# **Electron and Positron Induced Chemistry** (EPIC)

#### EU Network contract no. HPRN-CT-2002-00179

Commencement September 2002 (Funds received December 2002) Duration 36 months Period covered by this report: September 2002 to June 2004

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Network home page: <a href="http://physics.open.ac.uk/epic/EPIC%20home.html">http://physics.open.ac.uk/epic/EPIC%20home.html</a>

Location of the Mid-Term review meeting; Obergurgl, Austria

Date and timing of meeting: June 19<sup>th</sup> - June 23<sup>rd</sup> 2004,

#### Part A: Research Results

#### A1 Scientific Highlights;

The EU Framework V Network Electron and Positron Induced Chemistry (EPIC) is a network of internationally renowned research teams in Europe dedicated to the study of electron and position interactions with molecules. Its research is broadly divided into two sub-topics based upon the type of molecular target involved.

- 1. Studies of interactions with halogenated targets. Such molecules are relevant to industrial plasmas, in particular those used in the semiconductor industry.
- 2. Studies of interactions with biological molecules and in particular the nucleotide bases, their derivatives and water. This research is linked to the study of radiation damage in DNA and other biological systems.

#### Participating institutions are;

- 1. Centre of Molecular and Optical Sciences, The Open University, United Kingdom
- 2. Department of Physics and Astronomy, University College London, United Kingdom
- 3.Institut fur Ionenphysik, Leopold Franzens Universitaet Innsbruck, Austria
- 4. Department of Physical Chemistry, Freie Universitaet Berlin, Germany
- 5.Department of Chemistry, Universita di Roma 'La Sapienza', Universita di Roma 'La Sapienza', Italy
- 6. Department of Physics, University of Aarhus, Denmark
- 7. J Heyrovsky Institute of Physical Chemistry, Academy of Sciences of the Czech Republic, The Czech Republic.
- 8. Laboratoire des Collisions Atomiques et Moléculaires Université Paris-Sud, Paris, France

#### Together with collaborators within:

Department of Physics, Trento University, Italy Department of Physics, University of Bonn, Germany Department of Physics, Charles University, Prague, Czech Republic Institute of Physics Belgrade, Serbia Department of Physics, Comenius University, Slovakia CSIC, Madrid, Spain

The Network officially started in September 2002 although funds were only received in December 2002 and many network staff were not therefore appointed until 2003. The Network has nevertheless in the first year shown itself to be a dynamic and rapidly evolving Network of the leading scientists in Europe. In the second year the research programme has developed rapidly with the employment of a number of excellent and dynamic Younger researchers funded by the Network. The Network's study of electron impact with biomolecules has received particular attention with two recent PRL publications from Institut fuer Ionenphysik, Leopold Franzens Universitaet and Frei Universitaet Berlin on dissociative attachment to nucleotide bases receiving coverage in the international media. A complementary theoretical calculation (performed by URLS) on the dynamics of Uracil fragmentation after electron attachment has likewise been published in PRL and received widespread publicity. These results provide

significant consequences for the molecular description of genotoxic effects in living cells due to low-energy electrons, which are found to be the most abundant secondary species formed from ionizing radiation.

The second highlight concerns the potential of slow electrons to act as a soft tool to control a chemical reaction in the condensed phase. By setting the energy of a well defined electron beam to values below 3 eV the FUB team have shown that the surface of a thin film of  $1,2\text{-}C_2F_4Cl_2$  molecules can be completely transformed into molecular chlorine (and byproducts, possibly perfluorinated polymers). At higher energies (above the threshold for electronic excitation, > 6 eV) some equilibrium composition between product and initial molecule can be achieved, however, accompanied by a gradual overall degradation of the film. The effect of complete transformation is based on both the *selectivity* and particular *energy dependence* of the *initial* step of the reaction which is dissociative electron attachment (DEA) to  $C_2F_4Cl_2$  but also the fact that the initial molecule is efficiently decomposed by subexcitation electrons while the product  $Cl_2$  is virtually unaffected.

Due to this rapid progress in the scientific research amongst the teams three further networks based upon the core research in the EPIC network have been awarded. An EU COST Action RADAM (Physics P9) commencing in November 2003 to study radiation damage at the molecular level. This five year programme links the electron/positron community with those studying ion and photon damage of biological molecules and brings EPIC network members together with radiation chemists and medical researchers. A joint meeting between EPIC and RADAM is to be held in Lyons 24th to 27th June 2004 <a href="http://costp9-radam.in2p3.fr/index.html">http://costp9-radam.in2p3.fr/index.html</a>. In 2005 EPIC will participate in the international Miller conference on Radiation chemistry to be held in Nice in September.

An ESF Funded Programme entitled Electron Induced Processing at the Molecular level (EIPAM) bringing EPIC members together with researchers in the Scanning Tunnel Microscopy (STM) community to study how nanoscale physics and chemistry may be developed using STM techniques. This five year programme will start in July 2004 and the first meeting will be held as part of the 332nd Wilhelm and Else Heraeus Seminar, "Processes Driven by Low Energy Electron-Molecule Interactions" 1st-4th September, 2004 at Bad Honnef, Germany. Once again EPIC members will participate in this meeting and younger participants of the Network will present their work in oral and poster sessions.

