

# STAND-ALONE PROJECT - FINAL REPORT

**Project title**            Fragmentation of Biomolecular Ions

**Project leader**        Univ.Prof.Mag.Dr. Paul Scheier

**Project number**       

**Part 1** of the project report is intended for interested members of the public; **parts 2-4** are addressed to reviewers and must be submitted in the language of the original application.

**Part 5** provides an opportunity to report to the FWF on interactions with the administration during the course of the project.

**The complete report must be submitted in hardcopy and on electronic medium (CD or floppy disc) in Word for Windows format.** Guidelines and forms for the final report can be downloaded from the FWF web site

(<http://www.fwf.ac.at/de/faq/einzelprojekte/evaluierung.html> )

# 1. Summary for public relations work

Die Stabilität von Biomolekülen nach Ionisation spielt eine wichtige Rolle bei der Bestrahlung von organischem Gewebe durch ionisierende Strahlung. Komplexe Moleküle zerfallen oft nicht unmittelbar nach dem Ionisierungsprozess, sondern bis zu Sekunden verzögert. Auf der molekularen Ebene bedeutet diese Zeitspanne eine Ewigkeit. Im vorliegenden Projekt wurden solche Zerfallsprozesse von einfachen Bausteinen des Lebens, wie DNS-Basen und Aminosäuren untersucht. Für isolierte Biomoleküle in der Gasphase konnten eine Vielzahl an verzögerten Zerfallskanäle sowohl für positive wie negativ geladene Ionen entdeckt werden. Durch Einbetten der Biomoleküle in winzige Tröpfchen aus Helium zeigte sich, dass praktisch alle verzögerten Zerfallsprozesse unterdrückt werden. Anstelle von kleinen Bruchstücken wurde ein schweres Fragment beobachtet, welches als Zwischenprodukt in der Gasphase weiter zerfällt, jedoch in den Tröpfchen stabilisiert wurde. Durch dieses neuartige Verfahren lassen sich komplexe chemische Prozesse Schritt für Schritt untersuchen. Eine wichtige Schlussfolgerung aus den vorliegenden Ergebnissen ist, dass umgebende Atome bzw. Moleküle einen beträchtlichen Einfluss auf die durch Strahlenschäden entstehenden Produkte haben. Bisherige Ergebnisse aus der Gasphase lassen sich nicht unmittelbar auf biologische Zellen und organisches Gewebe anwenden. Die extrem niedrige Temperatur im Inneren eines Heliumtröpfchens von 0.37K bietet eine Fülle an interessanten Möglichkeiten. So können Experimente an zustandsselektierten Molekülen und Komplexen auf relativ einfache Art und Weise gemacht werden, deren Ergebnisse für den Vergleich mit theoretischen Rechnungen von großer Bedeutung sind. Weiters können neutrale Partikel erzeugt werden, die eisbedeckten mikroskopisch kleinen Staubteilchen in kalten und dichten interstellaren Wolken entsprechen. Elektronen- und ioneninduzierte Prozesse, die zur Synthese von komplexen Molekülen in diesen interstellaren Wolken führen, lassen sich so im Labor untersuchen.

The stability of biomolecules upon ionization is an important issue for the interaction of ionizing radiation with organic tissue. Complex molecules often do not decay immediately after the ionization event. Delayed fragmentation may be observed up to seconds after the excitation process. On the molecular level this time corresponds to an eternity. In the present project delayed decay reactions of simple biomolecules such as DNA bases and aminoacids upon the inelastic interaction with free electrons were studied. For both, cations and anions several delayed decay reactions were observed. Experiments with the same molecules embedded in helium droplets revealed that basically all delayed decay reactions are quenched. Instead of several of low-mass fragments only the dehydrogenated closed-shell parent anion is formed. In the gas phase this product can be considered as an intermediate reaction product that is stabilized inside the helium droplets by efficient cooling. This property of helium droplets can be utilized to investigate chemical reactions step by step by freezing intermediate products. An important consequence of the present results is that solvent atoms or molecules may have a surprisingly large effect on the final reaction products formed by radiation damage. Furthermore, gas phase results that have been obtained both experimentally and theoretically may deviate significantly from the liquid environment in cells and organic tissue.

The ultra-low temperatures inside the helium droplets of 0.37K provide a wealth of interesting possibilities. Experiments with state selective molecules and clusters can be performed quite easily. The results of such experiments can be directly compared with quantum chemical calculations and can serve as benchmarks to test theory. In addition, neutral particles can be formed that can serve as models for ice covered dust particles in cold interstellar clouds. Electron and ion induced processes at the surface of these dust particles that are expected to be the origin of complex molecules in space can be investigated in a laboratory experiment.

## 2. Brief project report

In the last three years the research funded by this project was leading to exciting discoveries and results that have been published in several high-impact journals. Pickup of biomolecules and subsequently also other molecules in superfluid He droplets turned out to be a highlight that will be investigated in the following years. High sensitivity of the mass spectrometer system in Innsbruck and the appropriate conditions of the He cluster source made it possible to investigate for the first time anion formation in He droplets upon free electron attachment combined with mass spectrometry. Until now Innsbruck is still the only place in the world where anions from doped He droplets can be analyzed mass spectrometrically. This technique opens a wide field of interesting applications such as state selectivity, formation of exotic complexes, micro and nano-solvation, freezing of intermediate and normally unstable reaction products, laboratory experiments to simulate cold and dense interstellar clouds and ultra-cold chemistry, just to mention a few. Our first study on electron attachment to clusters of the DNA bases thymine and adenine embedded in He droplets was published in *Physical Review Letters* and demonstrates that predominantly intact and dehydrogenated parent anions are formed. In a later work with improved experimental conditions, i.e., a fully differentially pumped pickup cell, much better results concerning fragments originating from non-embedded monomers could be obtained. In a recent paper (S. Denifl, et al., *ChemPhysChem* 9 (2008) 1387) we reported that basically all low-mass fragments formed upon dissociative electron attachment to gas phase molecules are completely suppressed in He droplets. Instead, the dehydrogenated parent anion is formed at these core excited resonances. This demonstrates that solvated molecules may behave completely differently compared to isolated molecules and has to be considered for the extrapolation of gas phase data to the cellular level concerning radiation damage.

In order to obtain a more detailed insight into the process of electron attachment to molecules and clusters embedded in He droplets we performed a series of experiments with simple molecules such as  $\text{CCl}_4$ ,  $\text{CHCl}_3$ ,  $\text{H}_2\text{O}$ ,  $\text{CO}_2$ ,  $\text{C}_{60}$  and several amino acids. The results on water and chloroform ( $\text{CHCl}_3$ ) were published this year in *JACS*. In the case of  $\text{CO}_2$  we discovered a well pronounced shift of the position of the low-energy resonance of the parent cluster anions from about 2 eV down to almost 0 eV by shrinking the He droplets via increase of the nozzle temperature from 9K to 14K. Currently we try to repeat these measurements with improved electron energy resolution utilizing an electron monochromator combined with an improved He droplet source and pickup cell.

Until now many anions turn out to have a high affinity to bind one or more He atoms. In several cases even the size of a coordination shell by a pronounced decrease of the anion yield above a certain number of attached He atoms could be observed. These results are currently prepared for publication and enable the experimental determination of the size of the ionic core. In addition the salvation of He atoms to ions demonstrates that these ions are extremely cold and in the case of anions photoelectron spectroscopy could provide interesting additional information about the effect of the number of He atoms attached to an anion.

A proposal, based on our results presented above, describing a new photoelectron spectroscopy experiment with ultra-cold anions formed in doped He droplets was granted within the infrastructure initiative IV. Currently we are building a new experiment where for the first time the binding energy of electrons of mass selected anions formed upon electron attachment to doped He droplets can be measured.

Concerning the stability of positive and negative ions formed upon the inelastic interaction of free electrons with gas phase biomolecules the following results were achieved:

In collaboration with the group of O. Ingolfsson from Iceland we could demonstrate that the metastable decay pathways of the dehydrogenated closed shell anion of the amino acid valine does not depend on the formation mechanism, i.e., dissociative electron attachment or deprotonation in MALDI (H. D. Flosadottir, et al. *Angew. Chem. Int. Ed.* 46 (2007) 8057). Furthermore, unimolecular and collision induced fragmentation of anions formed at different

resonances allows to determine the structure of different isomeric forms of anions. Two additional papers (F. Zappa et al. ChemPhysChem 9 (2008) 607 and K. Graupner et al. J. Chem. Phys. 128 (2008) 104304) have been published in 2008 in collaboration with the group of T. Field in Belfast investigating the stability of anions formed upon free electron attachment. These first results suggest the inclusion metastable decay reactions for all upcoming systems.

For both, cations and anions of aromatic molecules we discovered a pronounced isotope effect for selected metastable decay reactions. In order to exclude experimental artefacts that are possible with 2-sector field mass spectrometers a 5-sector field instrument was purchased from the money of this project. This instrument was installed in Innsbruck in December 2007 and currently we are performing first measurements with cations. Several modifications of the electronics of this instrument have to be done in order to enable the formation of anions at very low electron energies and to optimize the instrument for the planned experiments. Besides the investigation of the stability of ions from biomolecules this instrument opens new possibilities for decay measurements of cluster ions.

