

## MO 24: Poster: Experimental Techniques

Time: Thursday 17:00–19:00

Location: Tent C

MO 24.1 Thu 17:00 Tent C

**Ionic Liquids with Three-Valent Cations: Spectroscopic Studies Towards Their Use as Reaction Media** — ●MAX SCHADENFROH, CARINA ALLACHER, SELINA REIGL, MANUEL ROTHE, WERNER KUNZ, and PATRICK NÜRNBERGER — Institut für Physikalische und Theoretische Chemie, Universität Regensburg, 93040 Regensburg

Ionic liquids (ILs) are defined as salts with a melting point below 100 °C [1]. ILs are multifaceted systems with highly customizable physical and chemical properties, and thus offer a plethora of applications. While classical ILs are often toxic and environmentally harmful, a new class of ILs was introduced in 2018 [2], which better satisfies the principles of Green Chemistry. These compounds rely on the **CO**ncept of **M**elting **P**oint **L**owering due to **E**thoxylation (**COM**PLET). More recently, this concept could be extended to three-valent cations [3].

Here, we present spectroscopic studies of ionic liquids containing  $\text{Eu}^{3+}$ ,  $\text{Y}^{3+}$ , and  $\text{La}^{3+}$  cations. Combining excitation and emission spectroscopy, an energy transfer from the anionic ligand to the metal upon photoexcitation can be corroborated. This ligand-metal interaction may be exploited in photochemical organic synthesis by utilization of these ILs as solvent environment. The approach to combine catalyst and solvent in one compound could be beneficial for confinement-controlled synthesis and an alternative to conventional photocatalysts.

[1] H. Weingärtner, *Angew. Chem. Int. Ed.* **47**, 654–670 (2008).

[2] E. Müller *et al.*, *J. Mol. Liq.* **251**, 61–69 (2018).

[3] M. Rothe *et al.*, *Chem. Eur. J.*, **27**, 13052–13058 (2021).

MO 24.2 Thu 17:00 Tent C

**Ultrafast dynamics of Metanil Yellow studied by time-resolved transient absorption and XUV photoelectron spectroscopies in solution** — ●ALINA KHODKO<sup>1,4</sup>, MATTHEW MGBUKWU<sup>3</sup>, CAMILO GRANADOS<sup>1,3</sup>, EVGENII TITOV<sup>2</sup>, NATALIYA KACHALOVA<sup>4,5</sup>, VALERII VOITSEKHOVYCH<sup>4</sup>, IGOR DMYTRUK<sup>4,6</sup>, STEFAN HAACKE<sup>3</sup>, OLEG KORNILOV<sup>1</sup>, and JÉRÉMIE LÉONARD<sup>3</sup> — <sup>1</sup>Max Born Institute, Berlin, Germany — <sup>2</sup>Institute of Chemistry, University of Potsdam, Germany — <sup>3</sup>Institut de Physique et Chimie des Matériaux de Strasbourg, Université de Strasbourg, France — <sup>4</sup>Institute of Physics, Kyiv, Ukraine — <sup>5</sup>L.M. Litvinenko Institute of Physical and Organic Chemistry and Coal Chemistry, Kyiv, Ukraine — <sup>6</sup>Taras Shevchenko National University of Kyiv, Ukraine

The excited-state dynamics of the Metanil Yellow (MY) were studied by ultrafast transient absorption (TA) spectroscopy and state-of-the-art XUV time-resolved photoelectron spectroscopy (TRPES). Here the TA experiments were carried out with two excitation wavelengths,  $\lambda=370$  nm and  $\lambda=490$  nm, to investigate the non-hydrated and hydrated forms of the molecule and reveal differences in their dynamics in two solvents: water and ethanol. In TRPES experiments the dynamics were studied in water solution, using a  $\lambda=400$  nm pump, thus exciting both forms. In general, the timescales from the TRPES experiments are in good agreement with the results from the TA measurements. Based on quantum chemical calculations, the dynamics are tentatively assigned to the  $S_2^*S_1$  conversion followed by relaxation to a long-lived state, the nature of which remains to be confirmed.

