

## MO 8: Poster: Collisions

Time: Tuesday 17:00–19:00

Location: Tent C

MO 8.1 Tue 17:00 Tent C

**Excitation and dissociation of astrophysically relevant molecules by ion impacts** — ●MASATO NAKAMURA — College of Science and Technology, Nihon University, Funabashi, Japan

Collision-induced dissociation of molecules by ion impacts plays an important role in the chemical evolution in molecular clouds. To reveal the mechanism of such processes, the energy transfer and fragmentation of molecules by ion impacts at hyperthermal energies are theoretically studied. The classical trajectory (CT) calculation and the spectator model are applied to estimate the energy transfer from translational to internal degrees of freedom. The model predicts the energy-transfer from the translational to the internal degrees of freedom with less efficiency. The threshold energy for CID of CO molecule by ion impacts is calculated for various projectiles. When the projectile is much lighter than the target, it is found that the spectator model works well. The probability of CID depends strongly on the orientation angle at the moment of the contact. Calculation and analysis are extended to other astrophysically relevant molecules.

MO 8.2 Tue 17:00 Tent C

**Intermolecular Coulombic Decay from organic dimers** — ●DEEPHY MARIA MOOTHERIL<sup>1</sup>, XUEGUANG REN<sup>2</sup>, THOMAS PFEIFER<sup>1</sup>, and ALEXANDER DORN<sup>1</sup> — <sup>1</sup>Max-Planck-Institute of Nuclear Physics, Heidelberg, 69115, Germany — <sup>2</sup>School of Physics, Xi'an Jiaotong University, Xi'an, 710049, China

Inter-atomic/intermolecular Coulombic decay (ICD) is an important electronic relaxation mechanism after inner-valence ionization of atoms or molecules with weakly bound neighbours. Here we study ICD in organic heterocycle dimers like thiophene dimers and pyridine-water complexes induced by electron collisions (109 eV) using the (e,e+2ion) coincidence technique [1]. Collisions with electrons causes ionization of the inner valence orbital. It is observed that the energy released after relaxation to the inner valence vacancy is transferred to the neighbouring molecule, mainly via ICD, ionizes the outer valence orbital of the neighbor and thus inducing Coulomb explosion of the dimer. Comparison of projectile energy loss spectra with theoretical single ionization spectra shows the ICD mainly proceeds from the C 2s<sup>-1</sup> inner valence vacancy in thiophene dimers and from the O 2s<sup>-1</sup> and the N 2s<sup>-1</sup> inner-valence vacancies in pyridine-water clusters [2].

References:

- [1] X. Ren et al 2018 Nature Physics 14(10) 1062- 1066  
 [2] A. D. Skitnevskaya et al 2023 J. Phys. Chem. Lett. 14(6) 1418-1426

MO 8.3 Tue 17:00 Tent C

**Dynamics of methane CH<sub>4</sub> activation by tantalum cations Ta<sup>+</sup> in gas phase** — MARCEL META<sup>1</sup>, MAXIMILIAN HUBER<sup>1</sup>, ●MAURICE BIRK<sup>1</sup>, MARTIN WEDELE<sup>1</sup>, MILAN ONČÁK<sup>2</sup>, and JENNIFER MEYER<sup>1</sup> — <sup>1</sup>RPTU Kaiserslautern-Landau, Fachbereich Chemie und Landesforschungszentrum OPTIMAS, Kaiserslautern, Germany — <sup>2</sup>Universität Innsbruck, Institut für Ionenphysik und Angewandte Physik, Innsbruck, Austria

To understand reactions on an atomic-level, we make use of well-defined model systems in the gas phase. We are interested in the rearrangement of atoms during a reaction, i.e. the atomistic dynamics which we investigate by measuring energy and angle differential cross sections [1,2].

The reaction Ta<sup>+</sup> + CH<sub>4</sub> → TaCH<sub>2</sub><sup>+</sup> + H<sub>2</sub> in its quintet ground state is endothermic and spin forbidden. However the reaction is still observed at room temperature. An efficient crossing from the quintet surface over to the triplet surface leads to the exothermic formation of TaCH<sub>2</sub><sup>+</sup> [3-6]. The title reaction was investigated by measuring experimental energy and angle differential cross sections via crossed beam velocity map imaging supported by quantum chemical calculations.

