

MO 25: Cluster

Zeit: Donnerstag 16:30–19:00

Raum: Poster C1

MO 25.1 Do 16:30 Poster C1

Photoionization of He Dimers — ●TILO HAVERMEIER, TILL JAHNKE, ROBERT GRISENTI, KATHRINA KREIDI, MARKUS SCHÖFFLER, SVEN SCHÖSSLER, NADINE NEUMANN, JASMIN TITZE, MATHIAS KÜHNEL, JÖRG VOIGTSBERGER, HENDRIK SANN, ROBERT WALLAUER, STEFAN VOSS, FELIX STURM, LUTZ FOUCAR, JUAN MORILLAS, HORST SCHMIDT-BÖCKING, and REINHARD DÖRNER — Institut für Kernphysik, University Frankfurt, Max von Laue Str. 1, 60438 Frankfurt, Germany.

The helium dimer is one of the most weakly bound systems in the universe. This makes it an interesting quantum mechanical object for investigation. These Van der Waals Clusters can be produced in an expansion of a cryogenic gas jet through a small nozzle into vacuum. In the present experiment we examine the interaction of He dimers with synchrotron radiation at an energy range from 64 to 78 eV. We observed different pathways leading to single ionization of both He atoms of the dimer compound. This two close standing ions begin now to dissociate in cause of their coulomb potential. All charged fragments were detected in coincidence with a COLTRIMS system. Especially Interatomic Coulombic Decay (ICD) and the two step process (TS1) were clearly identified. Furthermore a distribution of the internuclear distance was obtained from the measured Kinetic Energy Release (KER).

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Elektronenspektroskopie an Wasserclustern — ●MARKO FÖRSTEL, SILKO BARTH, VOLKER ULRICH, TORALF LISCHKE, MELANIE MUCKE und UWE HERGENHAHN — Max-Planck-Institut für Plasma-physik, EURATOM association, Boltzmannstr. 2, 85748 Garching

In schwach gebundenen (van der Waals oder H-Brücken) Clustern sind Autoionisationsprozesse möglich, die direkt in einen Zustand mit zwei positiven Ladungen an zwei verschiedenen Konstituenten führen. Dieser Mechanismus ist als Interatomarer oder Intermolekularer Coulomb Zerfall (ICD) bekannt geworden. Der Vorhersage nach läuft er in sehr vielen Arten von Clustern ab, gut erforscht ist er aber bis jetzt nur für die van der Waals Cluster aus Edelgasen. Im Poster werden erste Hinweise auf ICD in Wasser gezeigt.

Dotierte Wasser-Cluster sind ebenfalls von großem Interesse, da sie als Modell für die Solvatation von Substanzen in flüssigem Wasser dienen können. In dem Beitrag wird ein neuer Aufbau zur Herstellung alkali-dotierter, positiv geladener Wasser-Cluster vorgestellt und erste experimentelle Ergebnisse diskutiert.

MO 25.3 Do 16:30 Poster C1

Untersuchung der Lokalisation von K-Schalen Photoelektronen in Neon-Dimeren — ●K. KREIDI^{1,2}, T. JAHNKE¹, T. WEBER³, T. HAVERMEIER¹, R. GRISENTI¹, X.-J. LIU⁴, Y. MORISITA⁵, S. SCHÖSSLER¹, L. SCHMIDT¹, M. SCHÖFFLER¹, M. ODENWELLER¹, N. NEUMANN¹, L. FOUCAR¹, J. TITZE¹, B. ULRICH¹, F. STURM¹, C. STUCK¹, R. WALLAUER¹, S. VOSS¹, I. LAUTER¹, H.-K. KIM¹, M. RUDLOFF¹, H. FUKUZAWA⁴, G. PRÜMPER⁴, N. SAITO⁵, K. UEDA⁴, A. CZASCH¹, O. JAGUTZKI¹, H. SCHMIDT-BÖCKING¹, S. K. SEMENOV⁶, N.A. CHEREPKOV⁶ und R. DÖRNER¹ — ¹Institut für Kernphysik, J. W. Goethe Universität, Max-von-Laue-Str. 1, 60438 Frankfurt, Germany — ²DESY, Notkestrasse 85, 22607 Hamburg, Germany — ³Lawrence Berkeley National Laboratory, Berkeley CA 94720, USA — ⁴Institute of Multidisciplinary Research for Advanced Materials, Tohoku University, Sendai 980-8577, Japan — ⁵National Metrology Institute of Japan, AIST, Tsukuba 305-8568, Japan — ⁶State University of Aerospace Instrumentation, 190000 St. Petersburg, Russia

Mit der COLTRIMS-Technik wurde der Zerfall von Neodimeren nach der K-Schalen-Ionisation mit einer Photonenenergie von 881.2 eV untersucht. Die Zerfallsmechanismen, die zu den Aufbrüchen des Dimers (Ne^+/Ne^+ und $\text{Ne}^+/\text{Ne}^{2+}$) führen, wurden identifiziert. Die Lokalisation des K-Schalen Photoelektrons wurde anhand der Symmetrie der Winkelverteilung um die Molekülachse untersucht. Die Winkelverteilung der ICD-Elektronen liefert durch ihre asymmetrische Struktur Aufschluss über die Art des ICD-Zerfalls.