An ESF Network entitled 'Collisions in Atom Traps (CATS)' will bring together members of the cold atom community and members of EPIC to investigate electron/positron interactions with cold atoms and cold molecules, while also exploring the new world of ultracold plasmas! A three year programme commenced in October of 2003 and has led to the design of several novel experiments which will become active in late 2004.

Network members have also been successful in developing research links with other members of the academic community and with applied/industrial partners. The OU team in particular has provided results on several fluorocarbon replacements for the semiconductor industry that have received widespread interest amongst the industrial community particularly in Japan. The set of data collected by network members on electron interactions with fluorocarbons species is amongst the most comprehensive set of data collected for these species. We are therefore developing links with Japanese industry, hosting a special workshop (organised by EPIC members) in Stockholm July 21-22, 2003 between European and Japanese researchers. In

February several members of the EPIC Network attended a second meeting in Tokyo and a regular conference series is now planned entitled EU Japan Symposium on Plasma Processing. The third meeting will be held in Slovakia in January 2005. The Network Co-ordinator was invited to the first meeting of Centres of Excellence in Plasma Technology in Nagoya in April 2004. A formal agreement between such CoE's is being established with the intention of exchanging staff and students between such centres. It is expected that some of the Young Researchers employed by the Network will take advantage of these exchanges and travel to Japan to conduct further research, their training in the EPIC Network having made them highly suitable personnel for such a programme.

Thus EPIC is definitely fulfilling the hopes of its participants in acting as a forum and focus for development of electron and positron research within the European Community. In the next two years EPIC will seek to develop still further and explore links with research groups worldwide to ensure that a truly international research programme in electron and positron physics is developed with applications exploited from astrophysics to life sciences.

The development of such a vibrant research community is ideal for the training of young research scientists. The major goal of EPIC is to train the next generation of researchers such that research in electron and positron research will continue to grow and develop in the next decade. The network has been fortunate to recruit a unique set of talented younger researchers whose work in the next two years will provide much of the momentum and creativity of the research programme. Training of these younger researchers has, and will, require a set of workshops, the first of which was held in the UK in September 2003 dedicated to training researchers in the study of biological systems and included practical courses in DNA extraction and analysis. A Vacuum training course was held in December 2003 and a theoretical methods school is planned for later in 2004. Presentation and communication skills have been developed by their attendance at Network meetings where younger researchers present their work to the Network members and other senior researchers. All younger researchers employed by July 2003 gave presentations at the EPIC network meeting in Prague in July 2003 and will do so again at the Mid-term review meeting in Obergurgl together with presentations by more recently employed research fellows.

Thus the network has made an impressive start to its activities and will continue to develop as our younger researchers are increasingly integrated into and develop the research programme. Further details please see the Network webpage and those of the partners (<a href="http://physics.open.ac.uk/epic/EPIC%20home.html">http://physics.open.ac.uk/epic/EPIC%20home.html</a>)

#### **Difficulties encountered to date**

No major difficulties have been encountered to date; the Network being judged a great success by its participants and by the wider research community.

Recruitment was slow for some groups with delays in obtaining the funding from the EC (received only in December 2002) leading to the loss of two young researchers who had in principle agreed to join the network but who took other posts in October 2002 where funds were *immediately* available. This has led to a slower than expected start for positron based research at UCL (partner 2) and for partner 5 (ULRS, Rome). However all posts are now filled or have candidates under consideration. The staggered appointment schedule required some alteration in the order of training courses with the experimental programme being accelerated and theoretical

slightly retarded, reflecting the appointment of experimental researchers ahead of theoretical appointees.

In October 2002 the Network co-ordinator left University College London to take up a new post as Professor of Physics and Director of Research at the Open University. Since the original application involved a joint experimental and theoretical training programe at UCL this requires some alteration in the training arrangements between UCL and OU with UCL continuing training in theoretical aspects of the programme and OU undertaking the experimental. For this reason Postdoc appointments were not made until July 2003 (for experiment) and January 2004 (for theory). The two institutes are only an hour travel time apart so the two teams are in weekly contact. Some rearrangement of funds between OU and UCL was also necessary to meet these arrangements.

The largest 'difficulty' of the network to date has been its success! Many other European groups as well as USA, Japanese, Australian, Brazilian and Indian groups have requested observer status to allow them to integrate with the research programme. We have been pleased to welcome them to our meetings (unpaid) and are delighted by the subsequent research that has evolved from these links. The success in obtaining support for an ESF Networks, an ESF programme, a COST Action and a collaboration partnership with Japanese government/industry ASET consortia has shown that the EPIC Network is achieving its stated goal of integrating European research in Electron and Positron Chemistry making Europe the international leader in this area. It is an environment in which the young researchers can and do thrive! We thank the EU for their support.

### **A2 Publications:**

Those in italics are publications involving one or more network partners. Brackets refer to partner numbers listed as in A1.Underscore indicates younger member of the network.