- [1] J. Meyer, R. Wester, Annu. Rev. Phys. Chem. 2017, 68, 333;  
 [2] M. Meta et. al., J. Phys. Chem. Lett. 2023, 14, 24, 5524; [3] J. F. Eckhard et. al., J. Phys. Chem. 2021, 125, 5289; [4] J. M. Bakker et. al., J. Mol. Spectrosc. 2021, 378, 111472; [5] L. G. Parke et. al.,

J. Phys. Chem. 2007, 111, 17773; [6] E. Sicilia et. al., Phys. Chem. Chem. Phys. 2017, 19, 16178

MO 8.4 Tue 17:00 Tent C

**Dynamics of the oxygen atom transfer reaction between Ta<sup>+</sup>/Nb<sup>+</sup> and carbon dioxide** — ●MARCEL META<sup>1</sup>, MAXIMILIAN E. HUBER<sup>1</sup>, MAURICE BIRK<sup>1</sup>, TIM MICHAELSEN<sup>2</sup>, ATILAY AYASLI<sup>2</sup>, MILAN ONČÁK<sup>2</sup>, ROLAND WESTER<sup>2</sup>, and JENNIFER MEYER<sup>1</sup> — <sup>1</sup>Fachbereich Chemie und Forschungszentrum OPTIMAS, RPTU Kaiserslautern-Landau, Kaiserslautern, Germany — <sup>2</sup>Institut für Ionenphysik und Angewandte Physik, Universität Innsbruck, Innsbruck, Austria

The four atom reaction M<sup>+</sup> + CO<sub>2</sub> presents a benchmark system for CO<sub>2</sub> activation in the gas phase and has been investigated throughout the last decades with different methods and along the periodic table. Recent crossed beam experiments on the reaction dynamics of the oxygen atom transfer (OAT) reaction between Ta<sup>+</sup> + CO<sub>2</sub> → TaO<sup>+</sup> + CO showed dominantly indirect dynamics despite the thermal rates being close to collision rate and the reaction being highly exothermic.[1] Here, we compare the dynamics of the OAT reaction for the tantalum cation Ta<sup>+</sup> and its lighter homologue niobium Nb<sup>+</sup> as a means to alter spin-orbit coupling. The main focus is to gain insight into the nature of the bottle-neck for Ta<sup>+</sup> + CO<sub>2</sub>: If it is a submerged transition state or a crossing point between the quintet and triplet surfaces. Ultimately, a multi-method approach of experiment and theoretical modelling is used to better assign a nature to the bottleneck.

[1] M. Meta, M. E. Huber, T. Michaelsen, A. Ayasli, M. Ončák, R. Wester, J. Meyer, J. Phys. Chem. Lett. 24, 5524 (2023)

MO 8.5 Tue 17:00 Tent C

**Setup for improved resolution in ion-molecule crossed beam imaging** — ●JERIN JUDY, DASARATH SWARAJ, TIM MICHAELSEN, FABIO ZAPPA, ROBERT WILD, and ROLAND WESTER — Institut für Ionenphysik und Angewandte Physik, Universität Innsbruck, Innsbruck, Austria.

Crossed-beam experiments have proven to be a powerful tool for investigating reaction dynamics in the gas-phase [1]. Our group specializes in the study of ion-molecule reactions in combination with a velocity map imaging (VMI) spectrometer to record energy and angle dependent differential cross-sections [2]. Currently we focus on reactions involving laser ionized hydrogen molecules with argon using a newly commissioned crossed-beam experiment, where our aim is to resolve the different vibrational levels in the molecular products. We will present preliminary results on this system and describe the new experimental setup.

- [1] N. Balucani *et al.*, Int.Rev. Phys. Chem. 25, 109 (2006).  
 [2] R. Wester, Phys. Chem. Chem. Phys. 16, 396 (2014).

MO 8.6 Tue 17:00 Tent C

**Auger spectrum of the ultra-fast dissociating 2p<sub>3/2</sub><sup>-1</sup>σ\* resonance in HCl in the semi-classical one-center approximation** — ●MATEJA HRAST<sup>1,2</sup> and MATJAZ ŽITNIK<sup>1,3</sup> — <sup>1</sup>Jozef Stefan Institute, Ljubljana, Slovenia — <sup>2</sup>Institute of Science and Technology Austria (ISTA), Klosterneuburg, Austria — <sup>3</sup>Faculty of Mathematics and Physics, University of Ljubljana, Slovenia

We present an ab-initio theoretical L-VV resonant Auger spectrum of the ultrafast dissociating 2p<sub>3/2</sub><sup>-1</sup>σ\* resonance in HCl. The decay rates are derived in one-center approximation and a semi-classical description of dissociation is considered. The calculated profiles of Auger spectral lines resemble those of atomic Auger decay but with the characteristic tails extending towards lower electron kinetic energies. The calculated line asymmetries reflect dissociation dynamics along the potential energy curve of the initial state and its relative position with respect to the potential energy curves of the corresponding final states. For some transitions, the line shape is also strongly affected by the variation of Auger decay rate with the internuclear distance.