MO 25.4 Do 16:30 Poster C1

Ligand-binding motifs in hydroxybenzene-ligand cation complexes — ALEXANDER PATZER, HARALD KNORKE, JUDITH LANGER,

and ●OTTO DOPFER — Institut für Optik und Atomare Physik, TU Berlin, Hardenbergstrasse 36, 10623 Berlin

The competition between hydrogen-bonding and π -stacking is of fundamental importance for molecular recognition. In this contribution, we present IR spectroscopic and quantum chemical results for resorcinol cation complexes with inert ligands (e.g., Ar, N₂). IR spectra of mass-selected complexes are obtained via photodissociation in a tandem mass spectrometer [1]. The combined spectroscopic and quantum chemical approach provides detailed insight into the preferred ion-ligand binding motif, the actual binding site (isomer), and the strength of the intermolecular bond as a function of the ligand type, the number of ligands, and the resorcinol isomer. Comparison with the corresponding phenol complexes [2] reveals the effects of the second hydroxy group on the intermolecular interaction potential.

[1] O. Dopfer, *Int. Rev. Phys. Chem.* 22, 437 (2003).[2] O. Dopfer, *Z. Phys. Chem.* 219, 125 (2005).

MO 25.5 Do 16:30 Poster C1

Nonclassical versus classical structures of the ethyl cation probed by IR spectroscopy — HORIA-SORIN ANDREI, NICOLA SOLCA, and ●OTTO DOPFER — Institut für Optik und Atomare Physik, TU Berlin, Hardenbergstrasse 36, 10623 Berlin

The competition between classical and nonclassical geometries is a fundamental issue for hydrocarbon molecules. The ethyl cation (C_2H_5^+ , protonated ethene) represents the most simple example for protonation of a C=C double bond. Calculations predict the nonclassical structure to be slightly more stable than the classical structure. However, spectroscopic evidence for this conclusion is still lacking. The present work reports IR photodissociation spectra [1] of size selected clusters of the ethyl cation with Ar, N₂, CO₂, and CH₄. The IR spectra recorded in the CH stretching range provide detailed information on the degree of delocalization of the excess proton between the two C atoms. Significantly, the structure of the additional proton depends sensitively on the microsolvation environment. Whereas Ar is a negligible perturber [2], leaving C_2H_5^+ in the most stable nonclassical geometry, the stronger interaction with N₂ induces a switch from a nonclassical to a classical C_2H_5^+ ion core. The latter ligand appears to form a weak covalent bond to one C atom of the ethyl cation. The interpretation of the IR spectra is supported by rotational line profile simulations and ab initio calculations.

[1] O. Dopfer, *Int. Rev. Phys. Chem.* 22, 437 (2003). [2] H.S. Andrei, N. Solca, O. Dopfer, *Angew. Chem.*, in press, DOI: 10.1002/anie.200704163 (2007)

MO 25.6 Do 16:30 Poster C1

Electronic structure and optical properties of ideal diamond clusters - diamondoids — LASSE LANDT¹, KATHRIN KLÜNDER¹, ●MATTHIAS STAIGER¹, JEREMY DAHL², ROBERT CARLSON², THOMAS MÖLLER¹, and CHRISTOPH BOSTEDT¹ — ¹Technische Universität Berlin, Germany — ²MolecularDiamond Technologies, Richmond (CA), USA

Diamondoids can be considered a new form of ideal diamond clusters in the (sub-)nanometer size regime. Because they can be perfectly size and isomer selected fundamental investigations about size and shape effects in neutral clusters known with atomic precision are now becoming possible.

We have investigated highest occupied and lowest unoccupied states as well as optical absorption across the gap for a series of diamondoids from adamantane up to hexamantane. The combination of these three investigations paints a comprehensive picture of their electronic structure. All experiments have been performed in the gas phase reproducing the same idealized boundary conditions of interaction-free and neutral clusters typically assumed in theoretical investigations.

We find that the lowest unoccupied states do not show any particle size. The highest occupied states, however, show strong size but only minor isomeric dependencies. These findings are explained with the localization of the lowest unoccupied states on the surface and the highest occupied states in the core of the cluster. The absorption measurements across the gap in the VUV energy regime reveal strong changes of the spectra with the particle shape and symmetry.