## 2.1 Report on the scientific work

### 2.1.1 information on the development of the research work (2000 characters excl. spaces)

- **overall scientific concept and goals**

The stability of biomolecular ions, both positively and negatively charged, has been investigated with a 2-sector-field mass spectrometer system. Possible artefacts caused by decay reactions in the sector fields and other field free regions become a real problem for large molecules. With help of a 5-sector-field mass spectrometer that could be purchased from the funding of this project this problem can be reduced almost completely.

Pickup of biomolecules with large rare gas droplets enables the formation of cold and complex neutral targets. Superfluid He droplets were utilized in this project and the inelastic interaction of free electrons with doped He nano-droplets was studied. Both positive and negative ion formation was observed and investigated. Recently discovered site selectivity upon free electron attachment to gas phase biomolecules is conserved in the doped droplets and clusters of biomolecules.

- **was there a change of direction in the field between the start and the end of the project?** – If so, what form did the change take and what effect did it have on the work?

Throughout the whole project the development of a neutral spray source was carried out. Starting with a design similar to electro-spray we moved to sonic- and thermo-spray. Additionally ultrasonic nebulization was tried out but all methods failed to provide a stable and intense beam of neutral molecules free of solvents. For simple molecules such as caffeine some preliminary results with a spray source could be achieved. However, extensive heating was required which would destroy more complex biomolecules such as polypeptides that were planned to be vaporized gently by this technique. In Berlin laser acoustic desorption was successfully utilized to vaporize delicate biomolecules and in the future it is planned to build such a source also in Innsbruck.

In contrast pickup of biomolecules in He droplets turned out to form intense beams of ultra-cold complex and neutral targets of biomolecules. We performed a series of experiments utilizing this technique until the end of this project and plan to continue with this research for the next years. Especially the effect of various solvents and the number of solvent molecules surrounding a biomolecule can be studied quite easily with this method.

2.1.2 most important results and brief description of their significance (main points) with regard to (8000 characters excl. spaces)

- **contribution to the progress of the field** (e.g. did the results contribute to an increased importance for the field and in what way?);  
In this project it was possible to demonstrate that molecular anions with a certain complexity are often not formed immediately after the attachment of the electron but require several microseconds. Delayed decay reactions can be investigated in the field free regions of sector field mass spectrometers.
- **breaking of new scientific ground** (i.e. to what extent and in what respect?);  
Experiments with molecular anions that are formed via free electron attachment to doped He droplets where the neutral molecule is solvated by He or even a certain number of solvent molecules show that excited intermediates transfer their excess energy fast enough to the surrounding solvent molecules which stabilizes intermediate and in the gas phase unstable reaction products. In organic tissue and the cellular environment surrounding water molecules will have a similar effect and this project demonstrates that gas phase results cannot be transferred to biological systems without inclusion of the surrounding solvent molecules.
- **most important development of hypotheses** (what relevance did the project have for the development of scientific hypotheses, e.g. were new hypotheses developed or old hypotheses disproved?);  
Surrounding solvent atoms or molecules have a surprisingly large effect on the resulting reaction products upon inelastic interaction of electrons with large molecules. For biomolecules and other hydrogen containing molecules low mass fragment anions are strongly suppressed and instead the dehydrogenated closed-shell anion which is an intermediate reaction product is stabilized by the surrounding solvent. Thus results obtained in the gas phase often do not apply in the condensed phases.
- **development of new methods**;  
The inelastic interaction of free electrons with doped He droplets turns out to be a powerful technique with a variety of scientifically interesting aspects. (i) At the temperature of 0.37K most species are in their ground state and thereby state selective experiments become possible. (ii) Complex targets can be preformed such as fullerenes decorated with simple molecules (water, ammonia, etc.) that can serve as models for dust particles in cold and dense interstellar clouds. (iii) intermediate reaction products can be stabilized by the surrounding He which enables the investigation of chemical reactions in a direct way step by step.
- **relevance for other (related) areas of science** (transdisciplinary issues and methods).  
Radiation damage to biological tissue on the molecular level has to include surrounding water molecules. Fragmentation with complex rearrangement of the constituents where many bonds are cleaved and others formed are unlikely to happen for solvated molecules.

2.1.3 information on the running of the project, use of the available funding and where appropriate any changes to the original project plan relating to (2000 characters excl. spaces)

- **duration**;  
The project duration was exactly three years as expected.
- **use of personnel**;  
Dr. Sylwia Ptasinska was contributing to this project for almost one year and started to build a neutral spray source. It was possible to pay her salary from a European project. Dr. Fabio Zappa who worked for more than two years in my group was financed from the Brazilian agency CNPq. He was contributing to all parts of this

project. Thus it was not necessary to hire an additional post doc researcher as expected in the proposal.

- **larger items of equipment purchased;**

A 5-sector field mass spectrometer was purchased with money that was initially intended for personnel costs. Post doc scientists could be paid from other sources which enabled this possibility. Although the instrument was purchased quite late within this project and first results cannot be included in this report the additional features of this mass spectrometer will be frequently used for future studies including the FWF-funded project P19073.

- **other significant deviation<sup>1</sup> .**

none

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<sup>1</sup> The assessment of what should be regarded as a "significant deviation" is the responsibility of the project leader. As a guideline, any deviation of more than 25% from the original financial plan or work schedule should be accounted for.

## **2.2. Personnel development – importance of the project for the scientific careers of those involved (including the project leader)**

(2000 characters excl. spaces)

Dr. Sylwia Ptasinska, although not funded by this project spent one and a half years in the laboratories of Prof. Sanche in Sherbrooke, Canada and recently got a tenure track position in Milton Keynes where she is leading a small independent group. Several diploma theses could be successfully finished by the following students: Manuel Winkler (technician at a MSE in the Southern Tyrol), Manuel Beikircher (teacher at a high school in the Southern Tyrol), Andreas Mauracher (Ph.D. student in Innsbruck) and Ingo Mähr (employee at a MSE in Vorarlber). Furthermore, Philipp Sulzer finished his Ph.D. thesis with distinction in February 2008 and is now working as a physicist at a MSE in Innsbruck.

This project supported research that fits into the lines of research of several European networks and thus helped to establish and intensify collaborations with other European groups in Iceland, Portugal, Germany, the UK and Slovakia. With all of these groups joint publication have been accepted in international refereed journals. Particularly the experiments with doped He droplets turned out to be exciting and opened a completely new field with interesting questions and topics for the future. Last but not least the research supported by this project was leading to a position on the short list for a position of a Max-Planck director for the PI of this project.

## **2.3 effects of the project outside the scientific field**

(2000 characters excl. spaces)

Some of the themes covered by this project attracted the interest of the media and were leading to contributions in local and international newspapers and to a contribution in a science telecast of the Austrian broadcast ORF. Furthermore, the students supported by this project participated actively at several activities for the public, such as “Lange Nacht der Forschung”.



### 3. Information on project participants

not funded by the FWF			funded by the FWF (project)		
co-workers	number	Person-months	co-workers	number	Person - months
non-scientific co-workers	1	9	non-scientific co-workers		
diploma students	6	54	diploma students	5	15.5
PhD students	12	108.25	PhD students	6	21.75
post-doctoral co-workers	4	72.25	post-doctoral co-workers	2	2
co-workers with "Habilitation" (professorial qualifications)			co-workers with "Habilitation" (professorial qualifications)		
professors	2	10.8	professors		

## 4. Attachments

### List 1

#### 1.a. scientific publications<sup>2</sup>

with an indication of the status (published, in press, submitted, in preparation)

