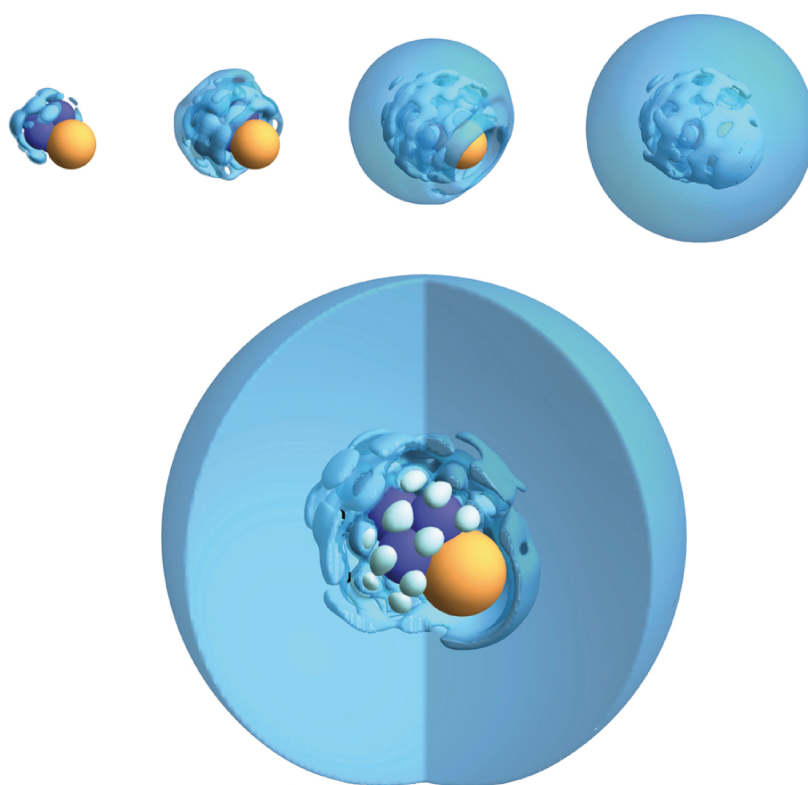


International Conference on  
**Quantum Fluid Clusters 2015**



June 7 - 11, 2015, Toulouse, France

**Scientific organisation**

Nadine Halberstadt, Marius Lewerenz, Alexandra Viel

**Local organisation**

Patricia Bordais, Sylvie Boukhari, Nadine Halberstadt

This is the 10th edition in a series of international conferences which was initiated in 1989 as an informal workshop in Trento to bring together researchers in the emerging field of quantum fluid clusters. With the spectacular expansion of this field of research the workshop has evolved into a broader biannual conference which now covers topics from fundamental physics to molecular physics, nanophysics, chemical physics and physical chemistry.

We are happy to host this exciting meeting for the first time in France and we thank all invited speakers and the authors of the oral and poster contributions to have made it possible to compile a diverse and very interesting program.

The 33 oral presentations are organised in 9 sessions which are dedicated to

- Finite Size Superfluidity
- Nanoparticle Formation
- Magnetism and Solvation
- Nanodroplet Ionization
- Photoexcitation and Spectroscopy
- Spectroscopy
- Time-Resolved Processes
- Dynamics: Theory and Simulation
- Reactivity

Generous support from a long list of sponsors is gratefully acknowledged. Their generosity made it possible not only to organise this event without a registration fee but also to provide financial support to a certain number of participants. Special thanks go to Europhysics Letters for sponsoring a poster award to encourage young scientists.

Organising this event would not have been possible without the help of the people at Université Paul Sabatier. We hope that you will enjoy not only the science but also the beautiful town of Toulouse.

Last but not least a very special contribution to this community comes from the City of Toulouse, which will award the 'Médaille d'Or de la Ville de Toulouse' to Jan Peter Toennies in recognition of his pioneering contributions to this field and many others and as a co-founder and long time supporter of this conference series.

Bienvenue à Toulouse!

Nadine Halberstadt, Marius Lewerenz, and Alexandra Viel



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## The Many Fascinating Quantum Effects of Helium

J. Peter Toennies

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Helium is the smallest of all atoms and the only atom for which no chemistry is known. Although very rare on earth it is the second most abundant element (after hydrogen) in the universe. The very weak forces between the light bosonic  $^4\text{He}$  atoms explains why it is the only substance that remains liquid down to the lowest temperatures but also why it exhibits many remarkable quantum effects.

The most spectacular is the *superfluidity* of the liquid below 2.27 K. The dramatic story behind this discovery started in 1908 when the Leiden physicist Heike Kamerlingh-Onnes won the race to liquify helium. Thirty years later Jack Allen and Don Miesener in Cambridge and Pyotr Kapitsa in far away Moscow not quite independently, but simultaneously, reported convincing evidence that the strange behaviour of the liquid observed since 1908 marked the transition of the liquid to a new state of matter called “superfluidity”. It took another forty years before the discovery was recognized by the Nobel committee when they gave the prize to Kapitsa. Already in 1938 Fritz London speculated about the possible role of a new type of quantum “condensation” proposed by Bose and Einstein in 1924 for explaining the strange new phenomenon. Surprisingly since then and even today a completely satisfactory first principles theory of superfluidity is still not available. In 1969 Andreev and Lifshitz proposed that even the solid could become a superfluid. The first experimental evidence reported in 2004 was considered definitive until it was questioned in 2012 and today the search is still going on.

The ultra-weak bond between He atoms also leads to unexpected quantum effects in gas phase interactions which were first observed in free jet expansions in 1977. The unusually sharp velocity distributions of  $< 1\%$  lead to the realization that the atom-atom cross section, at  $T \rightarrow 0$  K was an extraordinary  $259,000 \text{ \AA}^2$  making it the largest cross section for scattering of ground state atoms. Subsequently the average bond distance of the dimer was measured by matter-wave-diffraction to be  $52 \text{ \AA}$  making it by far the largest ground state molecule. The He trimer is an even more exotic molecule. In 1970 Efimov predicted that a zero-energy (barely) bound trimer, could have an extremely vastly extended excited quantum state which after a long search was finally confirmed in this month (May 2015) and found to have an extension of more than  $300 \text{ \AA}$ !

At this meeting we are concerned with the remarkable dynamical behaviour of chromophore molecules which, when embedded in very cold (0.38 K) superfluid nanodroplets consisting of only hundreds of atoms, behave as if they were in vacuum. Similar effects have since been found in clusters with only a dozen atoms. These experiments challenge the long standing view that superfluidity is a macroscopic phenomenon and raise new challenges for a satisfactory first principles theory.

In the final section of my lecture I will briefly describe my favorite of the many exciting current helium nanodroplet experiments. I will also mention some history of the QFC meetings and analyse the development of the nanodroplet field in recent years.

# Shapes and Vorticities of Superfluid Helium Nanodroplets

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Helium nanodroplets have long been considered ideal model systems to explore quantum hydrodynamics in self-contained, isolated superfluids. However, the dynamic properties of individual droplets, such as vorticity, remained beyond the reach of experimentalists. Here, we investigate the rotation of single, superfluid  $^4\text{He}$  droplets ( $D=200\text{-}2000$  nm) via single-shot femtosecond X-ray coherent diffractive imaging.<sup>1</sup> The angular velocities,  $\omega$ , of the droplets span a range from vanishing to those close to the disintegration limit. The droplets exhibit large centrifugal deformations but retain axially symmetric shapes at  $\omega$  well beyond the stability range of viscous classical droplets. The formation of quantum vortex lattices inside the droplets is confirmed by observing characteristic Bragg patterns from Xe clusters trapped in the vortex cores. The vortex densities are up to five orders of magnitude larger than observed in bulk liquid He, accessing a previously unattainable regime of quantum rotation. The images of the vortex filaments in the droplets with small vorticity were obtained from the diffraction images via phase retrieval techniques. This collaborative work was performed at Linac Coherent Light Source, the free electron laser within SLAC National Accelerator Laboratory.

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# Quantum dynamics of confined molecules

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We will provide an account of the available methodologies designed to simulate the quantum dynamics of confined molecules. We are interested in providing an interpretation of spectroscopic experiments that probe to rotational, vibrational, and translational motions of molecules trapped in quantum fluids and nano-cavities. Of particular interest is the behaviour of molecular rotors as probes of superfluidity in helium and hydrogen clusters and droplets [1,2,3]. The quantum nature of hydrogen molecules trapped in clathrate hydrates and the dynamics of water molecules trapped in matrices such as C60 cages will also be considered. For the latter case, issues such as nuclear spin conversion will be addressed. The formal and computational tools that enable these investigations range from exact basis set methods for few degrees of freedom systems, to path integral based techniques for larger system sizes. Both finite temperature and ground state path integral methods will be described. Observables such as effective rotational constants, vibrational shifts, the superfluid fraction, and quantum entanglement entropies can be obtained from such techniques and will help shed light on the nature of confined quantum systems.

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## Vortex arrays in nanoscopic superfluid helium droplets

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We have studied the appearance of vortex arrays in a rotating He-4 nanodroplet at zero temperature within density functional theory. Our results are compared with those for classical rotating fluid drops used to analyze the shape and vorticity in recent experiments [L.F. Gomez et al., Science 345, 906 (2014)], where vortices have been directly seen in superfluid droplets for the first time. In agreement with the experiments, we find that the shape of the droplet changes from pseudo-spheroid, oblate-like for a small number of vortices to a peculiar "wheel-like" shape, delimited by nearly flat upper and lower surfaces, when the number of vortices is large. Also in agreement with the experiments, we find that the droplet remains stable well above the stability limit predicted by classical theories for axially-symmetric shapes.

