** SYHD 1.1 Wed 11:00 E415

**Structure and field-induced dynamics of small helium clusters** — ●MAKSIM KUNITSKI<sup>1</sup>, JAN KRUSE<sup>1</sup>, QINGZE GUAN<sup>2</sup>, DÖRTE BLUME<sup>2</sup>, and REINHARD DÖRNER<sup>1</sup> — <sup>1</sup>Institut für Kernphysik, Goethe-Universität Frankfurt am Main, Max-von-Laue-Straße 1, 60438 Frankfurt am Main, Germany — <sup>2</sup>Homer L. Dodge Department of Physics and Astronomy, University of Oklahoma, 440 W. Brooks St., Norman, OK 73019, USA

Small helium clusters are peculiar few body quantum systems. The helium dimer has a single weakly bound state of a huge spatial extent. About 80% of its probability distribution resides in the classically forbidden tunnelling region. This is why such objects are termed “quantum halos”. The helium trimer has two bound states, one of which is of Efimov nature. We utilize laser-triggered Coulomb explosion imaging for measuring spatial probability distributions of these quantum objects. Application of an additional laser pulse in a pump-probe manner allows us to observe the structural response dynamics of small helium clusters to a strong laser field on a picosecond time scale.

The results of our experimental approach on He<sub>2</sub>, He<sub>3</sub> and He<sub>4</sub> will be discussed.

**Invited Talk** SYHD 1.2 Wed 11:30 E415

**Coherent Diffraction Imaging of isolated helium nanodroplets and their ultrafast dynamics** — ●DANIELA RUPP — ETH Zurich

Isolated helium nanodroplets are used as ideal model systems for exploring light-matter interaction and provide fascinating possibilities to embed dopant atoms or molecules and study their arrangement and properties at ultracold temperatures. Via single-pulse single-particle coherent diffractive imaging (CDI) with the intense femtosecond pulses from short-wavelength free electron lasers (X-FELs) and high-harmonic generation (HHG) sources, it is possible to study single specimen in free flight. The elastically scattered photons form an interference pattern, encoding the particle’s structure and the light-induced dynamics during and after pulsed laser excitation. In this presentation, an overview on the young and thriving field of helium nanodroplets in intense short-wavelength pulses will be given and recent results on their ultrafast changes in the electronic and geometric structure will be discussed.

**Invited Talk** SYHD 1.3 Wed 12:00 E415

**Clustering dynamics in superfluid helium nanodroplets: A theoretical study** — ●NADINE HALBERSTADT<sup>1</sup>, ERNESTO GARCÍA ALFONSO<sup>1</sup>, MARTÍ PI<sup>2,3</sup>, and MANUEL BARRANCO<sup>2,3</sup> — <sup>1</sup>LCAR, CNRS and Université Toulouse 3, F-31062 Toulouse, France — <sup>2</sup>Departament FQA, Facultat de Física, Universitat de Barcelona, Barcelona, Spain — <sup>3</sup>Institute of Nanoscience and Nanotechnology

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In this work we study the collision of heliophilic atoms with a superfluid helium droplet, followed by their solvation and clustering. We use time-dependent Helium density functional theory (<sup>4</sup>He-TDDFT), which has proven to be the best compromise between accuracy and feasibility to study the stability and real time dynamics of doped helium droplets with a size comparable to experiments.

We also investigate the effect of the presence of a quantum vortex on the pickup and clustering process, in relation with the pioneering experiment by Vilesov’s group which used atom doping to visualize quantum vortices.

Our simulations reveal rather surprising final cluster configurations, very different from the gas phase ones. This is due to the fast cooling property associated to superfluidity, which quenches metastable configurations, and to the high density shell building around each dopant atom which can prevent dopant-dopant bond formation.

They also reproduce the attractivity of dopant atoms to the vortex lines, with a cluster building along them but in a final configuration very different from the gas phase one.

**Invited Talk** SYHD 1.4 Wed 12:30 E415

**Messenger spectroscopy of molecular ions – Development of a new experimental setup** — ●ELISABETH GRUBER — Institute of Ion Physics and Applied Physics, Universität Innsbruck, A-6020 Innsbruck, Austria

Helium nanodroplets (HNDs) provide an inert matrix with outstanding properties to isolate diverse molecular ions, to grow complexes and clusters at sub-Kelvin temperature and to study the latter spectroscopically. Here, we present a newly developed experimental setup, which allows the formation of mass-selected and helium-tagged molecular ions, perfectly suitable for messenger-spectroscopy, by using HNDs instead of the commonly used RF-multipole trap technique. The setup combines an in-house-assembled helium nanocluster source with a commercially available quadrupole time-of-flight mass spectrometer. In the first step, HNDs are highly ionized by electron impact and afterwards doped with the molecules of interest. A gentle shrinking of the helium matrix of the doped HNDs by collisions with helium gas delivers helium-tagged molecular ions, detached from the helium droplets due to Coulomb repulsion. A subsequent quadrupole mass filter allows the selection of a specific dopant-helium-complex, which is then analysed spectroscopically. In contrast to previous studies, where the absorption spectra are predominantly obtained from the precursor ion depletion, the new setup enables the detection of the photoproduct from virtually zero background signal. This enables high quality spectra even for weak absorption lines at reduced data acquisition times. Recent results obtained with the new setup will be presented.