##### 1.a.1. Peer-reviewed publications (journals, contribution to anthologies, working papers, proceedings etc.)

- 1) Aleem, A.; Mauracher, A.; Sulzer, P.; Denifl, S.; Zappa, F.; Bacher, A.; Wendt, N.; Märk, T.D.; Scheier, P.: Relative partial cross sections for anions formed upon electron attachment to nitrotoluene. *Int. J. Mass Spectrom.* **271** (2008) 36-44
- 2) Denifl, S.; Zappa, F.; Mähr, I.; Mauracher, A.; Probst, M.; Märk, T.D.; Scheier, P.: Inelastic Electron Interaction with Chloroform Clusters Embedded in Helium Droplets. *J. Am. Chem. Soc.* **130** (2008) 5065-5071
- 3) Denifl, S.; Zappa, F.; Mauracher, A.; Ferreira da Silva, F.; Bacher, A.; Echt, O.; Märk, T.D.; Bohme, D.K.; Scheier, P.: Dissociative electron attachment to DNA bases near absolute zero: freezing dissociation intermediates. *ChemPhysChem* **9** (2008) 1387-1389
- 4) Zappa, F.; Denifl, S.; Mähr, I.; Bacher, A.; Echt, O.; Märk, T.D.; Scheier, P.: Ultracold Water Cluster Anions. *J. Am. Chem. Soc.* **130** (2008) 5573-5578
- 5) Denifl, S.; Mauracher, A.; Sulzer, P.; Bacher, A.; Märk, T.D.; Scheier, P.: Free electron attachment to the chloromethane CHCl<sub>3</sub>. *Int. J. Mass Spectrom.* **265** (2007) 139-145
- 6) Denifl, S.; Sulzer, P.; Huber, D.; Zappa, F.; Probst, M.; Märk, T.D.; Scheier, P.; Injan, N.; Limtrakul, J.; Abouaf, R.; Dunet, H.: Influence of Functional Groups on the Site-Selective Dissociation of Adenine upon Low-Energy Electron Attachment. *Angew. Chem. Int. Ed.* **46** (2007) 5238-5241
- 7) Flosadottir, H.D.; Denifl, S.; Zappa, F.; Wendt, N.; Mauracher, A.; Bacher, A.; Jonsson, H.; Märk, T.D.; Scheier, P.; Ingolfsson, O.: Combined experimental and theoretical study on the nature and the metastable decay pathways of the amino acid ion fragment [M-H]<sup>-</sup>. *Angew. Chem. Int. Ed.* **46** (2007) 8057-8059
- 8) Mauracher, A.; Denifl, S.; Aleem, A.; Wendt, N.; Zappa, F.; Cicman, P.; Probst, M.; Märk, T.D.; Scheier, P.; Flosadottir, H.D.; Ingolfsson, O.; Illenberger, E.: Dissociative Electron Attachment to Gas Phase Glycine: Exploring the Decomposition Pathways by Mass Separation of Isobaric Fragment Anions. *Phys. Chem. Chem. Phys.* **9** (2007) 5680-5685
- 9) Sulzer, P.; Mauracher, A.; Denifl, S.; Probst, M.; Märk, T.D.; Scheier, P.; Illenberger, E.: Probing Di-Nitrobenzene by Low Energy Electrons Identification of Isomers via Resonances in Dissociative Electron Attachment. *Int. J. Mass Spectrom.* **266** (2007) 138-148
- 10) Sulzer, P.; Mauracher, A.; Denifl, S.; Zappa, F.; Ptasinska, S.; Beikircher, M.; Bacher, A.; Wendt, N.; Aleem, A.; Rondino, F.; Matejcek, S.; Probst, M.; Märk, T.D.; Scheier, P.: Identification of Isomers of Nitrotoluene via Free Electron Attachment. *Anal. Chem.* **79** (2007) 6585-6591
- 11) Zappa, F.; Denifl, S.; Mähr, I.; Lecointre, J.; Rondino, F.; Echt, O.; Märk, T.D.; Scheier, P.: Electron impact ionization of thymine clusters embedded in superfluid helium droplets. *Eur. Phys. J. D* **43** (2007) 117-120
- 12) Burrow, P.D.; Gallup, G.A.; Scheer, A.M.; Denifl, S.; Ptasinska, S.; Märk, T.; Scheier, P.: Vibrational Feshbach resonances in uracil and thymine. *J. Chem.*

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<sup>2</sup> The publication list must mention for each work: all authors; full title; series/journal title; year; volume; and page numbers.

- Phys.* **124** (2006) 124310; selected for *Virtual Journal of Biological Physics Research* 11 Issue 7
- 13) Denifl, S.; Zappa, F.; Mähr, I.; Lecointre, J.; Probst, M.; Märk, T.D.; Scheier, P.: Mass Spectrometric Investigation of Anions Formed upon Free Electron Attachment to Nucleobase Molecules and Clusters Embedded in Superfluid Helium Droplets. *Phys. Rev. Lett.* **97** (2006) 043201
  - 14) Feil, S.; Winkler, M.; Sulzer, P.; Ptasinska, S.; Denifl, S.; Zappa, F.; Kräutler, B.; Märk, T.D.; Scheier, P.: Single, double and triple ionization of tetraphenyl iron(III) porphyrin chloride. *Int. J. Mass Spectrom.* **255-256** (2006) 232-238
  - 15) Huber, D.; Beikircher, M.; Denifl, S.; Zappa, F.; Matejcek, S.; Bacher, A.; Grill, V.; Märk, T.D.; Scheier, P.: High resolution dissociative electron attachment to gas phase adenine. *J. Chem. Phys.* **125** (2006) 084304
  - 16) Ipolyi, I.; Cicman, P.; Denifl, S.; Matejcek, V.; Mach, P.; Urban, J.; Scheier, P.; Märk, T.D.; Matejcek, S.: Electron impact ionization of alanine: Appearance energies of the ions. *Int. J. Mass Spectrom.* **252** (2006) 228-233
  - 17) Ptasinska, S.; Denifl, S.; Gohlke, S.; Scheier, P.; Illenberger, E.; Märk, T.D.: Decomposition of Thymidine by Low-Energy Electrons: Implications for the Molecular Mechanisms of Single-Strand Breaks in DNA. *Angew. Chem. Int. Ed.* **45** (2006) 1893-1896
  - 18) Sulzer, P.; Ptasinska, S.; Zappa, F.; Mielewska, B.; Milosavljevic, A.R.; Scheier, P.; Märk, T.D.; Bald, I.; Gohlke, S.; Huels, M.A.; Illenberger, E.: Dissociative electron attachment to furan, tetrahydrofuran, and fructose. *J. Chem. Phys.* **125** (2006) 044304; selected for *Virtual Journal of Biological Physics Research* 12 Issue 3
  - 19) Ptasinska, S.; Denifl, S.; Scheier, P.; Illenberger, E.; Märk, T.D.: Bond- and Site-Selective Loss of H Atoms from Nucleobases by Very-Low-Energy Electrons (<3 eV). *Angew. Chem. Int. Ed.* **44** (2005) 6941-6943
  - 20) Ptasinska, S.; Denifl, S.; Grill, V.; Märk, T.D.; Illenberger, E.; Scheier, P.: Bond- and Site-Selective Loss of H- from Pyrimidine Bases. *Phys. Rev. Lett.* **95** (2005) 093201
  - 21) Ptasinska, S.; Denifl, S.; Mroz, B.; Probst, M.; Grill, V.; Illenberger, E.; Scheier, P.; Märk, T.D.: Bond selective dissociative electron attachment to thymine. *J. Chem. Phys.* **123** (2005) 124302

**1.a.2. Non peer-reviewed publications (journals, contribution to anthologies research reports, working papers, proceedings, etc.)**

- 1) Edtbauer, A.; Ferreira da Silva, F.; Schöbel, H.; Mauracher, A.; Probst, M.; Denifl, S.; Märk, T.D.; Scheier, P. (2008): Biomolecules inside superfluid helium droplets at 0.37 K. In: *RADAM 2008, Radiation Damage in Biomolecular Systems. 13th-15th June 2008, Debrecen, Hungary. Eigenverlag.*
- 2) Ferreira da Silva, F.; Schöbel, H.; Denifl, S.; Märk, T.D.; Scheier, P. (2008): DEA of clusters of amino acid in He droplets and triggering of peptide formation due to low energy electrons. In: *RADAM 2008, Radiation Damage in Biomolecular Systems. 13th-15th June 2008, Debrecen, Hungary. Eigenverlag.*
- 3) Probst, M. (2008): Dissociative electron attachment to biomolecules. In: *Kendl, A.; Schindler, S. (Hrsg.): Introduction to Computer Science and Applied Computing. Innsbruck: innsbruck university press (IUP) (= IAC Series Volume 1), 59 - 60.*
- 4) Alizadeh, E.; Mauracher, A.; Sulzer, P.; Denifl, S.; Probst, M.; Märk, T.D.; Scheier, P. (2008): Dissociative Electron Attachment to Biomolecules and Explosives. In: *LEEMI-EIPAM'08. Eigenverlag, 35.*
- 5) Eden, S.; Tabet, J.; Bruny, G.; Farizon, B.; Farizon, M.; Ouaskit, S.; Märk, T.D. (2008): Electron transfer in proton collisions with DNA bases. In: *LEEMI-EIPAM'08. Eigenverlag, 39.*