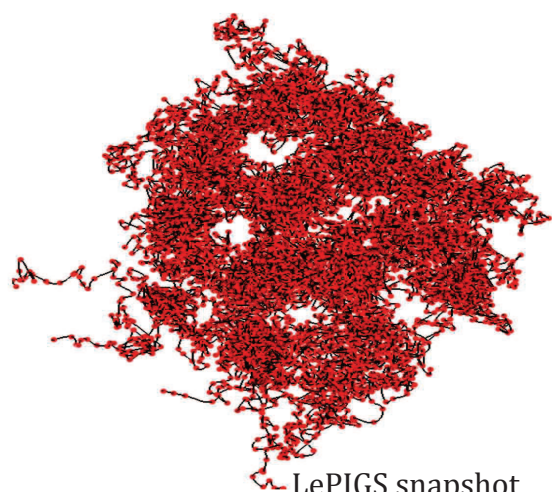
## Quantum molecular dynamics study of ground state properties of parahydrogen clusters and their bosonic isotopologues

Matthew Schmidt, Stephen Constable, Nabil Faruk and P.-N. Roy

We examine properties of parahydrogen clusters and their bosonic isotopologues (ortho-deuterium and para-tritium) in the zero temperature limit using a quantum molecular dynamics method known as the Langevin equation Path Integral Ground State (LePIGS) [1,2]. We examine cluster sizes in the range of  $N=4 - 40$ . A number of questions of interest include the quantification of the “liquid-like” or “solid-like” nature of parahydrogen clusters and the correct shape of the chemical potential. We compare our results to DMC [3] and PIGS-MC (a Monte Carlo version of PIGS) [4], which give conflicting results.

We also construct an accurate 1D pair potential for each isotopologue in the ground vibrational state using a 6D potential from Hinde [5]. We perform LePIGS simulations and calculate, using perturbation theory [6], the vibrational frequency shift of parahydrogen clusters from  $N=4-40$  and for ortho-deuterium and para-tritium from  $N= 4-10$  [7]. We compare our results to those calculated using other potential energy surfaces in our simulations and also to experiment. By accurately calculating vibrational frequency shifts, we may be able to assist experimentalists in correct assignment of cluster sizes.

Future work involves calculating the dissociation energy of the water dimer and extending this work to hydrogen clusters in hydrate clathrates.



LePIGS snapshot of  $N=33$  para-tritium cluster

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# Helium-mediated growth: from clusters to nanoparticles and nanowires

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# AN AB-INITIO-MOTIVATED SCHEME FOR VAN-DER-WAALS ADSORBATE-SURFACE INTERACTIONS: APPLICATION TO TIME-RESOLVED SIMULATIONS OF SOFT, $^4\text{He}$ -DROPLET-ASSISTED, DEPOSITION ON SOLID SURFACES

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The ultra-cold  $^4\text{He}$  droplet-assisted synthesis and deposition of embedded metal nanoparticles (NPs) on solid surfaces, originally proposed by Vilsesov's group [1], attracts nowadays strong attention [1-5]. This is due to both the exciting fundamental physics revealed via the technique, including earlier traces of quantum vorticity in superfluid  $^4\text{He}$  droplets [1,5], and the potential applications in nanoscience and nanotechnology [2,3]. For instance, it can be exploited to induce the formation of ultrathin wires of metal NPs [1,5] with special special electro-, magneto-optical, and catalytic properties. To control the metal NPs film formation, it is important to understand the basic mechanism regulating the  $^4\text{He}$  droplet-mediated deposition of the metal NPs and their subsequent diffusion and aggregation. Of course, this process is much influenced by the specific He-metal, He-surface, and surface-metal interactions so that their accurate descriptions is a prerequisite for realistic first-principles simulations. The first focus of this talk will be on an ab-initio-grounded scheme to van der Waals-dominated adsorbate-surface interactions [6-9,11], with application to the He-surface [7,8,11] and silver-surface systems [9]. Next, we will discuss the dispersionless and dispersion-accounting (time-dependent) density functional and molecular dynamics simulations of  $^4\text{He}$  droplets at impact with graphene and  $\text{TiO}_2(110)$  surfaces [8,10,11]. Finally, theoretical evidences for the  $^4\text{He}$  droplet-assisted-sticking of an embedded metal atom at very low landing energies will be presented [11] (see figure).

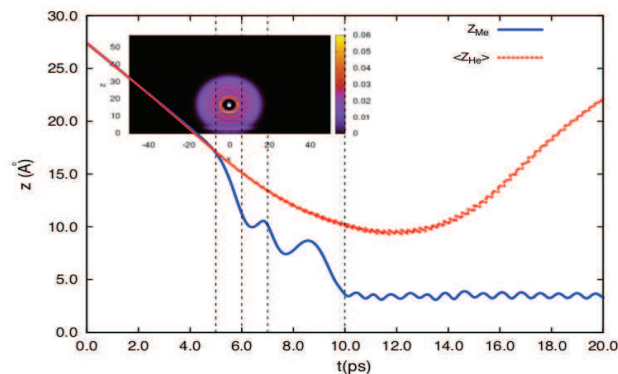


Figure illustrating the  $^4\text{He}$ -droplet-assisted sticking of a metal atom to a solid surface at very low landing energy. Red and blue lines indicate the position (distance to the surface) of the metal atom and the  $^4\text{He}$  droplet mass-center as a function of time, respectively.

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## The mechanism of Nanowire Production in Quantized Vortices of Superfluid Helium

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In 2009 the quantized vortices were proposed to be used as the universal 1D template for the growth of thin filaments by the condensation of impurities, in particular metals, embedded into HeII [1]. Starting from 2010 the nanowires of many metals and their alloys were grown in this way, the atoms and small clusters were created in HeII by laser ablation of submersed metallic targets ([2] and references there).

Recently the nanowires were detected as well under metal atoms capture into the cold liquid helium submicron droplets ([3] and references there). The quantized vortices were no doubt the templates inducing the growth of condensation product in one direction there too.

The diameters of the nanowires, their structure and morphology of nanowires formed by condensation of metals in superfluid bulk helium, have been studied in sufficient detail. The electrical conductivities of nanowires and individual nanowires were measured in a wide temperature range for normal and superconducting metals, the mechanism of nanowire nucleation and growth in the core of quantized vortices, explaining their structure and thickness, has been proposed and justified.

Nanowires formed in cold helium droplets are still described only qualitatively. Thus the question still exists whether these nanowires are similar to that produced by laser ablation in bulk HeII or not. Despite the reasons for nanowire production in these systems are very close, the answer to this question is not obvious. Firstly, the temperature in helium droplets (0.37K) is much lower than in that in the bulk experiments (1.5 - 2.0 K). On the one hand, it facilitates the capture of atoms into the core of vortex, but on the other hand hinders the motion of trapped atoms and clusters along the vortex core. Secondly, no interaction of vortices with each other exists in the droplets.

This problem will be analyzed in the present report by using the extensive data from experiments performed in the bulk superfluid helium.

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# From quantized vortices to nanowires: new experiments in superfluid helium droplets

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Although still in its infancy, superfluid helium droplets have now emerged as a uniquely powerful tool for the fabrication of nanoparticles and nanowires, and a number of metallic nanoparticles have been synthesized in this way, such as Ag,[1-3] Au,[1] and Ni[1] nanoparticles. In particular, the sequential addition of dopants to helium droplets eases to form core-shell nanoparticles, for example, Ag/Si nanoparticles.

At Leicester we have carried out a series of experiments on large superfluid helium droplets, inside which quantized vortices are now identified as an intrinsic feature. Starting with the addition of Ag atoms to the droplets, we have seen long chains of spherical nanoparticles on the TEM images.[4] As spherical nanoparticles do not possess anisotropy, the guiding force to align these particles can only be provided by quantized vortices in superfluid helium. Therefore, this experiment provided firm evidence for quantized vortices in large helium droplets.Following this idea we have added several other materials to the droplets including Au, Si, Cr and Ni,[5] and have exploited quantized vortices as a tool to fabricate 1D nanostructures.Finally, we report a striking observation on quantized vortices in superfluid helium droplets by TEM imaging of Ag nanoparticles deposited on a surface. The TEM images have shown scattered small particles at the vicinity of the vortex lines, suggesting multiply quantized vortices have been generated, which can survive in the vacuum for at least a few milliseconds.

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# Solvation dynamics of metallic dopants in helium droplets

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# Quantum Monte Carlo studies of atomic and molecular clusters embedded in He nanodroplets

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## A thermodynamic model to predict the formation, sizes and mobilities of electron clusters and positively charged ('snowball') clusters in all fluid phases of helium

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*Van der Waals-type thermodynamic state equations are developed for description of mobilities of electron and ion impurities in supercritical, normal liquid and superfluid helium. The state equations allow to calculate an effective size of the impurities, i.e. the 'hydrodynamic' radius. The mobilities derived from the impurity sizes and the known dynamic viscosities match experimental data with unsurpassed accuracy. This model can be extended to low densities where Knudsen numbers are greater than one by reformulating the Millikan-Cunningham factor to account for size changes. With the ability to predict hydrodynamic radii in different thermodynamic regimes and over large pressure and temperature ranges we are able to simulate growth of clusters formed by the attractive interaction between impurities and solvent atoms or molecules. In the supercritical regime of helium we observe distinct regimes of growth and subsequent compression with further increasing pressure. The compressibility derived from the change of hydrodynamic radius with pressure allowed us to identify a liquid-like phase for positively-charged 'snowball' clusters in normal liquid and supercritical helium for lower pressures. For higher pressures, the 'snowballs' solidify.*

Electrons and positive ions are microscopic probes frequently used to explore transport, diffusion and quantum properties of liquid helium. Electrons introduced into liquid helium localise and build clusters with ground state helium atoms due to attraction. Inside these electron-helium clusters there are large cavities with radii up to 20 Å (at 4.2 K and 1 bar), depending on the pressure. The formation of the void results from the repulsive interaction between ground state helium atoms and electrons at short range caused by the Pauli principle and the much longer ranged van der Waals-like attraction. Positive ions in liquid helium behave the opposite way. At short range, electrostrictive forces between the positive charge and the surrounding polarised helium atoms dominate and attract the helium atoms towards the positive centre. As a consequence a dense shell of helium is built, which is why the term 'Atkins-snowball' is often used.

