

## MO 1: Electronic

Time: Monday 10:45–12:15

Location: H2

**Invited Talk**

MO 1.1 Mon 10:45 H2

**Long-range interactions between polar molecules and Rydberg atoms** — ●MARTIN ZEPPENFELD — MPI für Quantenoptik, Hans-Kopfermann Str. 1, 85748 Garching

Due to large dipole moments in polar molecules and huge dipole moments in Rydberg atoms, strong interactions between polar molecules and Rydberg atoms persist for separations beyond  $1\ \mu\text{m}$ . This provides exciting opportunities in quantum science, with applications such as cooling of internal or motional molecular degrees of freedom, nondestructive molecule detection, and quantum information processing.

In my talk, I will provide an overview of these opportunities and present my work on realizing such ideas experimentally. In particular, we have investigated Förster resonant energy transfer between molecules and Rydberg atoms at room temperature in the past, observing huge interaction cross sections and electric-field-controlled collisions. Currently we are setting up a new experiment to investigate interactions between cold molecules and Rydberg atoms, providing many new opportunities.

MO 1.2 Mon 11:15 H2

**Optical Properties of Gold Cations** — ●MARKO FÖRSTEL<sup>1</sup>, KAI POLLW<sup>1</sup>, TAARNA STUEMUND<sup>1</sup>, NIKITA KAVKA<sup>2</sup>, ROLAND MITRIC<sup>2</sup>, and OTTO DOPFER<sup>1</sup> — <sup>1</sup>Technische Universität Berlin, Berlin, Deutschland — <sup>2</sup>Universität Würzburg, Würzburg, Deutschland

The scientific interest in gold clusters and nanoparticles is very high, especially due to their manifold catalytic properties. In order to understand these in detail, it is necessary to have precise knowledge of the electronic structure of gold-containing systems. We probe the optical properties of small gold clusters in unprecedented detail using highly sensitive photodissociation spectroscopy and compare our results with various theoretical methods to provide a better understanding of these systems. In this talk we summarize our findings on  $Au_2^+$  [1,2],  $Au_3^+$  and  $Au_4^+$  [3,4] clusters.

[1] Förstel et al., *Angewandte Chemie Int. Ed.* 123 48, 2020

[2] Förstel et al., submitted to *Eur. J. Chem.*

[3] Förstel et al., *Angewandte Chemie Int. Ed.* 58 11, 2019

[4] Förstel et al., *Rev. Sci. Instr.* 88 12, 2017

MO 1.3 Mon 11:30 H2

**Exploration of the Optical Properties of Small Cationic Silicon Carbides: The Optical Spectrum of  $Si_4C_2^+$**  — ●ROBERT G. RADLOFF, MARKO FÖRSTEL, KAI POLLW, TAARNA STUEMUND, and OTTO DOPFER — Institut für Optik und Atomare Physik, Technische Universität Berlin, Berlin, Germany

It is known that a great number of molecules are present in space. Some of these molecules have already been identified, others remain to be discovered. In the environment of carbon stars like IRC+ 10216, where carbon is more abundant than oxygen, not all carbon is bound into CO and thus a variety of carbon bearing molecules exists in the

outer layers of these stars. We focus our research on silicon carbide aggregates. Observations show that small silicon carbide molecules like SiC, Si<sub>2</sub>C, SiC<sub>2</sub>, SiC<sub>3</sub> and SiC<sub>4</sub> are present in the circumstellar medium around the IRC+ 10216. Furthermore, its spectrum shows an emission feature around  $12\ \mu\text{m}$  that is tentatively attributed to silicon carbide dust grains.

In our study we are aiming to gain insight into the optical and structural properties and the photochemistry of small cationic silicon carbides as well as a better understanding of their role in astrochemistry and their influence on the formation of silicon carbide dust grains. We present the photofragmentation behavior of various cationic silicon carbides and the first optical spectrum of  $Si_4C_2^+$  recorded by means of photodissociation spectroscopy in the range of 208-330 nm [1].

[1] M. Förstel et al., *J. Mol. Spectrosc.*, 2021, 377, 111427

MO 1.4 Mon 11:45 H2

**Near-infrared spectrum of the first excited state of  $Au_2^+$**  — ●KAI MARIO POLLW, MARKO FÖRSTEL, TAARNA STUEMUND, and OTTO DOPFER — Technische Universität Berlin, Berlin, Deutschland

We recently observed and published the optical spectrum of the gold dimer cation which resembles the simple  $H_2^+$  molecule in its electronic configuration.[1] Due to the highly irregular spectral structure, multi-reference methods, spin-orbit coupling and relativistic corrections need to be taken into account to understand the PES of this seemingly simple dimer. By tagging with Ar we are able to investigate the otherwise not accessible 1st excited state in the near-infrared. Surprisingly, this state shows a regular vibronic structure that can be well reproduced by DFT calculations. In this talk we will present our experimental and computational results on the  $Au_2^+ - Ar$  system.

[1] Förstel et al., *Angewandte Chemie Int. Ed.* 123 48, 2020

MO 1.5 Mon 12:00 H2

**X-ray L-edge absorption spectroscopy on gas phase diatomic iron halide systems beyond the oxidation state** — ●MAX FLACH<sup>1,2</sup>, VICENTE ZAMUDIO-BAYER<sup>1</sup>, KONSTANTIN HIRSCH<sup>1</sup>, MARTIN TIMM<sup>1</sup>, OLESYA ABLYASOVA<sup>1,2</sup>, MAYARA DA SILVA SANTOS DA SILVA SANTOS<sup>1,2</sup>, MARKUS KUBIN KUBIN<sup>1</sup>, CHRISTINE BÜLOW<sup>2</sup>, BERND VON ISSENDORFF<sup>2</sup>, and TOBIAS LAU<sup>1,2</sup> — <sup>1</sup>Helmholtz-Zentrum, Berlin, Germany — <sup>2</sup>Albert-Ludwigs-Universität, Freiburg, Germany

Transition Metal L-edge spectroscopy is widely used to determine oxidation states of a wide range of samples, hence, an estimate of uncertainty contributions to assigned oxidation states from chemical shifts is of high importance. Here we use gas phase  $FeX^+$  ( $X=F, Cl, Br, I$ ) as a idealized model system to provide high resolution XAS spectra to quantify energy shifts of the Iron L<sub>3</sub>-edge and to study changes in electronic structure within the same oxidation state of Fe(II). Along with a change in line shape of the Iron L<sub>3</sub>-edge, we observe energy shifts of the intensity distributions median of the spectra along the series. The observed shifts hint towards a charge transfer to and from the halogen to the iron, involving orbitals of different symmetry.