MO 24.3 Thu 17:00 Tent C

**A through-flow cell for highly-resolved Stark effect measurements of Rydberg states in thermal nitric oxide** — ●FLORIAN ANSCHÜTZ<sup>1</sup>, ETTORE EDER<sup>1</sup>, FABIAN MUNKES<sup>1</sup>, ALEXANDER TRACHTMANN<sup>1</sup>, PHILIPP HENGEL<sup>2</sup>, YANNICK SCHELLANDER<sup>3</sup>, PATRICK SCHALBERGER<sup>3</sup>, MATTHEW RAYMENT<sup>4</sup>, STEPHEN HOGAN<sup>4</sup>, NORBERT FRUEHAUF<sup>3</sup>, JENS ANDERS<sup>2</sup>, ROBERT LÖW<sup>1</sup>, TILMAN PFAU<sup>1</sup>, and HARALD KÜBLER<sup>1</sup> — <sup>1</sup>5. Physikalisches Institut, Universität Stuttgart, Pfaffenwaldring 57, 70569 Stuttgart — <sup>2</sup>Institut für Intelligente Sensorik und Theoretische Elektrotechnik, Universität Stuttgart, Pfaffenwaldring 47, 70569 Stuttgart — <sup>3</sup>Institut für Großflächige Mikroelektronik, Universität Stuttgart, Allmandring 3b, 70569 Stuttgart — <sup>4</sup>Department of Physics and Astronomy, University College London, Gower Street, London WC1E 6BT, UK

We show the setup of a glass cell equipped for the electric readout of Rydberg states in nitric oxide (NO) at room temperature. The field distribution is discussed and our results on both the Stark effect and the collisional shift and broadening of Rydberg states in NO is

presented.

MO 24.4 Thu 17:00 Tent C

**Near field spectroscopy of molecular aggregates with topological phases** — ●SIDHARTHA NAYAK, ARITRA MISHRA, and ALEXANDER EISFELD — Max Planck Institute for the Physics of Complex Systems, Dresden, Germany

In this theoretical study, we focus on delocalized electronic excitonic states in molecular aggregates, particularly those exhibiting topological phases. It has been shown that a two-dimensional molecular aggregate, composed of two different sublattices and complex transition dipole moments, possesses topological edge states [1]. However, these states are predominantly 'dark' in traditional far-field absorption spectra. We consider a typical scattering scanning optical near-field microscopy (s-SNOM) setup, where the aggregate interacts with the near field stemming from a metallic tip [2, 3]. With the help of s-SNOM, we can not only excite these dark states but also record spatially resolved absorption spectra, revealing clear signatures of both excitonic edge states and bulk states.

[1] J.Y. Zhou, S. K. Saikin, N.Y. Yao and A. Aspuru-Guzik, *Nature materials* **13**, 1026-1032 (2014)

[2] X. Gao and A. Einfeld, *J. Phys. Chem. Lett.* **9**, 6003 (2018)

[3] S. Nayak, F. Zheng and A. Einfeld, *J. Chem. Phys.* **155**, 134701 (2021)

MO 24.5 Thu 17:00 Tent C

**Installation of a hollow cathode molecular ion source** — ●JULIAN RIMATZKI, SIMON REINWARDT, and MICHAEL MARTINS — Universität Hamburg, Hamburg, Deutschland

A research plan has been devised for studying inner-shell photoionization of molecular ions with a small thermal energy at the photon-ion spectrometer at PETRA III (PIPE)[1] of DESY in Hamburg. First result to characterise the plasma of a hollow cathode ion source will be shown. Such a characterisation can be obtained by studying  $\text{COH}^+$  and  $\text{HCO}^+$  isomers in the gas phase using soft X-Ray spectroscopy. The challenge of forming ions in a higher geometrical state like the  $\text{COH}^+$  can be solved by using a ion source with a plasma temperature below 18.000 K [2].

We are undergoing the construction and parametrization of our new Ion source at the PIPE-setup. We will present first results to form homogeneous ion beams with only one constitutional isomer.

[1] Schippers, S. *et al.*, *X-ray Spec.*, 2020, **49**, 11.

[2] Nobes, R. H., Radom, L., *Chem. Phys.*, 1981, **60**, 1.