Information of the size and structure of the electron and ion clusters in helium is difficult to obtain in a direct fashion. Thanks to the charged nature of electrons and ions, the measurement of their mobility is relatively straightforward when using electric fields. The mobility is related to a hydrodynamic radius,  $r$ , via the well known Stokes law for spherical objects flowing within a fluid of viscosity,  $\eta$ ,

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$$\mu_{Stokes} = \frac{e}{6\pi r\eta} \quad (1)$$

While the deduction of the radius requires no other knowledge than the viscosity of the fluid,  $\eta$ , a number of restrictions nevertheless apply. In particular at low densities where the Knudsen number is greater than one the more general Millikan-Cunningham equation must be used instead of eq. (1),

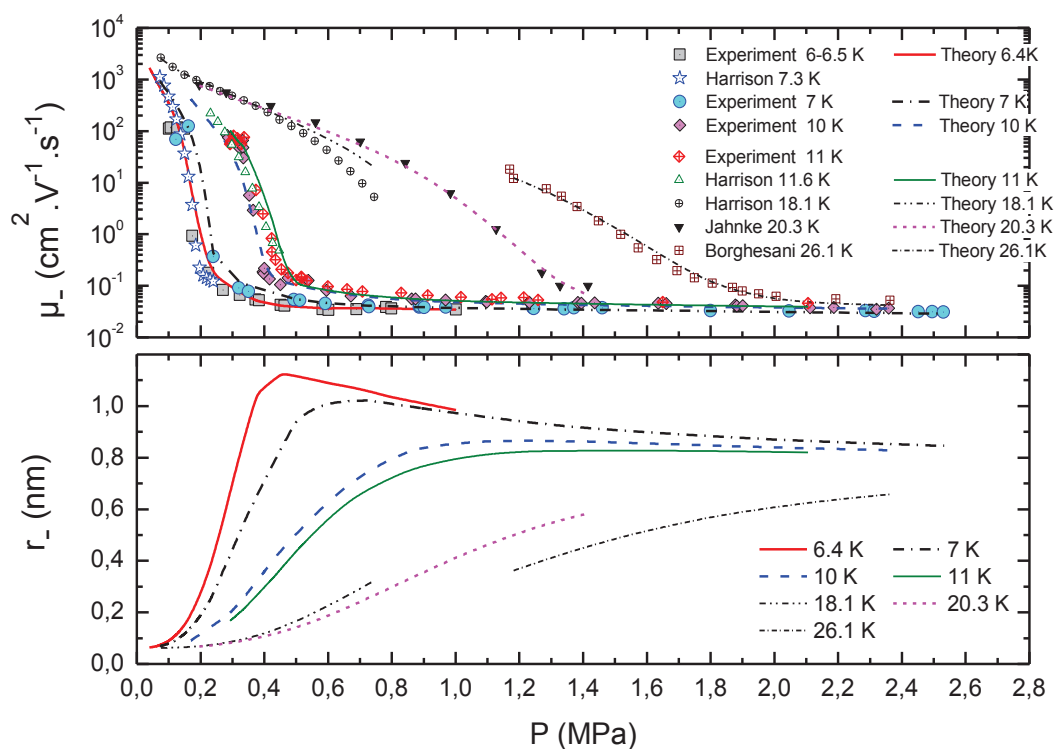
$$\mu_{MC} = \mu_{Stokes} (1 + \varphi) \quad (2)$$

where  $\mu_{MC}$  is the Millikan-Cunningham mobility and  $\varphi$  the Millikan-Cunningham factor.

Finding a coherent description of ion and electron mobility in different density regions, especially the crossover from gas kinetic to Stokes flow is a challenge. An implicit challenge is that ion and electron clusters in helium are expected to change their structure depending on the density.

We develop thermodynamic state equations for electrons and He ions in helium and employ the free volume model to derive the hydrodynamic radius. In general terms, the free volume model relates the size of foreign objects, i.e. solute molecules within a fluid to the size occupied by a free volume unit cell,  $(V-b)/N$ , using as the first approximation a simple power law between the two. The state equations of  $P$ ,  $V$  and  $T$  include two parameters which are calibrated using experimentally determined mobilities using one isotherm in the normal liquid phase, and one in the supercritical or the gaseous phase.

An example of this approach can be seen in Figure 1. The experimentally determined mobility of electrons is shown over a large range of temperatures and pressures. Both, the hydrodynamic radius and the mobility are nicely reproduced using the thermodynamic state equation approach [1]. Particularly, for sufficiently low temperatures in the supercritical phase one can observe a condensation region of the electron clusters and a compression region. Positively charged ions in supercritical helium behave in a very similar manner (not shown).



**Figure 1: Electron mobility and hydrodynamic radius in the supercritical region of helium. Experimental data of mobilities are taken from Harrison *et al.* (1973), Jahnke *et al.* (1971), Borghesani *et al.* (2002) and ourselves.**

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# Electron ionization of (doped) He nanodroplets: anions, cations and multiply charged species

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Low-mass cations and anions ( $m < 50$  kDa) formed upon electron bombardment of pristine and doped He nanodroplets (HNDs) were investigated utilizing high-resolution mass spectrometry. With an electrostatic sector-field massive charged HNDs containing up to  $10^7$  He ions were also analyzed. The formation of various charged or excited species inside the HNDs were identified, i.e., electron bubbles, metastable  $\text{He}^*$ ,  $\text{He}^{*-}$  [1] and  $\text{He}^+$ . For large droplets and/or high electron currents often two or more of these species can be formed inside one HND and interact with one another. Coulomb repulsion between charged species with the same polarity is expected to lead to the ejection of one of them from the HND. Ion-induced dipole interactions between  $\text{He}^*$  and  $\text{He}^{*-}$  lead to the formation of  $\text{He}^+$  at electron energies below 20 eV, which is below the ionization energy of a free He atom [2]. This surprisingly low threshold energy for the formation of  $\text{He}^+$  from HNDs was already reported in 1991 by Buchenau et al. [3]. The interaction of the primary charged and/or excited species with dopants inside or on the surface of HNDs provides a wide range of product ions, both positively and negatively charged. The formation of dications from doped HNDs can be explained via sequential Penning ionization [4] or the collision of  $\text{He}^{*-}$  with a positively charged dopant.  $\text{He}^{*-}$  is highly mobile [1] and provides, besides a loosely bound electron ( $\text{He}^*$  has an electron affinity of 77 meV), a potential energy of 19.7 eV, enough to positively ionize all dopants but Ne. Efficient formation of fullerene (cluster) dianions from HNDs doped with  $\text{C}_{60}$  and  $\text{C}_{70}$  has been observed and has been assigned to a concerted double electron transfer from  $\text{He}^{*-}$  [5]. Chemical reactions in heterogeneous dopant clusters driven by the charged and electronically excited species listed above have been studied. For mixed hydrogen-oxygen clusters only the formation of very few water molecules has been observed. However, a dopant cluster consisting of metal atoms and halogen- or oxygen-containing molecules is transformed into a salt nanocrystal with almost perfect stoichiometry [6]. Excess reactants of any kind are simply evaporated and do not show up in the mass spectra.

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## Clusters in Nanodroplets exposed to intense sculptured laser pulses

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The helium nanodroplet pick-up technique is used to generate small particles within an ultracold environment. Upon excitation with intense laser pulses the system transforms into a transient state called a nanoplasma. The process is highly nonlinear and show aspects of correlation and collective behavior. In particular the Mie resonance can be used to generate energetic and highly charged ion<sup>1</sup>. With the preparation of clusters in helium nanodroplets a core shell system is produced which allows to study the onset of collective excitations as function of size or the plasmonic responses of impurity and environment. We use sculptured ultrashort laser pulses to analyze and control the dynamics on a femtosecond timescale. The results of optimization experiments will be compared to molecular dynamics simulations<sup>2</sup>.

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# Trapping of ions, charged clusters, and microparticles under a free surface of superfluid helium and a mesoscopic network formation

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He<sup>+</sup> ions (snowballs) and free electrons (electron bubbles) can be trapped under a free surface of superfluid He by applying a suitable static electric field. We develop a new experimental technique for trapping positive ions of various metals under free He surface for their subsequent laser-spectroscopic studies. Our aim is to produce a two-dimensional pool of spin-polarized Ba<sup>+</sup> ions and to investigate their depolarization due to the interaction with the surface elementary excitations [1].