#### Partner 1; Open University

- 1. S Eden, P Limão-Vieira, N J Mason and S V Hoffmann. VUV spectroscopy of CF3Cl, CF3Br, CH3I and CH3Cl (2003) in preparation. (1,6)
- 2. T Mikoviny, M Kocan, S Matejcik, N J Mason and J D Skalny Complex study of negative corona discharge in pure carbon dioxide and its mixtures with oxygen. J Phys D (2004) 37 64-73
- 3. N J Mason and M J Hubin-Franskin, A Giuliani, I C Walker, J Delwiche, S V Hoffman, C Kech, P L Vieira, On the valence shell electronic spectroscopy of 2-vinyl furan J. Chem Phys (2004) **120** 10972-10982
- 4. Jan D. Skalny, Tomas Mikoviny, Stefan Matejcik, Nigel J. Mason An analysis of mass spectrometric study of negative ions extracted from negative corona discharge in air. Int J Mass Spec. (2004) **233** 317-24
- 5. J D Skalny, S Matejcik, T Mikoviny, S Eden and N J Mason Ozone generation in a negative corona discharge fed with N<sub>2</sub>O and O<sub>2</sub> J Phys D; Applied Physics (2004) **37** 1052-57
- 6. B K Antony, N J Mason and J Tennyson R-matrix calculation of low-energy electron collisions with LiH J Phys B (2004) 37 1689 1697.(1,2)
- 7. Y Itikawa and N J Mason Cross Sections for electron collisions with water molecules Journal Chem Phys Ref Data (2004) Submitted

- 8. I Rozum, N J Mason and J Tennyson Electron collisions with the CF3 radical using the R-matrix method New Journal of Physics (2003) **5** 155
- 9. P Limao Vieira, S Eden, N J Mason and S V Hoffmann Electronic State spectroscopy of acetaldehyde, CH<sub>3</sub>CHO by high resolution VUV photo-absorption Chem. Phys. Lett **376** 737-47 (2003)(1,6)
- 10. S Eden, P Limão-Vieira, N J Mason and S V Hoffmann. VUV photo-absorption of hexafluoropropene C3F6 Chem. Phys. Lett. (2003) in press (1,6).
- 11. S Eden, P Limão-Vieira, P Kendall, N J Mason, J Delwiche, M-J Hubin-Franskin, M Kitajima, H Tanaka, H Cho, S Hoffmann and S Spyrou. Electron excitation of tetrafluoroethylene, C2F4 Chem. Phys. Lett., (2003) in press.
- 12. R Balog, M Stano, P. Limão-Vieira, C Konig, I Bald, N J Mason and E Ilenberger J. Low energy (0-18eV) electron interaction with free and bound SF<sub>5</sub>CF<sub>3</sub>: Negative ion formation from single molecules, clusters and nanofilms Chem Phys (2003) **119** 10396
- 13. I C Walker, M H Palmer, J Delwiche, S V Hoffman, P Limão-Vieira, N J Mason, M F Guest, M-J Hubin-Franskin, J Heinesch and A Giuliani.

  The electronic states of isoxazole studied by VUV absorption, electron energy-loss spectroscopies and ab initio multi-reference configuration interaction calculations J. Chem. Phys., (2003) in press (1,6)
- 14. P Limão-Vieira, S Eden, N J Mason and S V Hoffmann. High resolution VUV photo-absorption of acetaldehyde, CH3CHO Chem. Phys. Lett. (2003) 376, 737-747.(1,6)
- 15. A Giuliani, I Walker, J Delwiche, S V Hoffmann, P Limão-Vieira, N J Mason, M-J Hubin-Franskin. Electronic spectroscopy of fufuryalcohol (1,6)
  - J. Chem. Phys. (2003) J. Chem. Phys. 119 (2003) 7282
- 16. A Giuliani, J Delwiche, S V Hoffmann, P Limão-Vieira, N J Mason, M-J Hubin-Franskin. 2-methylfurane: An experimental study of the excited electronic levels by electron energy loss spectroscopy, UV-VUV photo-absorption spectroscopy(1,6) J. Chem. Phys. (2003) in press.
- 17. P Limão-Vieira, S Eden, N J Mason.
  - Absolute photo-absorption cross sections and electronic state spectroscopy of selected fluorinated hydrocarbons relevant to the plasma processing industry Radiat. Phys. Chem. (2003) 68, 187-192.
- 18. P Limão-Vieira, P A Kendall, S Eden, N J Mason, J Heinesch, M-J Hubin-Franskin, J Delwiche, A Giuliani.
  - Electron and photon induced processes in SF5CF3
  - Radiat. Phys. Chem. (2003) 68, 193-197
- 19. P Limão-Vieira, S Eden, P A Kendall, N J Mason, A Giuliani, M-J Hubin-Franskin, J Delwiche and S V Hoffmann.
  - Electronic excitation and oscillator strength of SF5CF3 by high resolution VUV photoabsorption, electron energy loss and He(I) photoelectron spectroscopy Chem. Phys. Lett. (2003) submitted.
- 20. A Pelc, W Sailer, P Limão-Vieira, N J Mason, J Limtrakul, P Scheier, M Probst and T D Märk.
  - Low energy electron attachment to CH3CN Chem. Phys. Lett., (2003) in press (1,3).