- 6) Ptasinska, S.; Alizadeh, E.; Sulzer, P.; Abouaf, R.; Mason, N.J.; Märk, T.D.; Scheier, P. (2008): Formation of negative ions by low energy (< 20 eV) electron impact to gas phase 5-nitouracil. *In: LEEMI-EIPAM'08. Eigenverlag, 65.*
- 7) Denifl, S.; Ferreira da Silva, F.; Schöbel, H.; Zappa, F.; Märk, T.D.; Scheier, P. (2008): Inelastic electron interaction with doped helium droplets. *In: Solov'yov, A.V.: ISACC 2008 International Symposium "Atomic Cluster Collisions: structure and dynamics from the nuclear to the MesoBioNano scale". St. Petersburg (Russia), June 3-7 2008. Mulhouse: European Physical Society (= Europhysics Conference Abstracts 32B), 54 - 55.*
- 8) Denifl, S.; Ferreira da Silva, F.; Dampc, M.; Zappa, F.; Märk, T.D.; Scheier, P. (2008): Inelastic interaction of electrons with molecules inside cold helium droplets: detection of novel molecular aggregates. *In: LEEMI-EIPAM'08. Eigenverlag, 19.*
- 9) Reichsöllner, E.; Denifl, S.; Mauracher, A.; Zappa, F.; Probst, M.; Flosadottir, H.D.; Ingolfsson, O.; Jonsson, H.; Märk, T.D.; Scheier, P. (2008): Negative ion formation and fragmentation upon free electron attachment to amino acids. *In: Electron Controlled Chemical Lithography. Eigenverlag, 86.*
- 10) Probst, M.; Scheier, P.; Märk, T.D. (2008): Predicting the Sites of Electron Attachment to Biomolecules. *In: ECDM-V 5th European Charge Density Meeting. In conjunction with DFG 1178 Annual Meeting. Eigenverlag, 109 - 109.*
- 11) Denifl, S.; Sulzer, P.; Zappa, F.; Probst, M.; Märk, T.D.; Scheier, P.; Injan, N.; Limtrakul, J.; Abouaf, R.; Dunet, H. (2008): Site dependent dissociation of adenine: influence of functional groups upon dissociative electron attachment. *In: Beck, R.D.; Drabbels, M.; Rizzo, T.R.: 16th Symposium on Atomic and Surface Physics and Related Topics (SASP 2008). Contributions. Innsbruck: innsbruck university press (IUP) (= Conference Series), 1. 114 - 117.*
- 12) Mauracher, A.; Denifl, S.; Zappa, F.; Wendt, N.; Bacher, A.; Illenberger, E.; Probst, M.; Märk, T.D.; Scheier, P. (2007): Dissociative electron attachment to amino acids - theory and experiment. *In: Book of Abstracts - 4th Annual CMBI Meeting, Igls/Tirol, September 28.09.2007 - 29.09.2007. Innsbruck: Eigenverlag, 39.*
- 13) Alizadeh, E.; Mauracher, A.; Flosadottir, H.; Denifl, S.; Zappa, F.; Märk, T.D.; Scheier, P. (2007): Dissociative electron attachment to amino acids. *In: Rauch, H.; Vana, N.; Balcar, E.: 57. Jahrestagung der Österreichischen Physikalischen Gesellschaft. Book of Abstracts. Wien: Eigenverlag Technische Universität Wien, 82 - 83.*
- 14) Sulzer, P.; Mähr, I.; Denifl, S.; Zappa, F.; Märk, T.D.; Illenberger, E.; Scheier, P. (2007): Dissociative electron attachment to biomolecules: from gas phase to complex nanodroplets. *In: 25th Miller Conference on Radiation Chemistry. Eigenverlag, 24.*
- 15) Denifl, S.; Ptasinska, S.; Zappa, F.; Mähr, I.; Grill, V.; Probst, M.; Illenberger, E.; Märk, T.D.; Scheier, P. (2007): Dissociative Electron Attachment to Thymine: Bond and Site Selectivity in Different Molecular Environments. *In: AIP Conference Proceedings 901, 137 - 146.*
- 16) Denifl, S.; Zappa, F.; Echt, O.; Mauracher, A.; Probst, M.; Märk, T.D.; Scheier, P. (2007): Electron Driven Reactions at Ultra-Low Temperatures - Molecular Synthesis in Interstellar Clouds. *In: Book of Abstracts - 4th Annual CMBI Meeting, Igls/Tirol, September 28.09.2007 - 29.09.2007. Innsbruck: Eigenverlag, 12.*
- 17) Denifl, S.; Zappa, F.; Mähr, I.; Scheier, P.; Echt, O.; Märk, T.D. (2007): Electron Scattering on Clusters and Biomolecules Embedded in Helium Droplets. *In: Solov'yov, A.V. (Ed.): ISACC 2007 International Symposium "Atomic Cluster Collisions: structure and dynamics from the nuclear to the biological scale". Abstracts. Mulhouse: European Physical Society (= Europhysics Conference Abstracts 31D), 46 - 47.*

- 18) Sulzer, P.; Mähr, I.; Denifl, S.; Zappa, F.; Märk, T.D.; Illenberger, E.; Echt, O.; Scheier, P. (2007): Electron-driven damage to biomolecular systems. *In: Thomas, R.D.; Schmidt, H.T.; Fischer, D.: 2nd International Workshop on Electrostatic Storage Devices. Book of Abstracts. Eigenverlag, 21.*
- 19) Mähr, I.; Denifl, S.; Zappa, F.; Märk, T.D.; Scheier, P. (2007): Free electron attachment to nucleobases and amino acids embedded in superfluid helium droplets. *In: Symposium on Radiation Effects of Biomedical Interest. Thursday 22nd - Sunday 25th February 2007, Madrid. Eigenverlag, 41.*
- 20) Denifl, S.; Zappa, F.; Mähr, I.; Märk, T.D.; Scheier, P. (2007): Inelastic electron interaction (ionization/attachment) with biomolecules embedded in superfluid helium droplets. *In: Symposium on Size Selected Cluster 2007. Book of Abstracts. Eigenverlag, 62.*
- 21) Scheier, P.; Denifl, S.; Zappa, F.; Mähr, I.; Sulzer, P.; Ptasinska, S.; Illenberger, E.; Märk, T.D. (2007): Inelastic interactions of electrons with biomolecules: from gas phase to complex systems. *In: Symposium on Radiation Effects of Biomedical Interest. Thursday 22nd - Sunday 25th February 2007, Madrid. Eigenverlag, 9.*
- 22) Alizadeh, E.; Mauracher, A.; Denifl, S.; Zappa, F.; Flosadottir, H.D.; Ingolfsson, O.; Märk, T.D.; Scheier, P. (2007): Metastable Decay Pathways of Amino Acid Anions. *In: Book of Abstracts - 4th Annual CMBI Meeting, Igls/Tirol, September 28.09.2007 - 29.09.2007. Innsbruck: Eigenverlag, 40.*
- 23) Mauracher, A.; Beikircher, M.; Denifl, S.; Zappa, F.; Bacher, A.; Echt, O.; Märk, T.D.; Scheier, P. (2007): Metastable Decays of Negative Ions Formed Upon Electron Attachment to Small Biomolecules and Explosives. *In: Charalambidis, D.; Farantos, S.; Lambropoulos, P. (eds.): 9th European Conference on Atoms Molecules & Photons. ECAMP IX, 6-11th May 2007, Heraklion. Mulhouse: European Physical Society (= Europhysics Conference Abstracts 31C), Tu3-28.*
- 24) Sulzer, P.; Denifl, S.; Huber, D.; Zappa, F.; Probst, M.; Märk, T.D.; Scheier, P. (2007): Probing of derivatives of adenine with low energy electrons. *In: Book of Abstracts - 4th Annual CMBI Meeting, Igls/Tirol, September 28.09.2007 - 29.09.2007. Innsbruck: Eigenverlag, 41.*
- 25) Injan, N.; Probst, M.; Denifl, S.; Zappa, F.; Limtrakul, J.; Märk, T.; Scheier, P.; Urban, J.; Mach, P. (2007): Quantum Chemistry of Dissociative Electron Attachment to Adenine. *In: Matuska, J.; Matejčík, S.; Sklany, J.D.: Book of Abstracts of 16th Symposium on Application of Plasma Processes. Workshop on Research of Plasma Physics and Applications in Visegrad Countries. Bratislava: Library and Publishing Centre, Comenius University, 177 - 178.*
- 26) Mähr, I.; Mauracher, A.; Beikircher, M.; Denifl, S.; Zappa, F.; Bacher, A.; Grill, V.; Probst, M.; Märk, T.D.; Scheier, P. (2007): Stability of negatively charged biomolecules and explosives. *In: Symposium on Radiation Effects of Biomedical Interest. Thursday 22nd - Sunday 25th February 2007, Madrid. Eigenverlag, 43.*
- 27) Huber, D.; Lokuliyana, K.; Zappa, F.; Scheier, P. (2006): Development of a spray source for vaporization of low volatile biomolecules. *In: Ernst, W.; Neger, T.: 56. Jahrestagung der Österreichischen Physikalischen Gesellschaft. Book of Abstracts. Eigenverlag, 28 - 29.*
- 28) Huber, D.; Lokuliyana, K.; Zappa, F.; Scheier, P. (2006): Development of a spray source for vaporization of low volatile biomolecules. *In: Ernst, W.; Neger, T.: 56. Jahrestagung der Österreichischen Physikalischen Gesellschaft. Book of Abstracts. Eigenverlag, 118.*
- 29) Zappa, F.; Denifl, S.; Mähr, I.; Lecointre, J.; Rondino, F.; Echt, O.; Märk, T.D.; Scheier, P. (2006): Electron impact ionization of thymine clusters embedded in superfluid helium droplets. *In: Book of Abstracts of the 13th International Symposium on Small Particles and Inorganic Clusters (ISSPIC XIII Conference 2006), July, 23-28, 2006, Göteborg, Sweden. Eigenverlag, 96.*
- 30) Denifl, S.; Zappa, F.; Mähr, I.; Beikircher, M.; Sulzer, P.; Märk, T.D.; Scheier, P.; Ptasinska, S.; Bohme, D.K. (2006): Free electron attachment to nucleobases:

- reactions induced by hydride ions. *In: Tosi, P.; et al.: MOLEC XVI - European Conference on Dynamics of Molecular Systems. Book of Abstracts. Eigenverlag, 240 - 243.*
- 31) Denifl, S.; Zappa, F.; Mähr, I.; Scheier, P.; Märk, T.D. (2006): Inelastic electron interaction (ionization/attachment) of biomolecules embedded in superfluid He droplets. *In: Grill, V.; Märk, T.D. (eds.): 15th Symposium on Atomic and Surface Physics and Related Topics. Contributions. Innsbruck: innsbruck university press (IUP) (= Conference Series), 250 - 253.*
  - 32) Coupier, B.; Fedor, J.; Feil, S.; Zappa, F.; Denifl, S.; Scheier, P.; Märk, T.D. (2006): Inelastic electron interaction with water molecules. *In: Adoui, L.; Huber, B.A.; et al.: International Workshop on Radiation Damage of Water. Photons, electrons and ions colliding with water molecules, clusters, liquids and solids. Eigenverlag, 6 - 7.*
  - 33) Scheier, P.; Hochmair, E.; Märk, T.D.; Hansel, A.; Kuhn, S.; Probst, M.; Pulker, J.; Schöpf, K.; Schrittwieser, R.; Zierhofer, C. (2006): Ionen- und Plasmaphysik / Angewandte Physik. *In: Grumiller, M.; Märk, T.D.: Zukunftsplattform Obergurgl 2006: Forschungsk Kooperationen innerhalb der Leopold-Franzens-Universität Innsbruck. Innsbruck: innsbruck university press (IUP) (= Conference Series), 132 - 135.*
  - 34) Eden, S.; Tabet, J.; Ouaskit, S.; Farizon, B.; Farizon, M.; Scheier, P.; Märk, T.D. (2006): Ionization of water and biomolecules by protons in the bragg peak energy range: separation of direct ionization and electron capture processes. *In: Grill, V.; Märk, T.D. (eds.): 15th Symposium on Atomic and Surface Physics and Related Topics. Contributions. Innsbruck: innsbruck university press (IUP) (= Conference Series), 12.*
  - 35) Eden, S.; Tabet, J.; Ouaskit, S.; Farizon, B.; Farizon, M.; Scheier, P.; Märk, T.D. (2006): Ionization of water and biomolecules by protons in the Bragg peak energy range: separation of direct ionization and electron capture processes. *In: Adoui, L.; Huber, B.A.; et al.: International Workshop on Radiation Damage of Water. Photons, electrons and ions colliding with water molecules, clusters, liquids and solids. Eigenverlag, 8.*
  - 36) Feil, S.; Gluch, K.; Denifl, S.; Zappa, F.; Echt, O.; Scheier, P.; Märk, T.D. (2006): Metastable dissociation and kinetic energy release of helium clusters upon electron impact ionization. *In: Book of Abstracts of the 13th International Symposium on Small Particles and Inorganic Clusters (ISSPIC XIII Conference 2006), July, 23-28, 2006, Göteborg, Sweden. Eigenverlag, 92.*
  - 37) Zappa, F.; Ptasinska, S.; Denifl, S.; Grill, V.; Scheier, P.; Märk, T.D. (2006): Site selectivity in dissociative free-electron attachment to gas phase nucleobases. *In: Grill, V.; Märk, T.D. (eds.): 15th Symposium on Atomic and Surface Physics and Related Topics. Contributions. Innsbruck: innsbruck university press (IUP) (= Conference Series), 15 - 18.*
  - 38) Beikircher, M.; Ptasinska, S.; Feil, S.; Winkler, M.; Bacher, A.; Schustereder, W.; Echt, O.; Märk, T.D.; Scheier, P. (2006): Stability of uracil and thymine cations. *In: Grill, V.; Märk, T.D. (eds.): 15th Symposium on Atomic and Surface Physics and Related Topics. Contributions. Innsbruck: innsbruck university press (IUP) (= Conference Series), 166 - 169.*
  - 39) Scheier, P.; Ptasinska, S.; Denifl, S.; Candori, P.; Schustereder, W.; Hasan, V.G.; Cicman, P.; Feil, S.; Coupier, B.; Fedor, J.; Matejcik, S.; Illenberger, E.; Märk, T.D. (2005): Dissociative Electron Attachment to Biologically Relevant Molecules. *In: Hensel, K.; Matejcik, S.; Skalny, J.D.; Mason, N.J.: Book of Contributed Papers. 15th Symposium on Applications of Plasma Processes, 3rd EU-Japan Joint Symposium on Plasma Processing. Bratislava: Comenius University Press, 49 - 52.*
  - 40) Fedor, J.; Cicman, P.; Coupier, B.; Feil, S.; Gluch, K.; Winkler, M.; Scheier, P.; Märk, T.D. (2005): Dissociative Electron Attachment to Water Molecules. *In: Hensel, K.; Matejcik, S.; Skalny, J.D.; Mason, N.J.: Book of Contributed*

*Papers. 15th Symposium on Applications of Plasma Processes, 3rd EU-Japan Joint Symposium on Plasma Processing. Bratislava: Comenius University Press, 153.*

**1.a.3. Stand-alone publications (monographies, anthologies)**

1) Grill, V.; Märk, T.D. (eds.) 15th Symposium on Atomic and Surface Physics and Related Topics – Contributions. Innsbruck: innsbruck university press (IUP) (= Conference Series) 2006.

**1.b. publications for the general public and other publications**

such as films, exhibitions, preparation of a home page etc. with an indication of the status (published, submitted / in preparation)

1) <http://www.uibk.ac.at/ionen-angewandte-physik/nanobio/fwf-p18052> - Projekt-Homepage - published

**List 2 project-related participation in international scientific conferences**  
(with an indication of the conference date) – 4 subunits:

**2.1. Conference participations - invited lectures**

- 1) Denifl, S.: Inelastic electron interaction with doped helium droplets. *3rd International Symposium Atomic Cluster Collisions: structure and dynamics from the nuclear to the MesoBioNano scales (ISACC 2008)*, St. Petersburg, 03.06.2008 - 07.06.2008.
- 2) Alizadeh, E.: Dissociative electron attachment to biomolecules and explosives. *LEEMI-EIPAM'08, Roscoff*, 07.05.2008 - 11.05.2008.
- 3) Denifl, S.: Inelastic interaction of electrons with molecules inside cold helium droplets: detection of novel molecular aggregates. *LEEMI-EIPAM'08, Roscoff*, 07.05.2008 - 11.05.2008.
- 4) Märk, T.D.: Low Energy Electron Interaction with Biomolecules in Different Environments: from the Gas Phase to Droplets. *Isolated Biomolecules and Biomolecular Interactions (IBBI08)*, Valladolid, 13.04.2008 - 18.04.2008.
- 5) GRC
- 6) Märk, T.D.: Low energy electron interaction with biomolecules and biomolecular clusters. *Modelling Radiation Damage, Lyon*, 03.12.2007 - 06.12.2007.
- 7) Märk, T.D.: Electron Interaction With Biomolecules And Clusters Embedded In Helium Droplets. *COSTUK Meeting, Oxford*, 10.09.2007 - 12.09.2007.
- 8) Märk, T.D.: Electron Scattering on Clusters and Biomolecules Embedded in Helium Droplets. *2nd International Symposium "Atomic Cluster Collisions: structure and dynamics from the nuclear to the biological scale" (ISACC 2007)*, Darmstadt, 19.07.2007 - 23.07.2007.
- 9) Scheier, P.: Electron-driven damage to biomolecular systems. *2nd International Workshop on Electrostatic Storage Devices (ESD 2007)*, Stockholm, 17.06.2007 - 21.06.2007.
- 10) Probst, M.: Why is it so difficult to model water? *Mini-symposium in all aspects of "The Water Molecule"*, Uppsala, 15.05.2007 - 16.05.2007.
- 11) Scheier, P.: Dissociative electron attachment to biomolecules: from gas phase to complex nanodroplets. *25th Miller Conference on Radiation Chemistry, Buxton*, 14.04.2007 - 19.04.2007.
- 12) Märk, T.D.: Electrons and Biomolecules. *Symposium on Size Selected Clusters (S3C) 2007, Brand*, 12.03.2007 - 16.03.2007.
- 13) Probst, M.: Energetics and Geometries of Nucleic Acid Base Pairs in the Gas Phase and in Liquid Helium. *International Conference on Modeling in Chemical and Biological Engineering Science (CBES 2006)*, Bangkok, 25.10.2006 - 27.10.2006.
- 14) Fedor, J.: Dissociative electron attachment to water. *Second Annual Meeting of ESF Research Networking Programme on Electron Induced Processing at the Molecular Level (EIPAM Meeting 2006)*, Valletta, 16.09.2006 - 20.09.2006.
- 15) Scheier, P.: Formation and stability of anions upon free electron attachment to biomolecules in the gas phase and embedded in superfluid helium droplets. *Second Annual Meeting of ESF Research Networking Programme on Electron Induced Processing at the Molecular Level (EIPAM Meeting 2006)*, Valletta, 16.09.2006 - 20.09.2006.
- 16) Denifl, S.: Site-selective fragmentation of molecules induced by electron attachment. *International Symposium "Scattering, Coincidence and Absorption Studies of Molecules (SCASM)"*, Rio de Janeiro, 04.09.2006 - 06.09.2006.
- 17) Denifl, S.: Electron impact ionization mass spectrometry of nucleobases embedded in cold helium droplets. *1st Annual ITS LEIF Meeting, Sonderborg*, 07.07.2006 - 12.07.2006.
- 18) Märk, T.D.: Electron driven processes in molecules of biological relevance: bond, site, energy and state selectivity. *ESF-FWF Conference "Biomolecules -*