Ions, electrically charged metal clusters and microparticles are produced by laser ablation in superfluid <sup>4</sup>He and move upwards in a vertical static electric field. They become trapped under the free surface of superfluid He and are observed via light scattering (see Fig.1a). In a vertical electric field of 0.5 – 2.0 kV/cm, the charged liquid surface experiences various static and dynamic perturbations that are visualized using a fast video camera. In particular, we observe lifting of He surface, formation of static hillocks (see Fig.1a) and running waves. Under the electric field exceeding some threshold, the charges escape from the surface by forming jets or geysers of liquid He shooting upwards on a time scale of 1 ms and having a diameter of  $\approx 0.05$  mm. Similar behaviour is observed with positive and negative charges, under the electric field directed up and down, respectively.

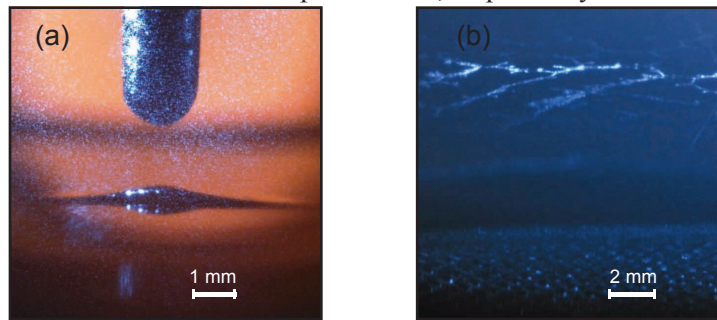


Fig1. (a) Charged liquid He surface in electric field; (b) metallic filaments trapped at liquid He surface

Very large number of trapped particles is generated also with the ablation target positioned in He gas above the liquid He surface and with the electric field directed downwards. At the surface, the trapped particles coalesce into larger structures: filaments with very large aspect ratios and mesoscopic networks (see Fig.1b). Since all the particles reaching the surface possess positive electrical charge, they must experience repulsive Coulomb forces that would prevent their coalescence. One possibility is that some positively charged particles first penetrate into the liquid and reach the bottom (negative) electrode. There they exchange their charge to negative and are driven back to the liquid surface by the electric field. Such particles could be stabilized under the liquid surface due to the surface tension and act as seeds for the coalescence of further positively charged particles arriving from above.

Formation of long filaments (nanowires) has been demonstrated earlier in several experiments involving laser ablation of metals in bulk superfluid He (see, *e.g.*, [2]) and doped He nanodroplets [3]. It was suggested that the filaments are formed via the coalescence of nanoparticles and/or single atoms trapped at the cores of quantized vortices. Considering the highly branched structure of the networks observed in the present experiment and their tendency to grow at a free surface rather than in the bulk liquid, we suggest that the formation process is dominated by the electrostatic interaction between charged micro- and nanoparticles and by their interaction with the He surface, rather than by trapping at quantized vortices.

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# Size Distributions of Helium Nanodroplets: An Ongoing Mystery

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Mass spectra of pure helium nanodroplets (HND) generally show small cluster ions with a maximum size of about 1000 helium atoms [1]. By deflecting the charged clusters in the electric field of a plate condensator in contrast, log normal distributions of these clusters have been reported [2], with huge droplets containing up to a few million helium atoms, depending on the temperature in the expansion region and the stagnation pressure of the helium gas.

Huge cluster ions can not be detected by mass spectrometric means because their high kinetic energy prevents them from reaching the detector region. At the same time it is still a mystery how the above mentioned low-mass cluster ions are ejected from large droplets as vaporization of a HND containing two-million He atoms requires more than 1 keV. The same problem goes for doped HNDs, where mass spectra reveal mostly "bare" ions [3] with the exception of helium attachment in a few cases [4].

For pure HNDs ejection mechanisms for  $He_2^+$  have been proposed [5], but the exact nature of this process still lies in the dark. Furthermore most ions are strongly heliophilic and thus prefer positions inside the HNDs which is in conflict to the preferred formation of low-mass and bare dopant ions.

In our experiments HNDs were ionized in a Nier-type ion source and were size selected using an electrostatic sector-field. We were able to detect log-normal-distributed charged HNDs containing up to  $10^7$  helium atoms and thus confirming the findings of [2]. By increasing the electron energy and/or the electron current the log-normal distribution was changed dramatically. When the ionizing voltage exceeds the double ionization threshold ( $49.2\text{ eV} = 2 \times 24.6\text{ eV}$ ), another peak in the distribution appears at a smaller droplet size, indicating Coulomb breakup

of the clusters due to multiple ionization. By further increasing the voltage/current this peak continues to grow and completely dominates the distribution in the end, leading to very narrow size distributions compared to those obtained at lower energies/currents (see fig.1).

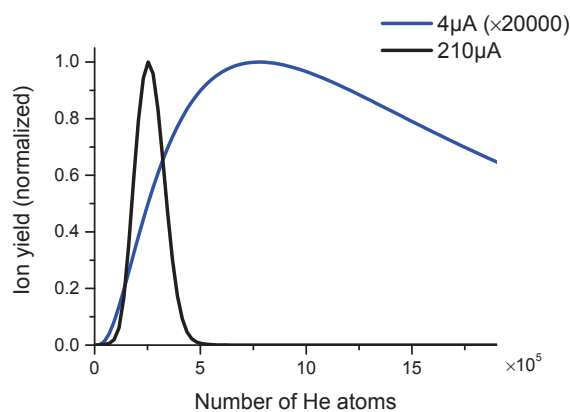


Figure 1. Electron Energy =200 eV, T= 8.5 K

Currently we perform experiments to unravel the nature of the Coulomb explosion of multiply charged HNDs.

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# **Spectroscopy and dynamics of atoms in and on helium droplets below and above the ionization limit**

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The spectroscopy and dynamics of excited atoms and ions in helium nanodroplets have been investigated by a variety of spectroscopic techniques such as time-of-flight mass-spectrometry, velocity map ion imaging, and photoelectron and ZEKE spectroscopy. Here I will give an overview of the various processes that have been observed and presentsome ofthe general trends that have emerged from these studies.

## Rotational dynamics of molecules in He droplets induced and probed by laser pulses

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Laser induced alignment, the method to confine the principal axes of molecules along axes fixed in the laboratory frame, is now used in a range of applications in physics and chemistry. With a few exceptions all studies have focused on isolated molecules in the gas phase.

Extension of alignment to molecules in He droplets is of interest for at least two reasons. First, alignment of molecules inside He droplets should enable studies or exploitation of the orientational dependence of molecular interactions as well as for extraction of molecular frame information in the presence of a dissipative environment. Second, the ability to control the degree of alignment implies being able to control the rotational angular momentum and coherence of the molecules inside the droplet. Some or all of the angular momentum and coherence may be transferred to the surrounding He atoms and as such open possibilities for laser-controlled excitation of collective angular momentum states, possibly quantized vortices [1].

The talk will present our experimental findings of laser-induced alignment of molecules in He droplets conducted both with femtosecond [2-3] and nanosecond pulses [4].

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# Dissociation and Recombination Dynamics of Chromium Molecules in Helium Nanodroplets

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The photoinduced dynamics of chromium dimers and small chromium clusters isolated in helium nanodroplets have been investigated with resonant multiphoton ionization (REMPI) spectroscopy and mass sensitive ion detection [1]. Electronic excitation of ground state ( $X^1\Sigma_g^+$ )  $\text{Cr}_2$  molecules to an excited state ( $A^1\Sigma_u^+$ ) induces dissociation into a ground state ( $a^7S_3$ ) and a metastable ( $a^5S_2$ ) atom. We find that the ground state atom remains solvated inside the droplet, while the metastable atom migrates to the droplet surface without desorbing from the droplet. This interpretation is based on the spectral REMPI signatures of both dissociation products and supported by density functional theory simulations [2]. We also find that REMPI of the surface located  $a^5S_2$  atom induces recombination of the two Cr atoms, which is evidenced by  $\text{Cr}_2^+$  detection. For small Cr clusters ( $\text{Cr}_{3,4}$ ), our results indicate that they may be composed of chromium dimers that exhibit the same dissociation and recombination behavior.

This demonstration of quantum state specific dopant locations, photoinduced transitions between solvated and surface locations, and the stable separation of two dopants open a possibility for the investigation of photoinduced chemistry in helium nanodroplets.

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## Spectroscopy in superfluid helium nanodroplets

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Helium droplets serve as cryogenic host system for atoms, molecules and clusters to study structures of molecules and van der Waals clusters and also low temperature chemistry. Unique properties of helium droplets are based on the superfluid phase and have been revealed by high resolution spectroscopy in the micro wave, the infra red, and the UVvis spectral range. [1]

Our initial approach to utilizing helium droplets as cryogenic reactor for the study of photochemical processes revealed surprising perturbations induced by the superfluid helium environment. [2] It drew our attention to the helium environment. Molecular spectra recorded in helium droplets always carry information on both the dopant species and the helium droplet. [3] In order to interpret the molecular contribution it is important to understand the helium induced part of spectra. We feed this enterprise entirely from the experimental side. Systematic studies as well as detailed study mostly by means of electronic spectroscopy reveal information on the dopant to helium interaction and, thus, provide insight into microsolvation of molecules in superfluid helium droplet [4]. We will critically discuss experimental details which have been interpreted according to the empirical model of microsolvation in helium droplets. It assumes a complex consisting of the dopant species surrounded by a non-superfluid helium solvation layer which rotates freely inside the superfluid helium droplet.