- 21. S Eden, P Limão-Vieira, P Kendall, N J Mason, S V Hoffmann, S M Spyrou. High resolution photo-absorption studies of acrylonitrile, C2H3CN, and acetonitrile, CH3CN Eur. Phys. J. D, (2003) in press. (1,6)
- 22. S Eden, N J Mason, P Limão-Vieira, M Kitajima, M Okamoto, H Tanaka, D Newnham and S Hoffmann.
  Electron and Photon Impact Studies of CF3I
  - in Electron Scattering from Atoms, Nuclei, Molecules and Bulk Matter, Ed.C T Whelan and N J Mason, Plenum Press, (2003) pp. 33-44.
- 23. P A Kendall, N J Mason, G A Buchanan, G Marston, P Tegeder, A Dawes, S Eden, P Limão-Vieira, D A Newnham.
  Temperature dependent high-resolution infrared photo-absorption cross sections of trifluoromethyl sulphur pentafluoride
  Chem. Phys., 287 (2003) 137-142.
- 24. I Rozum, N J Mason and J Tennyson Electron collisions with the CF radical using the R-matrix method J. Phys B **36** 2419-32 (2003)
- 25. N J Mason, P Limão-Vieira, S Eden, P Kendall, S Pathak, A Dawes, J Tennyson, P Tegeder, M Kitajima, M Okamoto, K Sunohara, H Tanaka, H Cho, S Samukawa, S V Hoffmann, D Newnham and S M Spyrou.
  VUV and Low Energy Electron Impact Study of Electronic State Spectroscopy of CF3I Int. J. Mass Spectrom., 223-224 (2003) 647-660.
- 26. P Limão-Vieira, S Eden, P A Kendall, N J Mason and S V Hoffmann. High resolution VUV photo-absorption cross-section for dimethylsulphide, (CH3)2S Chem. Phys. Lett., 366 (2002) 343-349. (1,6)
- 27. P Limão Vieira, S Eden, P A Kendall, N J Mason and S V Hoffmann. VUV photo-absorption cross section for CCl2F2 Chem. Phys. Lett., 364 (2002) 535-541. (1,6)
- 28. P Limão-Vieira, S Eden, N J Mason, R Balog, C König, I Bald and E Illenberger. Negative ion formation by low electron energy to condensed SF5CF3 molecules 13th Int. Symposium on Electron-Molecule Collisions and Swarms, Prague, Czech Rep. (2003). (1,4)
- 29. C T Whelan and N J Mason Electron Scattering from Atoms, Molecules, Nuclei and Bulk Matter Plenum Press published 2003
- 30. P A Kendall and N J Mason Electron Energy Loss spectroscopy of Trifluromethyl Sulphur Pentaflouride in Electron Scattering from Atoms, Molecules, Nuclei and Bulk Matter ed by C T Whelan and N J Mason Plenum Press 99-110 (2003)
- 31. N J Mason Electron Driven process: Scientific Challenges and Technological opportunities in Electron Scattering from Atoms, Molecules, Nuclei and Bulk Matter Ed by C T Whelan and N J Mason Plenum Press 179-190 (2003)
- 32. N J Mason Electron Scattering from Ozone. What do we know ? Physica Scripta (2003) **68** C37-43
- 33. A. Williart, P. A. Kendall, F. Blanco, P. Tegeder, G. García, and N. J. Mason Inelastic scattering and stopping power for electrons in O<sub>2</sub> and O<sub>3</sub> at intermediate and high energies, 0.3-5 keV Chem. Phys. Lett. (2003)
- 34. S Eden, P Limão-Vieira, P Kendall, N J Mason, M Kitajima, H Tanaka, H Cho, M-J Hubin-Franskin, J Delwiche and S Hoffmann.

  Spectroscopic studies of valence, Rydberg and ionic states of tetrafluoroethylene, C2F4 13th Int. Symposium on Electron-Molecule Collisions and Swarms, Prague, Czech Rep. (2003). (1,4)

35. P Limão-Vieira, S Eden, N J Mason, A Giuliani, M-J Hubin-Franskin, J Heinesch, J Delwiche, R Balog and Eugen Illenberger.

Electronic state spectroscopy of SF5CF3 by gas-phase and condensed phase conditions XXIII ICPEAC, Stockholm, Sweden, (2003). (1,4)

36. S Eden, P Limão-Vieira, N J Mason, M Kitajima, H Tanaka, H Cho, A Giuliani, M-J Hubin-Franskin, J Delwiche.

Electronic excitation of tetrafluoroethylene, C2F4

XXIII ICPEAC, Stockholm, Sweden, (2003).

37. P Limão-Vieira, P A Kendall, S Eden and N J Mason.

On the role of CCl2F2, (CH3)2S and SF5CF3 in stratospheric ozone depletion and global warming

VI Iberian Joint Meeting on Atomic and Molecular Physics, Madrid, Spain (2003).

38. S Eden, P Limão-Vieira and N J Mason.

High resolution VUV photo-absorption and electronic state spectroscopy of tetrafluoroethylene, C2F4

VI Iberian Joint Meeting on Atomic and Molecular Physics, Madrid, Spain (2003).

39. P Limão Vieira, P A Kendall, S Eden and N J Mason.

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2nd Conference on the Elementary Processes in Atomic Systems, Gdansk, Poland, (2002) 82.

40. S Eden, P Limão Vieira and N J Mason.

Absolute photo-absorption cross sections and electronic state spectroscopy of fluorinated selected hydrocarbons relevant to the plasma processing industry

2nd Conference on the Elementary Processes in Atomic Systems, Gdansk, Poland, (2002) 60.