*From Gas Phase Properties to Reactions relevant in Living Cells", Obergurgl, 24.06.2006 - 29.06.2006.*

- 19) Scheier, P.: Site Selective Bond Cleavage Upon Dissociative Electron Attachment - A Tool to Control Chemical Reactions. *37th Meeting of the American Physical Society Division of Atomic, Molecular and Optical Physics (DAMOP 2006), Knoxville, TN, 16.05.2006 - 20.05.2006.*
- 20) Scheier, P.: Bond and site selective fragmentation upon dissociative electron attachment. *231st American Chemical Society National Meeting (ACS), Atlanta, 26.03.2006 - 30.03.2006.*
- 21) Zappa, F.: Site selectivity in dissociative free-electron attachment to gas phase nucleobases. *SASP 2006: Symposium on Atomic and Surface Physics, Obergurgl, 04.02.2006 - 09.02.2006.*
- 22) Zappa, F.: Electron attachment to molecules of biological relevance. *58th Annual Gaseous Electronics Conference (GEC 2005), San Jose, California, 16.10.2005 - 20.10.2005.*
- 23) Scheier, P.: Isotope and site labeling for the identification of resonances in dissociative electron attachment to biomolecules. *52nd Annual Meeting of the Radiation Research Society (RRS), Denver, Colorado, 16.10.2005 - 19.10.2005.*
- 24) Scheier, P.: The use of isotope and site labeling for the identification of DEA peaks in biomolecules. *14th International Symposium on Electron-Molecule Collisions and Swarms (EMS 2005), Campinas, 27.07.2005 - 30.07.2005.*

## **2.2. Conference participations - lectures**

- 1) Ferreira da Silva, F.: DEA of clusters of amino acid in He droplets and triggering of peptide formation due to low energy electrons. *Radiation Damage in Biomolecular Systems (RADAM2008), Debrecen, 13.06.2008 - 15.06.2008.*
- 2) Ferreira da Silva, F.: The role of electron interaction with biomolecules embedded in superfluid helium droplets. *3rd Annual ITS LEIF Meeting & Summer School, Da Balaia, 18.05.2008 - 24.05.2008.*
- 3) Scheier, P.: Clusters and Biomolecules. *3rd Annual ITS LEIF Meeting & Summer School, Da Balaia, 18.05.2008 - 24.05.2008*
- 4) Scheier, P.: Electron driven reactions at ultra-low temperatures - Molecular synthesis in interstellar clouds. *4th Annual Meeting of the Center of Molecular Biosciences (CMBI), Igl, 28.09.2007 - 29.09.2007.*
- 5) Denifl, S.: Electron attachment to gas phase biomolecules in superfluid helium. *Annual Conference on Radiation Damage in Biomolecular Systems (RADAM'07), Dublin, 19.06.2007 - 22.06.2007.*
- 6) Denifl, S.: Inelastic electron interactions with biomolecules: from gas phase to complex systems. *Annual Conference on Radiation Damage in Biomolecular Systems (RADAM'07), Dublin, 19.06.2007 - 22.06.2007.*
- 7) Grill, V.: Molecular data for biological applications. *5th International Conference on Atomic and Molecular Data and Their Applications (ICAMDATA), Meudon, 15.10.2006 - 19.10.2006.*
- 8) Denifl, S.: Inelastic electron interaction with nucleobases: From the isolated molecules to base pairs. *3rd Annual Meeting of the Center of Molecular Biosciences (CMBI), Vill, 29.09.2006 - 01.10.2006.*
- 9) Huber, D.: Development of a spray source for vaporization of low volatile biomolecules. *56. Jahrestagung der Österreichischen Physikalischen Gesellschaft (ÖPG), Graz, 18.09.2006 - 21.09.2006.*
- 10) Denifl, S.: Inelastic electron interaction with water molecules. *International Workshop on Radiation Damage of Water "Photons, electrons and ions colliding with water molecules, clusters, liquids and solids", Saint Malo, 15.05.2006 - 16.05.2006.*
- 11) Denifl, S.: Inelastic electron interaction (ionization/attachment) of biomolecules embedded in superfluid He droplets. *Frühjahrstagung der Deutschen Physikalischen Gesellschaft (DPG), Frankfurt/Main, 13.03.2006 - 17.03.2006.*

- 12) Denifl, S.: Electron impact ionisation and attachment studies of biomolecules embedded in He droplets. *Second Working Group 1 Meeting (COST Action P9)*, Lissabon, 23.02.2006 - 25.02.2006.
- 13) Scheier, P.: Inelastic interactions of electrons with biomolecules: from gas phase to complex systems. *Symposium on Radiation Effects of Biomedical Interest*, Madrid, 22.02.2007 - 25.02.2007.
- 14) Grill, V.: Isotope and site labeling for the identification of DEA peaks in biomolecules. *2nd Annual Meeting of the Center for Molecular Biosciences (CMBI)*, Vill, 30.09.2005 - 01.10.2005.
- 15) Winkler, M.: Ultrakalte Uracilmoleküle. *55. Jahrestagung der Österreichischen Physikalischen Gesellschaft (ÖPG)*, Wien, 27.09.2005 - 29.09.2005.
- 16) Beikircher, M.: Unimolekularer Zerfall von Uracil und Thymin. *55. Jahrestagung der Österreichischen Physikalischen Gesellschaft (ÖPG)*, Wien, 27.09.2005 - 29.09.2005.
- 17) Sulzer, P.: Wechselwirkung von freien Elektronen mit Porphyrinen. *55. Jahrestagung der Österreichischen Physikalischen Gesellschaft (ÖPG)*, Wien, 27.09.2005 - 29.09.2005.
- 18)

### 2.3. Conference participations - posters

- 1) Edtbauer, A.; Ferreira da Silva, F.; Schöbel, H.; Mauracher, A.; Probst, M.; Denifl, S.; Märk, T.D.; Scheier, P.: Biomolecules inside superfluid helium droplets at 0.37 K. *Radiation Damage in Biomolecular Systems (RADAM2008)*, Debrecen, 13.06.2008 - 15.06.2008.
- 2) Probst, M.; Scheier, P.; Märk, T.: Predicting the Sites of Electron Attachment to Biomolecules. *5th European Charge Density Meeting*, Gravedona, 06.06.2008 - 11.06.2008.
- 3) Ptasinska, S.; Alizadeh, E.; Sulzer, P.; Abouaf, R.; Mason, N.J.; Märk, T.D.; Scheier, P.: Formation of negative ions by low energy (<20 eV) electron impact to gas phase 5-nitouracil. *LEEMI-EIPAM'08*, Roscoff, 07.05.2008 - 11.05.2008.
- 4) Denifl, S.; Mauracher, A.; Zappa, F.; Bacher, A.; Probst, M.; Scheier, P.; Märk, T.D.; Flosadottir, H.D.; Ingolfsson, O.; Illenberger, E.: Negative ion formation and fragmentation upon free electron attachment to simple amino acids. *Isolated Biomolecules and Biomolecular Interactions (IBBI08)*, Valladolid, 13.04.2008 - 18.04.2008.
- 5) Reichsöllner, E.; Denifl, S.; Mauracher, A.; Zappa, F.; Probst, M.; Flosadottir, H.D.; Ingolfsson, O.; Jonsson, H.; Märk, T.D.; Scheier, P.: Negative ion formation and fragmentation upon free electron attachment to amino acids. *Electron Controlled Chemical Lithography (ECCL)*, Lisbon, 12.03.2008 - 16.03.2008.
- 6) Denifl, S.; Sulzer, P.; Zappa, F.; Probst, M.; Märk, T.D.; Scheier, P.; Injan, N.; Limtrakul, J.; Abouaf, R.; Dunet, H.: Site dependent dissociation of adenine: influence of functional groups upon dissociative electron attachment. *16th Symposium on Atomic and Surface Physics and Related Topics (SASP 2008)*, Les Diablerets, 20.01.2008 - 25.01.2008.
- 7) GRC
- 8) Mauracher, A.; Denifl, S.; Zappa, F.; Wendt, N.; Bacher, A.; Illenberger, E.; Probst, M.; Märk, T.D.; Scheier, P.: Dissociative electron attachment to amino acids - theory and experiment. *4th Annual Meeting of the Center of Molecular Biosciences (CMBI)*, Igls, 28.09.2007 - 29.09.2007.
- 9) Alizadeh, E.; Mauracher, A.; Denifl, S.; Zappa, F.; Flosadottir, H.D.; Ingolfsson, O.; Märk, T.D.; Scheier, P.: Metastable Decay Pathways of Amino Acids Anions. *4th Annual Meeting of the Center of Molecular Biosciences (CMBI)*, Igls, 28.09.2007 - 29.09.2007.