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# Quasi-free and hindered rotation of single molecules in liquid helium and helium clusters

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The observation of free rotation of single molecules in superfluid helium droplets has caused considerable interest [1]. To understand the specific role of superfluidity experiments were performed with normal liquid <sup>3</sup>He droplets and mixed <sup>3</sup>He-<sup>4</sup>He droplets which, depending on the concentrations, provided a superfluid shell of variable thickness around an embedded molecule. These experiments showed that the width of rotational lines of OCS depended on the thickness of the superfluid <sup>4</sup>He layer in the <sup>3</sup>He droplets. 60 atoms of <sup>4</sup>He were needed to produce sharp lines, indicating free rotation. Droplets with less <sup>4</sup>He and pure <sup>3</sup>He droplets showed strongly broadened features with little resemblance of a rotational spectrum [2].

In another series of experiment the evolution of the effective moment of inertia with cluster size was investigated. These experiments showed the same trend for many different molecules: with addition of a few <sup>4</sup>He atoms the effective moment of inertia increased. Further addition brought this increase to a halt and even further addition reversed the trend, showing molecules whose rotation was largely decoupled from the rest of the cluster. The size range in which this happened was between two and fifteen helium atoms, much less than the 60 atoms needed to establish sharp lines [3, 4].

To resolve this apparent contradiction, to elucidate the nature of the line widths and their relation to the effective moment of inertia we have conducted experiments in bulk helium, using helium excimers as single-molecule probes. The excimers are short-lived and emit fluorescence, allowing the investigation of their rotational states using spectroscopy. To generate excimers in sufficient concentration and over a large pressure and temperature range a corona discharge in point-plane geometry was employed, allowing to control the interaction between molecule and environment by variation of pressure at thermal equilibrium.

Spectra of electronically excited <sup>4</sup>He were recorded between 3.8 K and 16 K and 0.3 bar and 5 bar. In the entire temperature range the spectra showed for low pressures well-resolved rotational lines. With increasing pressure the lines broaden and merge into a continuum, resembling the envelope of a rotational spectrum at pressures between 3 and 5 bar. The lines were also found to shift in frequency depending on the pressure and temperature. Changes in the rotational B-constant were not observed within our spectral resolution.

Line shifts and broadening were investigated carefully by fitting the rotational lines to Lorentzian functions. Below the critical temperature of helium the analysis of increase of pressure along isotherms showed distinct line shifts before the gas-liquid phase boundary was crossed, indicating the formation of helium clusters around the excimers and a stronger interaction between excimers and helium than helium and helium. These line shifts were observed for Q-transitions but not for P-transitions, indicating that two different types of environment exist at our experimental conditions.

We attribute the Q-lines to excimers that are caged in 7 Å-diameter voids. The sharp lines are attributed to excimers in larger gas bubbles that are not in thermal equilibrium with the environ-

ment and may display higher local temperatures. Reducing the temperature of the helium was found to reduce the concentration of these 'hot excimers'. The implication of our findings for probing the superfluid phase of helium will be discussed.

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# Rotational Superfluidity in Small Helium Droplets

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The first minimum appearing in molecular rotational constants as a function of helium droplet size has been previously associated with the onset of superfluidity in these finite systems. We investigate this relationship by bosonic density functional theory calculations of classical molecular rotors (OCS, N<sub>2</sub>O, CO and HCN) interacting with the surrounding helium. The calculated rotational constants are in fair agreement with the existing experimental data, demonstrating the applicability of the theoretical model. By inspecting the spatial evolution of the global phase and density, the increase in the rotational constant after the first minimum is shown to correlate with continuous coverage of the molecule by helium and appearance of angular phase coherence rather than completion of the first solvent shell. We assign the observed phenomenon to quantum phase transition between a localized state and one-dimensional superfluid, which represents the onset of rotational superfluidity in small helium droplets.



# Crystallization of Undercooled Quantum Liquids: *para*-H<sub>2</sub>, *ortho*-D<sub>2</sub>, and their mixtures with Ne

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We have extended the experimental production of liquid microjets (filaments) in vacuum, first realized by Faubel et al. [1], to studying the crystallization of undercooled quantum liquids: *para*-hydrogen (*p*H<sub>2</sub>), *ortho*-deuterium (*o*D<sub>2</sub>), and their mixtures with Ne. These highly collimated filaments, less than 10 microns in diameter, are an ideal medium to produce undercooled liquid samples and to investigate the homogeneous solidification process, free from wall effects [2]. The filaments exit from cryogenic capillary nozzles into vacuum, to cool down fast by surface evaporation, although with a temperature gradient across the jet due to their finite size radius and thermal conductivity. The filaments are monitored by laser shadowgraphy, and analyzed by means of high performance Raman spectroscopy [3], revealing their structure and temperature. The high spatial resolution of Raman spectroscopy allows observing in situ the structural changes of the liquid microjets, with a time resolution of ~10 ns. The filaments of pure *p*H<sub>2</sub> can be cooled down to 9 K (normal melting point at 13.8 K), before eventually solidifying at a crystal growth rate of ~33 cm/s [4]. Filaments of diluted mixtures of *o*D<sub>2</sub> and *p*H<sub>2</sub> show a significant slowdown in the crystallization kinetics with respect to the pure substances [5], which is more pronounced in their mixtures with small amounts of Ne impurity. In the case of the *p*H<sub>2</sub>/*o*D<sub>2</sub> mixtures, the observed slowdown can be interpreted in terms of a different effective size, caused by a purely mass-induced difference in zero-point quantum delocalization. This effect is confirmed in the mixtures with Ne, with a much larger quantum effective size ratio.

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# Time-resolved and XUV spectroscopy of helium nanodroplets

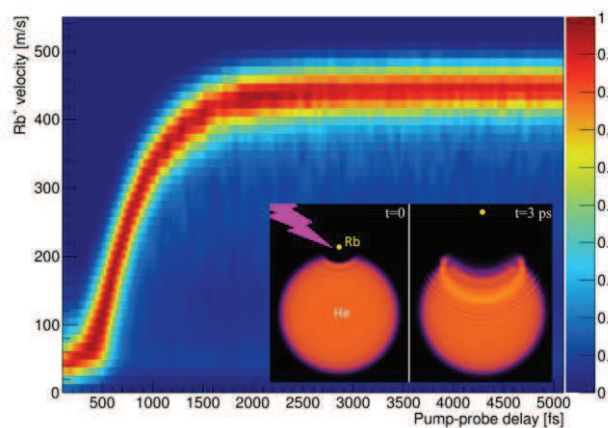
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**Synopsis** The ultrafast dynamics of pure and doped helium nanodroplets is studied using VIS and XUV femto-second pump-probe spectroscopy in combination with ion and electron imaging detection.

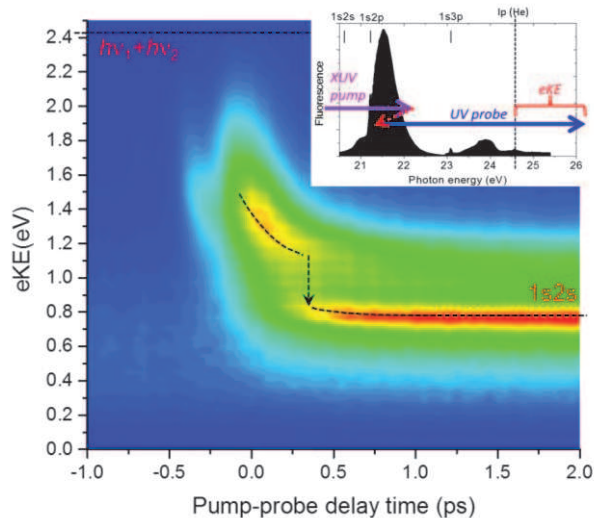
Helium (He) nanodroplets currently attract considerable interest mainly for two reasons. 1) Due to their quantum fluid nature He nanodroplets feature extraordinary properties such as microscopic superfluidity. 2) He nanodroplets can be considered as a nearly ideal matrix for spectroscopy of embedded molecules and aggregates due to their transparency for light up to the extreme ultraviolet (XUV) spectral range, and their ability to efficiently aggregate and cool embedded species.

However, the short-time dynamics of He nanodroplets is still largely unexplored. Recently, strong perturbations of the rotational motion of embedded molecules induced by the He droplet environment was observed for the case of impulsive excitation [1]. In this contribution we study the ultrafast response to laser excitation of a prototype system consisting of an alkali metal atom residing at the surface of He nanodroplets. Using femtosecond pump-probe spectroscopy in combination with ion and electron imaging detection we follow in real-time the desorption of the excited atom off the He droplet surface (see Fig. 1) as well as the formation of alkali-He exciplex molecules.



**Figure 1.** Time-evolution of the velocity of an excited Rb atom ejected off the surface of a He nanodroplet. Inset: TDDFT simulation [2].

Upon irradiation of He droplets with XUV light at  $h\nu \geq 21$  eV, where He droplets are strongly absorbing, a complex photo dynamics is initiated by the excitation or ionization of He atoms inside the droplets [3]. The dynamic of relaxation, fragmentation, as well as indirect ionization processes are studied using synchrotron and free-electron-laser (Fermi@Elettra) radiation. In particular, the real-time dynamics of pure He nanodroplets excited by tunable femtosecond XUV-pulses is studied in a pump-probe experiment. The time-resolved photoelectron spectra reveal ultrafast intra- as well as interband relaxation dynamics, see Fig. 2.



**Figure 2.** Pump-probe delay dependent photoelectron spectrum of pure He nanodroplets measured by XUV (22.2eV)/UV (4.8eV) fs pump-probe R2PI.