41. S Eden, P Limão Vieira and N J Mason.

Electron and photon induced processes in plasma etching gases

4th International Workshop on Fluorocarbon Plasmas, Col de Porte, Isère, France, (2002) 10.

42. N J Mason, S Eden, P Kendall. P Tegeder and P Limão Vieira.

Electron scattering from molecular systems relevant to plasma industry: A combined experimental and theoretical study

Int. Conf. on Current Develop. in Atomic, Mol. and Chem. Phys. with Appl., Delhi, India, (2002) 6.

43. P Limão Vieira, S Eden, and N J Mason.

Electron and photon induced processes in plasma etching gases

V Iberian Joint Meeting on Atomic and Molecular Physics, Lisbon, (2002) 49.

44. N J Mason, S Eden, P Limão Vieira, P Kendall, S Pathak, A Dawes, P Tegeder, M Kitajima. M Okamoto, H Tanaka, S Samukawa, H Cho and S Hoffmann.

Electron and Photon Impact Studies of CF3I

XIII International Symposium on Atomic, Cluster and Surface Physics, Going, Austria, (2002) 159.

#### Partner 2; University College London

1. I Rozum, NJ Mason and J Tennyson.

Electron collisions with the CF2 radical using the R-matrix method

J. Phys. B: At. Mol. Opt. Phys., 35, 1583-1591 (2002).(1,2)

2 JD Gorfinkiel, LA Morgan and J Tennyson.

Electron impact dissociative excitation of water within the adiabatic nuclei approximation J. Phys. B: At. Mol. Opt. Phys., 35, 543-555 (2002)

3. JD Gorfinkiel, LA Morgan and J Tennyson.

Electron impact dissociative excitation of water within the adiabatic nuclei approximation J. Phys. B: At. Mol. Opt. Phys., 35, 543-555 (2002)

4. A Faure and J Tennyson.

R-matrix calculations for polyatomic molecular ions: electron scattering by H3+ and H3O+ J. Phys. B: At. Mol. Opt. Phys., 35, 1865-1873 (2002).

5. CS Trevisan and J Tennyson.

Calculated rates for the electron impact dissociation of molecular hydrogen, deuterium and tritium

Plasma Phys. Controlled Fusion, 44, 1263-1276 (2002).

6. A Faure and J Tennyson.

Electron-impact rotational excitation of symmetric top molecular ions

J. Phys. B: At. Mol. Opt. Phys., 35, 3945-3956 (2002).

7. CS Trevisan and J Tennyson.

Calculated rates for the electron impact dissociation of molecular hydrogen: mixed isotopomers and scaling laws

Plasma Phys. Controlled Fusion, 44, 2217-2230 (2002).

8. A Faure and J Tennyson.

Rate coefficients for electron-impact rotational excitation of H3+ and H3O+ Mon. Not. Roy. astr. Soc., 340, 468-472 (2003).

9. I Rozum, NJ Mason and J Tennyson.

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*J. Phys. B: At. Mol. Opt. Phys.*, (in press) (1,2)

10. J Tennyson, JD Gorfinkiel, I Rozum, CS Trevisan and N Vinci.

Electron molecule collisions calculations using the R-matrix method

Radiation Phys. Chem., (in press).

11. A Faure, J Gorfinkiel and J Tennyson.

Electron-impact rotational excitation rates for the water molecule Mon. Not. Roy. astr. Soc., (submitted).

12. Laricchia, S Armitage, DE Leslie and P Van Reeth.

Positron and positronium interactions with atoms and molecules Radiation Physics and Chemistry (2003) in press

13. DE Leslie, S Armitage and G Laricchia.

Positronium Beam Production and Scattering contributed paper, Positron03 Workshop, Denmark

14. C Arcidiacono, A Kover and G Laricchia.

Electron ejection from collisions of positrons with helium contributed paper, Positron03 Workshop, Denmark

15. M Szluinska and G Laricchia

Ionization processes induced by positrons contributed paper, Positron03 Workshop, Denmark

16. M Szluinska, P Van Reeth and G Laricchia.

Empirical scaling of positron- and electron- impact ionization cross-sections contributed paper, Positron03 Workshop, Denmark

17. G Laricchia, S Armitage and DE Leslie

Positronium induced collisions

invited paper, Positron03 Workshop, Denmark

18. A Kover, C Arcidiacono and G Laricchia.

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invited paper, Positron03 Workshop, Denmark

19. DE Leslie, S Armitage and G Laricchia.

Production of collimated positronium from molecular nitrogen

J Phys B 35 (2002) 4819-4827

20. S Armitage, DE Leslie, AJ Garner and G Laricchia.

Fragmentation of positronium in collision with He atoms

Physical Review Letters 89 (2002) 173402-1

21. M Szluinska, P Van Reeth and G Laricchia.

Empirical scaling of positron- and electron-impact ionization cross sections J Phys B 35 (2002) 4059

22. G Laricchia, P Van Reeth, M Szluinska and J Moxom.

Total positron-impact ionization and positronium formation from the noble gases J Phys B 35 (2002) 2525