- 10) Sulzer, P.; Denifl, S.; Huber, D.; Zappa, F.; Probst, M.; Märk, T.D.; Scheier, P.: Probing of derivatives of adenine with low energy electrons. *4th Annual Meeting of the Center of Molecular Biosciences (CMBI), Igls, 28.09.2007 - 29.09.2007.*
- 11) Alizadeh, E.; Mauracher, A.; Flosadottir, H.; Denifl, S.; Zappa, F.; Märk, T.D.; Scheier, P.: Dissociative electron attachment to amino acids. *57. Jahrestagung der Österreichischen Physikalischen Gesellschaft (ÖPG), Krems, 24.09.2007 - 29.09.2007.*
- 12) Probst, M.; Injan, N.; Denifl, S.; Zappa, F.; Limtrakul, J.; Märk, T.D.; Scheier, P.; Urban, J.; Mach, P.: Dissociative Electron Attachment to Biomolecules. *16th Canadian Symposium on Theoretical Chemistry - 2007, St. John's, 04.08.2007 - 09.08.2007.*
- 13) Mauracher, A.; Wendt, N.; Sulzer, P.; Denifl, S.; Zappa, F.; Bacher, A.; Märk, T.D.; Scheier, P.; Probst, M.: Glycine - Theoretical and experimental studies. *Annual Conference on Radiation Damage in Biomolecular Systems (RADAM'07), Dublin, 19.06.2007 - 22.06.2007.*
- 14) Mauracher, A.; Beikircher, M.; Denifl, S.; Zappa, F.; Bacher, A.; Echt, O.; Märk, T.D.; Scheier, P.: Metastable Decays of Negative Ions Formed Upon Electron Attachment to Small Biomolecules and Explosives. *9th European Conference on Atoms Molecules and Photons (ECAMP IX), Heraklion, 06.05.2007 - 11.05.2007.*
- 15) Denifl, S.: Solvated biomolecules embedded in helium droplets: Ionisation and electron attachment. *2nd Annual ITS LEIF Meeting & Summer School, Heraklion, 30.04.2007 - 06.05.2007.*
- 16) Denifl, S.; Zappa, F.; Mähr, I.; Märk, T.D.; Scheier, P.: Inelastic electron interaction (ionization/attachment) with biomolecules embedded in superfluid helium droplets. *Symposium on Size Selected Clusters (S3C) 2007, Brand, 12.03.2007 - 16.03.2007.*
- 17) Probst, M.; Injan, N.; Denifl, S.; Zappa, F.; Limtrakul, J.; Märk, T.D.; Scheier, P.; Urban, J.; Mach, P.: Quantum Chemistry of Dissociative Electron Attachment to Adenine. *47th Sanibel Symposium, St. Simons Island, GA, 22.02.2007 - 27.02.2007.*
- 18) Injan, N.; Probst, M.; Denifl, S.; Zappa, F.; Mähr, I.; Beikircher, M.; Ptasinska, S.; Limtrakul, J.; Märk, T.D.; Scheier, P.: Energetics and Geometrics of Nucleic Acid Base Pairs in the Gas Phase and in Liquid Helium. *47th Sanibel Symposium, St. Simons Island, GA, 22.02.2007 - 27.02.2007.*
- 19) Mähr, I.; Denifl, S.; Zappa, F.; Märk, T.D.; Scheier, P.: Free electron attachment to nucleobases and amino acids embedded in superfluid helium droplets. *Symposium on Radiation Effects of Biomedical Interest, Madrid, 22.02.2007 - 25.02.2007.*
- 20) Mähr, I.; Mauracher, A.; Beikircher, M.; Denifl, S.; Zappa, F.; Bacher, A.; Grill, V.; Probst, M.; Märk, T.D.; Scheier, P.: Stability of negatively charged biomolecules and explosives. *Symposium on Radiation Effects of Biomedical Interest, Madrid, 22.02.2007 - 25.02.2007.*
- 21) Injan, N.; Probst, M.; Denifl, S.; Zappa, F.; Limtrakul, J.; Märk, T.; Scheier, P.; Urban, J.; Mach, P.: Quantum Chemistry of Dissociative Electron Attachment to Adenine. *16th Symposium on Application of Plasma Processes (SAPP XVI), Podbanske, 20.01.2007 - 25.01.2007.*
- 22) Kethsiri, L.; Huber, D.; Zappa, F.; Scheier, P.; Märk, T.D.: Development of a spray source for the vaporization of neutral low volatile molecules. *3rd Annual Meeting of the Center of Molecular Biosciences (CMBI), Vill, 29.09.2006 - 01.10.2006.*
- 23) Denifl, S.; Zappa, F.; Mähr, I.; Beikircher, M.; Sulzer, P.; Ptasinska, S.; Bohme, D.K.; Märk, T.D.; Scheier, P.: Free electron attachment to nucleobases: reactions induced by hydride ions. *3rd Annual Meeting of the Center of Molecular Biosciences (CMBI), Vill, 29.09.2006 - 01.10.2006.*

- 24) Mauracher, A.; Beikircher, M.; Denifl, S.; Zappa, F.; Bacher, A.; Grill, V.; Märk, T.D.; Scheier, P.: Stability of negatively charged biomolecules and explosives. *3rd Annual Meeting of the Center of Molecular Biosciences (CMBI), Vill, 29.09.2006 - 01.10.2006.*
- 25) Sulzer, P.; Ptasinska, S.; Denifl, S.; Grill, V.; Moser, S.; Kräutler, B.; Scheier, P.; Märk, T.: Low Energy electron interactions with labelled gas phase nucleobases. *3rd Annual Meeting of the Center of Molecular Biosciences (CMBI), Vill, 29.09.2006 - 01.10.2006.*
- 26) Denifl, S.; Zappa, F.; Mähr, I.; Beikircher, M.; Sulzer, P.; Märk, T.D.; Scheier, P.; Ptasinska, S.; Bohme, D.K.: Free electron attachment to nucleobases: reactions induced by hydride ions. *European Conference on Dynamics of Molecular Systems (MOLEC XVI), Levico Terme, Trento, 11.09.2006 - 15.09.2006.*
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- 34) Injan, N.; Probst, M.; Denifl, S.; Zappa, F.; Mähr, I.; Beikircher, M.; Ptasinska, S.; Limtrakul, J.; Märk, T.D.; Scheier, P.: Energetics of the base pairs TT, AA and AT. *XIIth International Congress of Quantum Chemistry (ICQC), Kyoto, 21.05.2006 - 26.05.2006.*
- 35) Ptasinska, S.; Denifl, S.; Zappa, F.; Grill, V.; Scheier, P.; Märk, T.D.: Site selectivity in dissociative free-electron attachment to gas phase nucleobases. *Frühjahrstagung der Deutschen Physikalischen Gesellschaft ( DPG ), Frankfurt/Main, 13.03.2006 - 17.03.2006.*
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- 37) Denifl, S.; Zappa, F.; Mähr, I.; Sulzer, P.; Scheier, P.; Märk, T.D.: Inelastic electron interaction (ionization/attachment) of biomolecules embedded in