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**Erreur ! Source du renvoi introuvable.** E-mail: [mudrich@physik.uni-freiburg.de](mailto:mudrich@physik.uni-freiburg.de)

## Dynamics in helium nanodroplets studied by ultrafast XUV and X-ray techniques

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Our work focuses on a deeper understanding of the electronic structure and, in particular, the coupled electronic and nuclear dynamics that occur in excited and/or ionized helium droplets. Two complementary projects are discussed. In a series of femtosecond high-harmonic generation based experiments, an XUV pump pulse excites droplets containing  $N_{\text{He}} \sim 2 \times 10^6$  He atoms up to  $\sim 24$  eV above the ground state. Excited droplets and relaxation products are ionized by a femtosecond infrared (IR) or UV probe pulse. Transient electronic configurations and the release of energy into atomic motion are probed by recording pump-probe delay dependent photoelectron angular and energy distributions as well as mass-resolved ion momenta. Distinctly different dynamics are observed with IR and UV probe photons. While IR probing provides a detailed picture of the ejection of Rydberg atoms and molecules, UV probing gives direct access to interband relaxation dynamics and trajectories that are associated with the formation of covalently bound molecular complexes inside the droplet. The results are discussed in the context of surface vs. bulk processes and connections to ab-initio molecular dynamics simulations are presented. A second project employs a pair of intense femtosecond X-ray pulses ( $\sim 840$  eV,  $\sim 10^{16}$  -  $10^{17}$  W/cm<sup>2</sup>) from the Linac Coherent Light Source (LCLS) to interrogate the coupled flow of charge and energy in highly ionized pure and doped He droplets. For each pulse pair, an ion mass spectrum and an X-ray diffraction pattern associated with a single He droplet are recorded. The results are analyzed as a function of the delay between the two X-ray pulses. Doping large ( $N_{\text{He}} \sim 10^6$  -  $10^{10}$ ) helium droplets with  $\sim 1\%$  of Xe atoms leads to dramatically different dynamic trends compared to both pure helium droplets and pure Xe clusters. The observations are discussed in the context of possible charge- and energy-transfer mechanisms between the host matrix and the embedded clusters.

## Dynamics of processes involving atoms or molecules and superfluid $^4\text{He}$ nanodroplets

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Although the study of chemical reactions in superfluid  $^4\text{He}$  nanodroplets (ND) is a very interesting topic and has been the subject of some experimental efforts, until now little attention has been paid to this problem from a theoretical perspective [1]. Here, we will present the most recent developments achieved in our laboratory on the quantum dynamics of a selection of relevant chemical and physical processes involving one or two impurities and a superfluid  $^4\text{He}$  ND ( $T \approx 0.37$  K). Thus, e.g., to investigate the photodissociation dynamics of diatomic molecules in  $^4\text{He}$  ND, a hybrid quantum mechanical theoretical approach that combines time dependent DFT (helium) and QM dynamics (molecule) has been developed [2]. This method has been applied to the study the  $\text{Cl}_2$  photodissociation arising from the  $B \leftarrow X$  transition, considering  $\text{Cl}_2(v=0, X) @ (^4\text{He})_N$  doped nanodroplets of different sizes ( $N=50-500$ ) [2]. In addition to the analysis of this interesting system, where the initial Cl-Cl chemical bond is broken, we will also present a rather wide set of results comprising, e.g., the  $(^4\text{He})_N$  relaxation process occurring in the after photodissociation time period, and other relevant processes (atomic pick up and chemical reaction). In all cases, the dynamic properties and microscopic mechanism have been examined considering a wide set of initial conditions. We hope that these results will encourage the experimentalists to investigate the dynamics of this kind of systems.

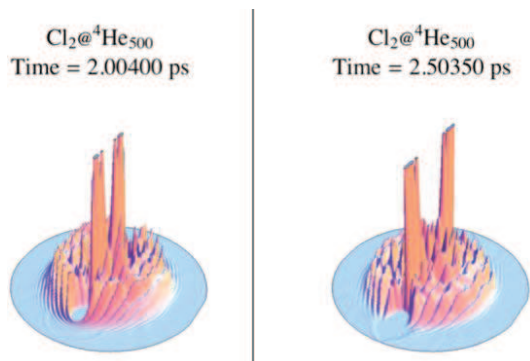


Fig. 1. Snapshots showing the helium density ( $xz$  plane), during the final of the  $[\text{Cl}_2(B) @ (^4\text{He})_{500}]^*$  photodissociation. The  $z$  axis corresponds to the Cl-Cl bond axis.

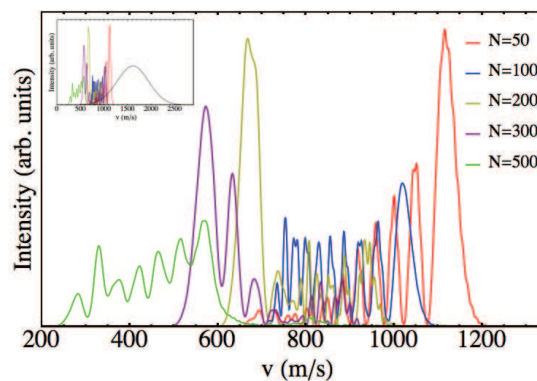


Fig. 2. Velocity distributions of the Cl photofragment for different ND sizes. The gas phase result (black line) is given in the small figure.

**Acknowledgments:** This work has been supported by the Spanish Ministry of Science and Innovation (projects refs. CTQ2011-27857-C02-01 and FIS2011-28617-C02-01). Thanks are also given to the Autonomous Government of Catalonia (A. V. predoctoral fellowship and projects refs. 2009SGR 17, 2014SGR 25 and XRQTC).

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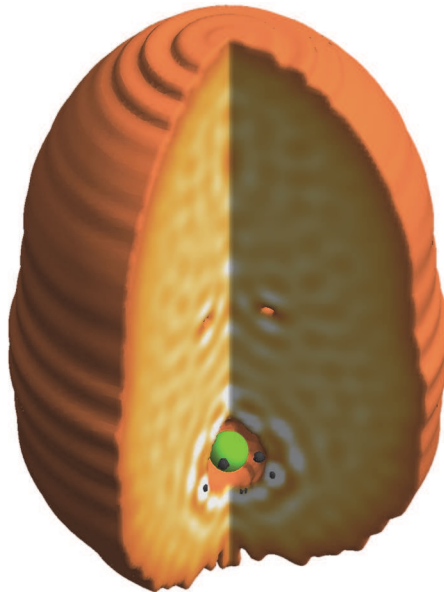
## Real-time dynamics of impurities in helium nano droplets

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I will present results of a series of simulations [1-7] obtained within TDDFT on the real time dynamics of neutral atoms and cations immersed in helium nano droplets, comparing them with experiments whenever possible. Potential applications and limitations of the method will be discussed.

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Dynamic evolution of a Ba<sup>+</sup> cation (green) immersed in a <sup>4</sup>He<sub>1000</sub> droplet. On top of it, near the center of the droplet, it can be seen a vortex ring nucleated during the sinking of the cation produced by photoionization of a neutral Ba atom at the surface of the droplet.

## Nonadiabatic Alignment of Molecules in Helium-4 and Superfluidity around Clusters

Robert E. Zillich

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Pump-Probe spectroscopy has been recently used for alignment of molecules in superfluid helium-4 droplets. In gas phase, a short non-adiabatic pulse leads to a coherent revival pattern of the molecule orientation. In  $4\text{He}$ , the dynamics is profoundly altered (e.g. the revivals are missing), hence the response to the helium environment to this highly nonlinear kick of the molecule cannot be understood in the familiar terms of superfluidity. We present our approach to solve the coupled dynamics of molecule and helium and show some early results. In a second part, we take the step from molecules to clusters in helium-4 and discuss the solvation of Mg and Na clusters. Using path integral Monte Carlo simulations, we demonstrate that the superfluid response around a larger dopant like a Mg11 cluster differs from the response around a small dopant: the decoupling of dopant rotation and helium motion can set in before the dopant is fully solvated. We calculate the helium solvation density and energy of various Mg and Na clusters, based on simple models for the interaction. As expected from experiments, small Na clusters form dimples on the He droplet surface rather than being surrounded by He, although the limit of large He droplets as encountered in experiments is out of reach in our simulations.



# Toward fast and efficient propagators for path integral simulations of hydrogen, water and more complex clusters

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More and more demanding applications of the path integral Monte Carlo method are needed to understand structural properties of clusters made of somehow complex molecules. They are also needed to study the spectra of trapped and embedded species, like organic molecules, in cryogenic environment (helium or hydrogen clusters or droplets), as well as the response properties of quantum fluid clusters to various kinds of probes. To meet this demand, different methods have been proposed. Some are dedicated to reduce the number of degrees of freedom and concentrate on those appropriate for the time scale of the problem, giving rise to curved manifold dynamics [1,2,3]. Others are designed to accelerate the convergence rate with respect to the time step by efficient numerical schemes [4]. During this talk, we will present new approximate propagators and energy estimators [5,6] that are accurate, requiring low memory during the computation, and practical for implementation.