23. G Laricchia.

Scattering of positrons and positronium by atoms and molecules in

The Physics of Electronic and Atomic Collisions

(Rinton Press, New York) (2002) 329

24. S Armitage and G Laricchia.

Positronium scattering from atoms and molecules

Nucl. Instr. Meth. B 192 (2002) 67

25. P Van Reeth, M Szluinska and G Laricchia.

On the normalization of the positron-impact direct ionization cross-section in the noble gases

Nucl. Instr. Meth. B 192 (2002) 220

26. A Kövér, K Paludan and G Laricchia.

Electron ejection by positron impact ionization

Nucl. Instr. Meth. B 192 (2002) 167

27. M Szluinska, P Van Reeth and G Laricchia.

Energy dependence of the total ionization and positronium formation cross-sections in e+- Xe collisions

Nucl. Instr. Meth. B 192 (2002) 215

28. JW Humberston, P Van Reeth and G Laricchia.

Correlations between cross sections and threshold energies for positronium formation and direct ionization

Nucl. Instr. Meth. B 192 (2002) 44

- 29. M. Szluinska and G. Laricchia Investigation into the energy dependence of the annihilation cross-section for Ne and Xe below the positronium formation threshold Nucl. Instr. Meth. B221 (2004) 100-106
- 30. G. Laricchia, S. Armitage and D. E. Leslie Positronium induced collisions Nucl. Instr. Meth. B221 (2004) 60-68

- 31. M. Szłuińska and G. Laricchia Positronium formation from Ar and Xe Nucl. Instr. Meth. B221 (2004) 107-111
- 32. Á. Kövér, <u>C. Arcidiacono</u> and G. Laricchia Differential ionization experiments on positron atom scattering Nucl. Instr. Meth. B221 (2004) 56-59
- 33. Z. D. Pešić, C. Arcidiacono, R. Hellhammer, N. Stolterfoht and G. Laricchia Ionisation and fragmentation of H2O molecule in the interaction with positrons and ions to be published in AIP conference series (2004)

#### 3. UIBK: Institut fuer Ionen Physik, University of Innsbruck

1. <u>L Feketeova</u>, DJ Skalny, G Hanel, B Gstir, M Francis, TD Märk.

Production of Cl via dissociative electron attachment to Cl2

Int. Mass Spectrom., 223/224 (2003) 661-668.

2. A Pelc, W Sailer, P Scheier, NJ Mason, E Illenberger, TD Märk.

Electron attachment to simple organic acids

Vacuum, 70 (2003) 429-433.(3,1)

3. B Gstir, S Denifl, G Hanel, M Rümmele, T Fiegele, M Stano, <u>L Feketeova</u>, S Matejcik, K Becker, P Scheier and TD Märk.

High resolution multiple electron impact ionisation of He, Ne, Ar, Kr and Xe atoms close to threshold: appearance energies and Wannier exponents

Nucl. Instr. Methods, submitted (2002)

4. G Hanel, B Gstir, S Denifl, D Muigg, T Fiegele, M Rümmele, W Sailer, A Pelc, N Mason, E Illenberger, S Matejcik, F Hagelberg, K Becker, A Stamatovic, M Probst, P Scheier, TD Märk. (3,4)

High resolution electron interaction studies with atoms, molecules, biomolecules and clusters

Book (N. Mason, ed.) Cambridge Univ. Press, in print (2002)

5. S Matt, R Parajuli, O Echt, C Lifshitz, A Stamatovic, P Scheier and TD Märk. Kinetics and energetics of spontaneous and electron-induced fragmentation of molecular

ions and cluster ions Book of Invited Papers of ICPEAC, in print (2002)

- 6. H Deutsch, K Becker, P Defrance, U Onthong, M Probst, S Matt, P Scheier and TD Märk. Calculated cross section for the electron impact ionisation of simple molecular ions Int. J. Mass Spectrometry, 223/224 (2003) 639-646.
- 7. JD Skalny, S Matejcik, T Mikoviny and TD Märk.

Effect of temperature on dissociative electron attachment to CCl2F2

Int.J.Mass Spectrom., 223/224 (2003) 217-228

8. P Cicman, M Francis, JD Skalny, TD Märk.

The Ion Extraction Efficiency in a Crossed Beams Experiment using a Trochoidal Electron Monochromator

Int. Mass Spectrom., 223/224 (2003) 271-278

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- 13. C.D. Marinica, J.P. Gauyacq, D. Teillet-Billy
  Inelastic electron scattering on a molecule embedded in a host medium: role of the
  electronic structure of the medium
  To be published
- 14. C.D. Marinica, C. Ramseyer, D. Teillet-Billy, J.P. Gauyacq Adsorbed molecule on a metal surface covered with a rare gas Ar monolayer : adsorption site effect on the  $N_2^{-2}\Pi_g$  resonance To be published

For further details please see the Network webpage and those of the partners (http://physics.open.ac.uk/epic/EPIC%20home.html)

#### Part B

#### **Comparison with the Joint programme of work (ANNEX 1 of the Contract)**

#### **B1: Project Objectives**

The major objectives of the proposed Network are to:

- (i) Train young researchers in the latest experimental and theoretical techniques for studying electron/positron induced chemistry by providing them with the opportunity to undertake research within internationally renowned research centres.
- (ii) Provide the most co-ordinated study ever undertaken, either experimental or theoretical, of the fundamental chemistry initiated by the irradiation by electrons and positrons of molecules (from diatomic to macromolecules) and
- (iii) To develop a new understanding of the basic processes by which such chemical reactions are induced and how such reactions are modified by their local environment.