MO 24.6 Thu 17:00 Tent C

**Characterization of a simple supersonic expansion source for small molecular ions** — ●LUKAS BERGER<sup>1</sup>, AIGARS ZNOTINS<sup>1</sup>, FLORIAN GRUSSIE<sup>1</sup>, DAMIAN MÜLL<sup>1</sup>, FELIX NÜSSLEIN<sup>1</sup>, ARNAUD DOCHAIN<sup>2</sup>, JOFFREY FRÉREUX<sup>2</sup>, XAVIER URBAIN<sup>2</sup>, and HOLGER KRECKEL<sup>1</sup> — <sup>1</sup>Max-Planck-Institut für Kernphysik, 69117 Heidelberg, Germany — <sup>2</sup>Institute of Condensed Matter and Nanosciences, Université Catholique de Louvain, Louvain-la-Neuve, B-1248 Belgium

The Cryogenic Storage Ring (CSR) at the Max Planck Institute for Nuclear Physics in Heidelberg is an electrostatic storage facility with a circumference of approx. 35 m that can be cooled to cryogenic temperatures ( $\sim 4$  K) by a closed-cycle liquid helium unit. The blackbody radiation field is strongly reduced compared to room-temperature experiments, and small infrared-active molecular ions will cool to their lowest rotational states within minutes in this environment, allowing for experiments with ions in defined quantum states. However, some astrophysically relevant molecular ions do not cool on accessible timescales, owing to the lack of a permanent dipole moment. To address this issue, we have developed a simple supersonic expansion ion source, based on a commercial pulsed valve and static discharge voltages. We have characterized the source performance with  $\text{N}_2\text{O}^+$  ions, conducting experiments at the STARGATE setup at UCLouvain (Louvain-la-Neuve, Belgium), which resulted in internal temperatures between 40 K and 200 K. The ion source was then integrated into the ion source platform of the CSR to deliver cold ions for merged beams experiments. The design and performance will be presented.

MO 24.7 Thu 17:00 Tent C

**Resonance Energy Transfer Involving Chiral Molecules and Macroscopic Environment** — ●JANINE C. FRANZ<sup>1,2</sup>, STEFAN YOSHI BUHMANN<sup>1</sup>, and A. SALAM<sup>3</sup> — <sup>1</sup>University Kassel, Germany — <sup>2</sup>University Freiburg, Germany — <sup>3</sup>Wake Forest University, Winston-Salem, USA

Resonance energy transfer between chiral molecules can be used to discriminate between different enantiomers. The transfer rate between chiral molecules consists of nondiscriminatory and discriminatory parts. We show that their ratio is usually larger in the far zone regime and that the degree of discrimination can be modified when considering a surrounding medium. We highlight the importance of local field effects on the degree of discrimination, predict the optimum dielectric medium for general identical chiral molecules for discrimination, and show that exotic media can even invert the discriminatory effect. When considering a chiral medium, the environment can actively participate in the discrimination, but the local-field corrections become more involved. We show that the local-field corrections in a chiral medium then lead to a surprising effect in the discrimination.

MO 24.8 Thu 17:00 Tent C

**Relayed hyperpolarization for zero- to ultralow-field nuclear magnetic resonance** — ●ERIK VAN DYKE<sup>1,2,3</sup>, JAMES EILLS<sup>1,2,3,4</sup>, ROMAN PICAZO-FRUTOS<sup>1,2,3</sup>, KIRILL SHEBERSTOV<sup>1,2,3,5</sup>, YINAN HU<sup>1,2,3,6</sup>, DMITRY BUDKER<sup>1,2,3,7</sup>, and DANILA BARSKIY<sup>1,2,3</sup> — <sup>1</sup>Helmholtz Institute Mainz, Mainz, Germany — <sup>2</sup>Johannes Gutenberg University, Mainz, Germany — <sup>3</sup>GSI Helmholtz Center for Heavy Ion Research, Darmstadt, Germany — <sup>4</sup>Institute for Bioengineering of Catalonia, Barcelona, Spain — <sup>5</sup>Ecole normale superieure, Paris, France — <sup>6</sup>Chinese Academy of Sciences, Beijing, China — <sup>7</sup>University of California at Berkeley, Berkeley, USA

Zero- to ultralow-field nuclear magnetic resonance (ZULF NMR) provides rich spectroscopic information in the absence of large magnetic fields. Still, signal acquisition requires a bulk magnetic moment for detection. We demonstrate that the parahydrogen-based Signal Amplification by Reversible exchange-Relay method (SABRE-Relay) can be used to generate hyperpolarized analytes for ZULF-NMR by observing J-spectra of methanol and ethanol (from vodka) at natural <sup>13</sup>C isotopic abundance. The magnetic-field dependence of SABRE efficiency is also shown.