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## **Motion of dopants in He-nanodroplets: Challenges and opportunities of a spacial confinement for cluster growth and cold chemistry**

Andreas W. Hauser, Johann Pototschnig, Martin Ratschek, Wolfgang E. Ernst

Helium nanodroplets can be considered as spatially confined nano-labs for studies of elementary chemical reactions or the formation of nanoparticles. We combine molecular dynamics simulations with bosonic He-density functional theory to describe the behavior of dopants in their superfluid confinement after pickup. Particle growth will be discussed for the example of the coinage metals Cu, Ag and Au.[1] As a template for studies of He-hindered chemical reactions, we refer to our work on Rb- and Xe-doped small droplets.[2] The fact that molecules with diffuse electron distributions, e.g. alkali metal atoms, prefer to reside on the surface, while others sink into the droplet center, might allow for the arrangement of pre-reactive setups, which could be triggered by photoexcitation. A simple model for electronic excitation of dopants in helium droplets is presented for selected states of the chromium atom.[3,4]

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# *Chemical Reactions in Helium Droplets: Past Successes and Future Prospects*

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The helium nanodroplet isolation method has been applied by several research groups to the study of chemical reactions, such as ion-molecule reactions, aggregation-induced transformations, and bond-forming barrierless reactions. Of course, the droplet method has also provided a versatile platform to study weakly bound 'entrance-channel' complexes, stabilized behind small barriers above the asymptotic energy of a bimolecular reaction. One of the goals of our field is to exploit helium droplets to study the photo-induced chemistry of these highly metastable species, which potentially can provide significant insight into issues such as bright state-reaction coordinate coupling and the mode-specificity of product branching ratios when multiple outcomes exist.

This talk will review some of the past successes and future prospects for studying chemistry in helium droplets. Infrared laser Stark and Zeeman spectroscopy has been applied in our group to several hydroxyl radical containing entrance-channel complexes. Recent results on these fascinating systems will be presented. These spectra highlight an already well-known, yet still amazing, truth about helium droplets: the rovibrational spectra of weakly bound open-shell systems can be satisfactorily simulated by assuming a gas-phase effective Hamiltonian.

# Understanding the ionic liquid $[\text{NC}_{4111}][\text{NTf}_2]$ from individual building blocks: An IR-spectroscopic study

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## Abstract:

This study explores at the molecular level the interactions underlying the IR spectra of the ionic liquid  $[\text{NC}_{4111}][\text{NTf}_2]$  and its deuterated isotope  $[\text{d}_9\text{-NC}_{4111}][\text{NTf}_2]$  by first isolating the spectra of charged ionic building blocks using mass-selective CIVP spectroscopy and then following the evolution of these bands upon sequential assembly of the ionic constituents. The spectra of the (1,1) and (2,2) neutral ion pairs are recorded using superfluid helium droplets as well as a solid neon matrix, while those of the larger charged aggregates are again obtained with CIVP. In general, the cluster spectra are similar to that of the bulk, with the (2,2) system displaying the closest resemblance. Analysis of the polarization-dependent band intensities of the neutral ion pairs in liquid droplets as a function of external electric field yields dipole moments of the neutral aggregates. This information allows a coarse assessment of the packing structure of the neutral pairs to be antiparallel at 0.37 K, in contrast to the parallel arrangement found for the assembly of small, high-dipole neutral molecules with large rotational constants (e.g., HCN).

# Ultra-low-temperature reactions of C( $^3P_0$ ) inside helium droplets

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Carbon atoms and ions are extremely abundant in the interstellar medium (ISM) [1]. The temperature of the ISM could be rather low. The lowest temperature found in space is 1 K [2]. In addition, it has been shown that there is no energy barrier for the reaction between atomic carbon and a broad variety of hydrocarbon molecules [3]. Therefore, the chemical inertness of molecules towards reaction with atomic carbon is an important property for them to reach a predominant abundance in the ISM.

We have initiated a project to study the reactivity of carbon atoms at ultra-low temperature. A technique to produce gas-phase carbon atoms with low kinetic energy suitable for the pick up by helium droplets has been developed [4]. It allows us to study the reactions of carbon atoms with acetylene, benzene [5], naphthalene, anthracene, and coronene molecules in liquid helium droplets at  $T = 0.37$  K. Mass spectrometry has been applied to characterize the products of the chemical reactions. A calorimetric technique was used to evaluate the amount of energy released in the reaction. The geometries and vibrational frequencies of the stationary points of the reactants, intermediates, and possible product isomers were determined using the B3LYP hybrid functional and the 6-311+G(d,p) basis set. Our results suggest that PAH molecules with aromatic rings, which have at least 4 common carbon atoms, could be resistant towards the reaction with carbon atoms. This may result in a predominant abundance of such PAH molecules in the ISM.

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# Conclusions

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## Poster presentations

# Nonadiabatic alignment and photoelectron spectroscopy of molecules in helium droplets

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We show that the alignment methods, based on moderately intense nonresonant laser pulses, can be transferred from isolated molecules in the gas phase to molecules embedded in superfluid Helium droplets. We show that nonadiabatic alignment inside helium droplets depends on the molecule studied, and the alignment dynamics are very different from the dynamics of isolated molecules.[1] It is shown that multiple short pulses, synchronized appropriately, can enhance the degree of alignment and provide information about the alignment dynamics. Our studies uses 1,4-diiodobenzene and I<sub>2</sub> as examples, but other molecules were studied as well.

In a second project, photoelectrons generated from 2-photon ionization of naphthalene molecules inside helium droplets were recorded and compared to studies on isolated molecules. The kinetic energy distributions of photoelectrons from molecules inside helium droplets deviate from the gas phase results. The motivation for the studies is to explore if photoelectron kinetic energy distributions from molecules in He droplets is an experimental observable that can provide useful information for femtosecond time-resolved studies of chemical reaction dynamics

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# Investigations of SF<sub>6</sub> with the Free Electron Laser FELIX

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Recently, we installed a helium nanodroplet apparatus for use with the Free Electron Laser for Infrared eXperiments (FELIX) at the Radboud University Nijmegen. The goal is to dope the nanodroplets with neutral dopants and in particular to study microsolvation processes over a broad spectral region.

As first experiment we studied the strong absorber SF<sub>6</sub> in the frequency range from 600 to 1000 cm<sup>-1</sup>. This spectral coverage allowed us to observe the two vibrational transitions at 615 cm<sup>-1</sup> and 945 cm<sup>-1</sup> of SF<sub>6</sub>. Using the highest power level (30 to 40 mJ) provided by FELIX the strongest band showed a broad absorption with a maximum depletion of 30% indicating a good overlap between helium droplet beam and the light source. At lower concentrations the line narrows. Similar results were obtained for the lower frequency mode at 615 cm<sup>-1</sup>. Effects of the laser power on the fragmentation pattern of SF<sub>6</sub> in He nanodroplets will be discussed.

# Physical and Chemical Properties of Thin Nanowires Grown in Superfluid Helium

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# **Ion and XUV emission from argon microdroplets exposed by intense laser pulses**

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Liquid jets are attractive targets for laser-generated plasma investigations. It gives a great opportunity to study properties of warm dense matter, as well as they are interesting as possible candidates for soft-Xray light sources. In the present study we investigate the process of ionization, heating and emission of XUV-radiation from liquid argon microdroplets, irradiated by ultra-short intense NIR laser pulses. The XUV emission spectra are recorded by home-build flat-field XUV spectrometer. The kinetic energies of the ions emitted from the droplets are simultaneously measured by field-free time-of-flight spectrometers located in laser propagation and counter-propagation directions. First results show a strong asymmetry. Ions with higher recoil energy are emitted predominately in the direction opposite to the laser propagation. In the XUV-spectra various atomic transitions can be identified which allows to determine the charge state of ions and plasma properties. The impact of the laser pulse parameters will be discussed.

# Seeded Multi-electron Ionization of Xenon Doped Helium Droplets

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# Dissociation and Recombination Dynamics of Chromium Molecules in Helium Nanodroplets

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The photoinduced dynamics of chromium dimers and small chromium clusters isolated in helium nanodroplets have been investigated with resonant multiphoton ionization (REMPI) spectroscopy and mass sensitive ion detection [1]. Electronic excitation of ground state ( $X^1\Sigma_g^+$ )  $\text{Cr}_2$  molecules to an excited state ( $A^1\Sigma_u^+$ ) induces dissociation into a ground state ( $a^7S_3$ ) and a metastable ( $a^5S_2$ ) atom. We find that the ground state atom remains solvated inside the droplet, while the metastable atom migrates to the droplet surface without desorbing from the droplet. This interpretation is based on the spectral REMPI signatures of both dissociation products and supported by density functional theory simulations [2]. We also find that REMPI of the surface located  $a^5S_2$  atom induces recombination of the two Cr atoms, which is evidenced by  $\text{Cr}_2^+$  detection. For small Cr clusters ( $\text{Cr}_{3,4}$ ), our results indicate that they may be composed of chromium dimers that exhibit the same dissociation and recombination behavior.

This demonstration of quantum state specific dopant locations, photoinduced transitions between solvated and surface locations, and the stable separation of two dopants open a possibility for the investigation of photoinduced chemistry in helium nanodroplets.

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# Resonant scattering from single He nanodroplets in intense XUV laser pulses

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# Dynamics of photo-excited Ba<sup>+</sup> cations in helium nanodroplets

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Within TDDFT, we have addressed the dynamics of Ba<sup>+</sup> cations in helium nanodroplets. The absorption spectra from S to P and D states, as well as the emission spectra from P to S and D states of the cation are discussed. The appearance of exciplexes is discussed and the dynamics of the excited Ba<sup>+</sup> cation in the P state has been investigated.

# Trapping of ions, charged clusters, and microparticles under a free surface of superfluid helium and a mesoscopic network formation

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He<sup>+</sup> ions (snowballs) and free electrons (electron bubbles) can be trapped under a free surface of superfluid He by applying a suitable static electric field. We develop a new experimental technique for trapping positive ions of various metals under free He surface for their subsequent laser-spectroscopic studies. Our aim is to produce a two-dimensional pool of spin-polarized Ba<sup>+</sup> ions and to investigate their depolarization due to the interaction with the surface elementary excitations [1].