#### In particular the Network will;

- 1. Study fundamental electron and positron energy transfer processes.
- 2. Study electron and positron impact dissociation processes yielding reactive neutral, anionic and cationic species.
- 3. Study how such processes are modified in the different phases of matter (gases, clusters and on surfaces.
- 4. Probe new reaction processes initiated in denser phases of matter e.g. nucleophilic substitution).

Different molecular compounds have been selected to illustrate these processes; halogenated hydrocarbons and fluorocarbons; simple biomolecules (e.g. DNA and RNA bases) and water. These objectives remained unchanged after the first year and excellent progress has been made towards achieving these objectives.

#### **B2** Research method and Work plan

#### **Experimental techniques**

Authoritative investigations of electron/positron-molecule interactions require the adoption of several different experimental methods within this Network. All the current state-of-the-art experimental techniques for probing electron/positron induced reactions with molecules are available to the researchers. In the first year of the Network these techniques have been developed still further making the participants amongst the leading pioneers of techniques or producing sources of biomolecules and ongoing work (led by younger researchers employed by the Network) is leading to the study of DNA itself with high resolution electron scattering apparatus (OU, FUB and UIBK) and the development of new techniques for probing DNA including use of Atomic Force Microscopy - AFM (OU and UAR).. The UAR group has pioneered the development of the first synchrotron based photo-ionisation electron source, a source that is capable of producing electron beams with resolutions of 2 meV at incident energies as low as 1 meV. With such a source it is possible to study electron impact induced rotational excitation and makes it possible to probe threshold phenomena at the onset of each mode of molecular excitation and has led to the investigation of a new class of scattering processes, named cold collisions with the electrons at temperature comparable to those of cold atoms .

The UCL team has developed corresponding methods for the investigation of single and multiply charged ionization (with and without positronium formation) including the first near-threshold measurements and the first complete (e,2e) type experiments with positrons. Techniques for generating positronium beams have also been developed and applied to the study of the interaction of simple atomic and molecular targets. Methods for extending these to more complex targets and probing those interactions that transfer energy directly into the target molecule are currently under development with the appointment of younger members of the research network.

Experimental teams in Berlin (FUB) and Paris (UPSO) have pioneered the transfer of gaseous phase experimental and theoretical techniques into the study of electron molecule collisions upon surfaces and are recognized as leaders in this field. Research performed this year through a collaboration of network members has led to a new understanding of state selective dissociation on surfaces with subsequent consequences for site selective chemistry using STM technology. In contrast the study of positron interactions in the condensed phase under single collision conditions has yet to be explored and this network is providing the first opportunity for developing techniques (both experimental and theoretical) to initiate such studies.

#### **Theoretical Methods**

The UCL team has led the modern development of the R-Matrix method for treating electron interactions with molecules. For diatomic molecules the R-matrix method has been extended to the nuclear coordinate which has allowed for the first time full, *ab initio* non-adiabatic treatments of vibrational excitation and dissociative electron attachment. UCL have recently developed a novel procedure for treating near-threshold electron impact dissociation. In addition the UCL group has recently extended their code to treat polyatomic molecules. This work is complemented by the team in Bonn (sub-node of FUB) who use a similar formalism. URLS have long employed methods based on single centre expansions to study electron interactions with polyatomic molecules. Such calculations may be used to study larger molecules still beyond the scope of the R-matrix method (eg biomolecules). Furthermore URLS have considerable experience of performing vibrational and rotational excitation calculations on polyatomics. UCL and URLS are collaborating in studies to provide cross sections for those targets for which experiments remain too difficult (eg radicals). The transfer of electron scattering methodologies from the gaseous phase to the treatment of inelastic electron scattering on molecules physisorbed on metal surfaces has been pioneered by the UPSO team.

The group at URLS have developed several dedicated scattering codes for treating the quantum dynamics of low-energy positron beams in a molecular gas, specifically one containing polyatomic molecules. These codes are now shared and have developed jointly with younger network members employed by ICP. This Network therefore contains the only research teams currently able to evaluate annihilation rates in polyatomic gases and who are able to evaluate total and differential elastic cross sections below the Ps formation threshold.

Thus the network has developed the research methods outlined in the original proposal with significant progress being made in the first year, progress that is expected to be accelerated still further in year 2 as younger members complete their initial training.

#### **B3** Schedule and Milestones

The work plan is set out in terms of three inter-linked scientific strands namely the study of:

- Electron and positron induced reactions in the gaseous phase.
- Reactions in molecular clusters and aggregates and
- Reactions in the condensed phase.

#### In the original Annex 1 the following milestones were declared

- **Year 1:** Advertising/ recruitment of Younger Researchers. Establishment of Network WWW site.
- (Month 1 -6) First Network meeting to determine specific project schedule and identify molecular targets to be studied by each partner laboratory.
- (Month 7-12) Experimental research programme on halogenated hydrocarbons and fluorocarbons commenced.
   Master class in 'Theory of Molecular dynamics and symmetry' organised by UCL Master Class in Theoretical Modelling organised by ULRS.

Master class in surface preparation and UHV techniques organised by FUB and UPSO.