- superfluid He droplets. *39. Jahrestagung der Deutschen Gesellschaft für Massenspektrometrie (DGMS), Mainz, 05.03.2006 - 08.03.2006.*
- 38) Denifl, S.; Zappa, F.; Mähr, I.; Scheier, P.; Märk, T.D.: Inelastic electron interaction (ionization/attachment) of biomolecules embedded in superfluid He droplets. *SASP 2006: Symposium on Atomic and Surface Physics, Obergurgl, 04.02.2006 - 09.02.2006.*
- 39) Beikircher, M.; Ptasinska, S.; Feil, S.; Winkler, M.; Bacher, A.; Schustereder, W.; Echt, O.; Märk, T.D.; Scheier, P.: Stability of uracil and thymine cations. *SASP 2006: Symposium on Atomic and Surface Physics, Obergurgl, 04.02.2006 - 09.02.2006.*
- 40) Sulzer, P.; Stano, M.; Feil, S.; Winkler, M.; Ptasinska, S.; Grill, V.; Zappa, F.; Krätler, B.; Märk, T.D.; Scheier, P.: Inelastic interaction of free electrons with gas phase porphyrins. *2nd Annual Meeting of the Center for Molecular Biosciences (CMBI), Vill, 30.09.2005 - 01.10.2005.*
- 41) Milosavljevic, A.R.; Sulzer, P.; Mielewska, B.; Rondino, F.; Zappa, F.; Marinkovic, B.P.; Märk, T.D.; Scheier, P.: Inelastic electron interaction (attachment/ionization) with furan and tetrahydrofuran. *LEEMI IV - Negative Ions: Experiment and Theory, Smolenice, 06.10.2005 - 09.10.2005.*
- 42) Ptasinska, S.; Denifl, S.; Mroz, B.; Probst, M.; Grill, V.; Märk, T.D.; Scheier, P.: Bond selective dissociative electron attachment to thymine. *2nd Annual Meeting of the Center for Molecular Biosciences (CMBI), Vill, 30.09.2005 - 01.10.2005.*
- 43) Sulzer, P.; Stano, M.; Feil, S.; Winkler, M.; Ptasinska, S.; Grill, V.; Zappa, F.; Krätler, B.; Märk, T.D.; Scheier, P.: Inelastic interaction of free electrons with gas phase porphyrins. *2nd Annual Meeting of the Center for Molecular Biosciences (CMBI), Vill, 30.09.2005 - 01.10.2005.*
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- 46) Ptasinska, S.; Denifl, S.; Mroz, B.; Wisthaler, A.; Grill, V.; Probst, M.; Illenberger, E.; Märk, T.D.; Scheier, P.: Bond-selective hydrogen abstraction from thymine. *24th International Conference on Photonic, Electronic and Atomic Collisions, Rosario, 20.07.2005 - 26.07.2005.*
- 47) Sulzer, P.; Stano, M.; Feil, S.; Winkler, M.; Ptasinska, S.; Grill, V.; Zappa, F.; Märk, T.D.; Scheier, P.: Inelastic interaction of free electrons with gas phase porphyrins. *Electron and Positron Induced Chemistry and Electron Induced Processing at the Molecular Level (EPIC-EIPAM 2005), S. Martino al Cimino (Viterbo), 25.06.2005 - 30.06.2005.*
- 48) Zappa, F.; Sulzer, P.; Mielewska, B.; Milosavljevic, A.; Ptasinska, S.; Denifl, S.; Scheier, P.; Märk, T.D.: Inelastic Electron Interaction with Sugar Molecules. *Electron and Positron Induced Chemistry and Electron Induced Processing at the Molecular Level (EPIC-EIPAM 2005), S. Martino al Cimino (Viterbo), 25.06.2005 - 30.06.2005.*
- 49) Ptasinska, S.; Denifl, S.; Grill, V.; Illenberger, E.; Scheier, P.; Märk, T.D.: Radiation Damage in Biomolecular Systems by Low Energy Electrons. *European Young Investigator Conference (EYIC 2005), Gniezno, 07.06.2005 - 12.06.2005.*
- 50)

#### 2.4. Conference participations - other

1)

### List 3 Development of collaborations

Indication of the most important collaborations (maximum 5), that took place (initiated or continued) in collaboration please give the name of the collaboration partner (name, title, institution) and a few words about the scientific content. Please also assign one of the following **categories** to each collaboration:

<b>N</b>			Nature	<b>N</b> (national); <b>E</b> (European); <b>I</b> (other international cooperation)
↓	<b>E</b>		Extent	<b>E1</b> <b>low</b> (e.g. no joint publications but mention in acknowledgements or similar); <b>E2</b> <b>medium</b> (collaboration e.g. with occasional joint publications, exchange of materials or similar but no longer-term exchange of personnel); <b>E3</b> <b>high</b> (extensive collaboration with mutual hosting of group members for research stays, regular joint publications etc.)
	↓	<b>D</b>	Discipline	<b>D</b> within the discipline <b>T</b> transdisciplinary

<b>N</b>	<b>E</b>	<b>D</b>	<b>Collaboration partner / content of the collaboration</b>
E	E2	D	1) Name: Oddur Ingolfsson Title: Stability of anions Institution: Department of Chemistry, University of Iceland, Reykjavík Content: chemical control and site selective bond cleavage upon electron attachment
E	E3	D	2) Name: Tom Field Title: Stability of anions Institution: Department of Physics and Astronomy, Queen's University of Belfast Content: metastable dissociation upon free electron attachment to molecules
E	E3	D	3) Name: Eugen Illenberger Title: Anion formation Institution: Institut für Chemie und Biochemie, Freie Universität Berlin Content: Electron attachment experiments with high electron energy resolution
E	E3	D	4) Name: Paulo Limao Vieira Title: Electron attachment Institution: Physics Department, New University of Lisbon Content: Anion formation upon free electron attachment and via collision with alkali atoms
I	E3	T	5) Name: Diethard K. Bohme Title: Chemistry of anions Institution: Department of Chemistry, York University, Toronto, Canada Content: Chemical reactions driven by low-energy electrons

**Note:** general scientific contacts and occasional meetings should not be considered as collaborations in the above sense.

**List 4 “Habitations” (professorial qualifications) / PhD theses / diploma theses**  
with an indication of the status (in progress / completed)

**Note:** it will not be possible to assign a “Habilitation” to a single project; what is required here is a mention of those “Habitations” for which the project was important. A similar caveat applies to PhD and diploma theses: the FWF does not support thesis work but rather funds the scientific work that forms the basis for theses.

**4.1. Professorial Qualifications**

1)

**4.2. PhD Theses**

- 1) **Sulzer, Philipp:** Dissociative Electron Attachment to Explosives and Biomolecules (2006 - 2008) - completed
- 2) **Aleem, Muhammad Abid:** in progress
- 3) **Alizadeh, Elahe:** in progress
- 4) **Edtbauer, Achim:** in progress
- 5) **Endstraßer, Nikolaus:** in progress
- 6) **Ferreira da Silva, Filipe:** in progress
- 7) **Mauracher, Andreas:** in progress
- 8) **Schöbel, Harald:** in progress

**4.3. Diploma Theses**

- 9) **Huber, Dieter:** Hochauflösende elektroneninduzierte Dissoziationsprozesse an Adenin - Entwicklung einer Sprayquelle zur Verdampfung schwerflüchtiger Biomoleküle (2005) – thesis completed, exam missing
- 10) **Winkler, Manuel:** Technische Verbesserungen zu massenspektrometrischen Untersuchungen von biologisch relevanten Molekülen (2005) - completed
- 11) **Beikircher, Manuel:** Tests und Weiterentwicklung eines hochauflösenden Massenspektrometers, Bestimmung der freiwerdenden kinetischen Energie für metastabiles Uracil, Propan und DNT und Aufnahme vollständiger Fragmentationsspektren für die dissoziative Elektronenanlagerung an Thymin und Adenin (2006) - completed
- 12) **Mauracher, Andreas:** Über theoretische und experimentelle Untersuchungen von MNT und DNB (2006) - completed
- 13) **Waldburger, Philipp:** in progress

**List 5 Effects of the project outside the scientific field** (where appropriate)

**Sections of the list:**

**5.1. Organization of scientific events**

- congresses, symposiums or workshops with participants from outside Austria  
Grill, V.; Naschberger, S.; Grabner, W.; Märk, T.D.; Matt-Leubner, S.;  
Weingartner, G.: Organisation, SASP 2006: Symposium on Atomic and Surface  
Physics, Obergurgl, Österreich, 04.02.2006 - 09.02.2006.

**5.2. Particular honours, prizes etc.**

Ptasinska, Sylwia: Anerkennungspreis der Dr. Maria Schaumayer Stiftung (2005).

**5.3. Information on results relevant to commercial applications**

**5.4. Other effects beyond the scientific field**

'Tanzende DNA', part of the ORF-Wissenschaftsmagazin NEWTON on Nov 5th,  
2006.

**5.5. Relevance of the project in the organization of the relevant scientific discipline**

The research carried out within this project fits into the direction of several  
European networks. This strengthened the position of Innsbruck within the scientific  
community and helped to establish several new international collaborations and  
continue and intensify existing ones.

**List 6. Applications for follow-up projects**

with an indication of the status (submitted / approved) and the funding organization.

**6.1 Applications for follow-up projects** (FWF projects)

(with an indication of the project type, e.g. stand-alone project, NFN, SFB, WK,  
fellowship, contribution to a stand-alone publication)

- 1) Bond and site selective dissociative electron attachment; stand alone project,  
approved
  - 2) Synthesis and Spectroscopic Characterization of Ultracold Molecular Anions,  
Translational brain power, submitted
- etc.

**6.2 Applications for follow-up projects** (Other national projects)

(e. g. FFG, CD Laboratory, a K-plus Centre, funding from the Austrian National  
Bank, the Federal Government, the provincial government or similar)

- 1)
  - 2)
- etc.

**6.3 Applications for follow-up projects** (International projects)

(eg. ERA project, ESF)

- 1) Electron Controlled Chemical Lithography, ESF COST Action CM0601, approved
- 2) Scientific and Technical Studies on Biomedical Uses of Radiation, ITN, submitted  
etc.