Ions, electrically charged metal clusters and microparticles are produced by laser ablation in superfluid <sup>4</sup>He and move upwards in a vertical static electric field. They become trapped under the free surface of superfluid He and are observed via light scattering (see Fig.1a). In a vertical electric field of 0.5 – 2.0 kV/cm, the charged liquid surface experiences various static and dynamic perturbations that are visualized using a fast video camera. In particular, we observe lifting of He surface, formation of static hillocks (see Fig.1a) and running waves. Under the electric field exceeding some threshold, the charges escape from the surface by forming jets or geysers of liquid He shooting upwards on a time scale of 1 ms and having a diameter of  $\approx 0.05$  mm. Similar behaviour is observed with positive and negative charges, under the electric field directed up and down, respectively.

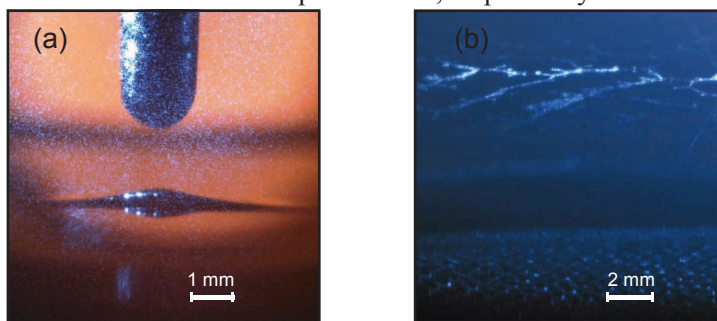


Fig1. (a) Charged liquid He surface in electric field; (b) metallic filaments trapped at liquid He surface

Very large number of trapped particles is generated also with the ablation target positioned in He gas above the liquid He surface and with the electric field directed downwards. At the surface, the trapped particles coalesce into larger structures: filaments with very large aspect ratios and mesoscopic networks (see Fig.1b). Since all the particles reaching the surface possess positive electrical charge, they must experience repulsive Coulomb forces that would prevent their coalescence. One possibility is that some positively charged particles first penetrate into the liquid and reach the bottom (negative) electrode. There they exchange their charge to negative and are driven back to the liquid surface by the electric field. Such particles could be stabilized under the liquid surface due to the surface tension and act as seeds for the coalescence of further positively charged particles arriving from above.

Formation of long filaments (nanowires) has been demonstrated earlier in several experiments involving laser ablation of metals in bulk superfluid He (see, *e.g.*, [2]) and doped He nanodroplets [3]. It was suggested that the filaments are formed via the coalescence of nanoparticles and/or single atoms trapped at the cores of quantized vortices. Considering the highly branched structure of the networks observed in the present experiment and their tendency to grow at a free surface rather than in the bulk liquid, we suggest that the formation process is dominated by the electrostatic interaction between charged micro- and nanoparticles and by their interaction with the He surface, rather than by trapping at quantized vortices.

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# Size Distributions of Helium Nanodroplets: An Ongoing Mystery

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Mass spectra of pure helium nanodroplets (HND) generally show small cluster ions with a maximum size of about 1000 helium atoms [1]. By deflecting the charged clusters in the electric field of a plate condensator in contrast, log normal distributions of these clusters have been reported [2], with huge droplets containing up to a few million helium atoms, depending on the temperature in the expansion region and the stagnation pressure of the helium gas.

Huge cluster ions can not be detected by mass spectrometric means because their high kinetic energy prevents them from reaching the detector region. At the same time it is still a mystery how the above mentioned low-mass cluster ions are ejected from large droplets as vaporization of a HND containing two-million He atoms requires more than 1 keV. The same problem goes for doped HNDs, where mass spectra reveal mostly "bare" ions [3] with the exception of helium attachment in a few cases [4].

For pure HNDs ejection mechanisms for  $He_2^+$  have been proposed [5], but the exact nature of this process still lies in the dark. Furthermore most ions are strongly heliophilic and thus prefer positions inside the HNDs which is in conflict to the preferred formation of low-mass and bare dopant ions.

In our experiments HNDs were ionized in a Nier-type ion source and were size selected using an electrostatic sector-field. We were able to detect log-normal-distributed charged HNDs containing up to  $10^7$  helium atoms and thus confirming the findings of [2]. By increasing the electron energy and/or the electron current the log-normal distribution was changed dramatically. When the ionizing voltage exceeds the double ionization threshold ( $49.2\text{ eV} = 2 \times 24.6\text{ eV}$ ), another peak in the distribution appears at a smaller droplet size, indicating Coulomb breakup

of the clusters due to multiple ionization. By further increasing the voltage/current this peak continues to grow and completely dominates the distribution in the end, leading to very narrow size distributions compared to those obtained at lower energies/currents (see fig.1).

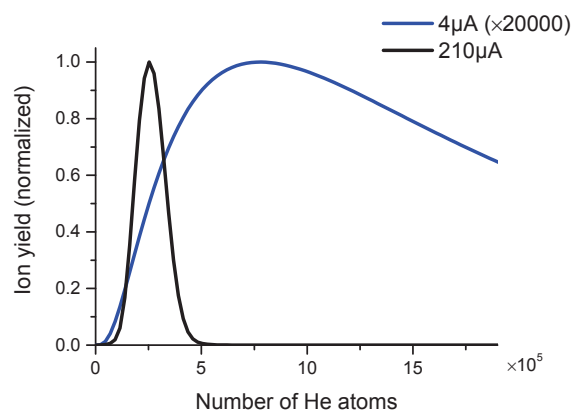


Figure 1. Electron Energy =200 eV, T= 8.5 K

Currently we perform experiments to unravel the nature of the Coulomb explosion of multiply charged HNDs.

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# Superradiance of organic molecules on neon clusters surfaces

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## **LASER INDUCED ALIGNMENT OF CS<sub>2</sub> MOLECULES SOLVATED INSIDE HELIUM DROPLETS**

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Laser-induced alignment of CS<sub>2</sub> molecules solvated inside liquid helium droplets has been investigated experimentally. The alignment is triggered by a 200 fs nonresonant, linearly polarized laser pulse and measured by timed Coulomb explosion with a delayed intense 30 fs laser pulse. The time resolved measurements reveal that for the first few picoseconds (ps) the rotational dynamics are almost as fast as that of isolated molecules. In particular, the degree of alignment reaches a maximum after just 1 ps compared to 0.7 ps for isolated molecules.

# Time resolved photoion/electron imaging spectroscopy of rubidium atoms attached to Helium nanodroplets

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This contribution will focus on the dynamics of rubidium (Rb) atoms attached to helium nanodroplets following upon excitation of the dopant to intermediately lying electronic states, i.e. the  $6P\Sigma$  and  $6P\Pi$  states in the pseudodiatomic model approach. This excitation, the first step in our femtosecond pump probe experiment, triggers the desorption of the Rb atom from the droplet surface. By subsequently ionizing the dopant and detecting the fragment ion masses, we observe  $\text{Rb}^+\text{He}_{n=0,1,2}$  ions at long and heavy cluster ions at short delay times, inferring submersion of the  $\text{Rb}^+$  ion into the droplet. This effect is caused by the attractive ion-droplet interaction and occurs on a timescale  $t \leq 2$  ps for all regarded excitation wavelengths.

To gain more insight into the involved dynamics, velocity map ion and electron images have been recorded for different pump probe delays.  $\text{Rb}^+$  and  $\text{RbHe}^+$  photofragments show an increasing kinetic energy and anisotropy leveling out at  $t \leq 10$  ps. Vice versa, photoelectron images show a decreasing energy asymptotically reaching the corresponding atomic transition. Additionally, relaxation into lower electronic states has been observed. The experimental results will be compared to a semiclassical model particularly focusing on the  $\text{RbHe}^+$  formation dynamics involving associative photoionization.

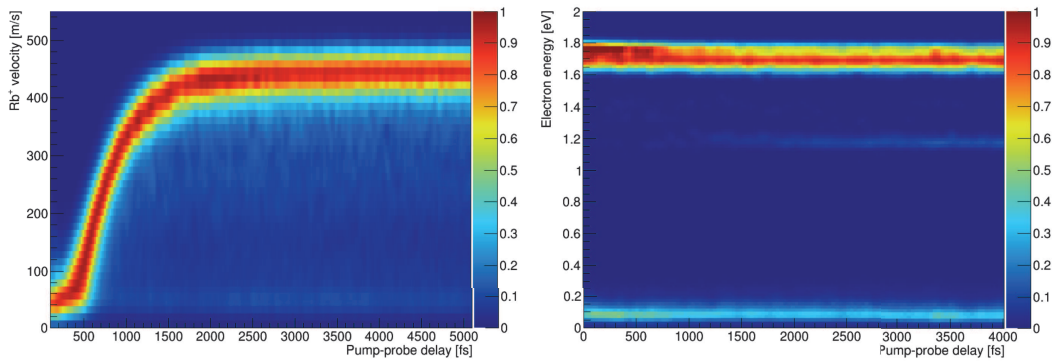


Figure 1: Left: Speed distribution of desorbing  $\text{Rb}^+$  ions at different pump probe delays for laser excitation to the pseudodiatomic  $6P\Sigma$  state. Right: Electron kinetic energy at different pump probe delays for laser excitation to the pseudodiatomic  $6P\Pi$  state.

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