The First Network meeting to determine specific project schedule and identify molecular targets to be studied by each partner laboratory was held at the coordinator's new institution in February 2002.

At this meeting it was agreed to continue to organise the research of this Network in this manner. For each of these strands four specific molecular targets have been chosen since these provide the opportunity to determine the reactivity as a function of particular site and/or chemical bond. The targets selected are:

- Halogenated hydrocarbons ( $CH_xR_y$  where R is any halogen species F, Cl, Br and I and x +y = 4 and the fluorocarbons ( $CF_xR_y$  where R is Br,Cl (or H) and x +y = 4).
- Simple bio-molecules that form the bases of DNA and RNA (adenine, cytosine, guanine, thymine and uracil) often called the *building blocks of life*.
- WATER, the universal solvent.

## 1. Electron and positron induced reactions in the gaseous phase Teams involved :OU, UCL, UIBK, FUB, ULRS, UAR, ICP

Experimental Programme: The different fragmentation patterns induced by low energy electrons and positrons have been explored many halogenated hydrocarbons and fluorocarbons. The electronic state spectroscopy has been extensively investigated by OU and differential cross sections measured. Yields of both anionic and cationic fragments have been measured together with their kinetic energy by UIBK and FUB. Total electron scattering cross sections have likewise been measured at low energy ( < 1eV) by UAR and provide a complementary means of determining the probability of a specified molecule to undergo dissociative attachment. This work has attracted the interest of many groups worldwide involved in plasma etching. This has led to the development of strong links with Japanese industry (see above).

Perhaps the most dramatic progress in the network has been in the study of electron scattering from bio-molecules, in particular the DNA bases adenine, cytosine, guanine, thymine and RNA base uracil and most recently the larger biomolecules including glycine, simple sugars and acids. This work has dramatic consequences for our understanding of radiation damage and has attracted worldwide attention with UIBK and FUB 's PRL publication being reported in international media.

We have also started an extensive study of water with completion of a comprehensive review of current state of knowledge of electron interactions with water. This work is seen to be pivotal to future research radiation damage. In particular the formation of anions by dissociative electron attachment has been shown to be an important problem in salvation chemistry. However the data for this mechanism is both rather old and conflictory such that it is necessary to repeat this work and compile authoritative cross sections. As part of this Network one of the Young researchers (from OU) in collaboration with researchers at another node (UIBK) have recently measured DEA in gaseous water. These results may also be compared with theoretical research at UCL and ULRS.

Theoretical Programme: Methodology and general purpose codes, built upon existing codes constructed by teams in the network, have been developed to study fundamental electron interactions with halogenated hydrocarbons and fluorocarbons leading to excitation and dissociation. These have highlighted the different electron attachment processes to the CF<sub>x</sub> radicals with CF supporting electron attachment but CF does not, the consequences of which are dramatic for design of future industrial semiconductor plasmas. The UCL group has also reported the first results for electron induced dissociation of the water molecule. ULRS have performed the first calculations on complex biological molecules (glycerine) pioneering new methods for probing radiation damage studies at the molecular level. In collaboration with ICP they have likewise developed methodology to study positron interactions with simple molecular targets, results that are now being tested by experiments performed at UCL.

## Task 2. Reactions in clusters and aggregates Teams: UCLE,ULCP,FUB,UIBK,UPSO

The goals of this research programme are to compare the electron induced reactions in the gas phase with those observed in simple cluster or aggregates and to determine the importance of intra-cluster scattering phenomena (electron transfer between the cluster components) in both primary and secondary chemical reactions. Some initial work in preparing clusters of halogenated hydrocarbons and fluorocarbons to study the role of such reactions as a function of cluster size and chemical composition have been performed by FUB some of which is in collaboration with OU. These studies have shown the dramatic changes to be found when electrons interact with even the simplest dimmers. This work is now to be extended to pioneering studies of electron attachment to bio-molecules and to targets consisting of a bio-molecule clustered either with water or simple organic molecules. The experimental research has been complemented by theoretical calculations at ULRS.

#### Task 3. Reactions in the condensed phase

**Teams: OU, UIBK, FUB, UPSO.** Electron induced reactions from molecules absorbed upon surfaces have been studied both theoretically and experimentally. Most recently one of us (OU) has provided the first evidence for the formation of a bio-molecule by electron impact of simple ice surfaces with the observation of glycine in an irradiated methylamine/water ice mixture. We

have also undertaken experimental studies on the formation and evolution of negative ion resonances in electron scattering from halogenated hydrocarbons and fluorocarbons absorbed on either metallic or ice surfaces (FUB). Dramatic changes in the dissociation pathways have been seen for molecules frozen on a surface compared to the gas phase. Such results suggest that with sufficient understanding it may be possible to perform selective bond breaking chemistry of surfaces using emerging STM technology, hence allowing truly nanoscale chemistry to be undertaken. This exciting prospect has led to the award of an ESF 5 year Programme starting in 2004.

Theoretical modelling of these systems will be developed using a new R-matrix method to investigate how the environment influences the molecular inelastic scattering properties i.e. vibrational excitation, electronic excitation and dissociative attachment processes. Investigation for extending techniques developed for electron studies to using positrons to probe surfaces is also planned.

#### **Network training:**

A Master class in preparation and synthesis of bio-molecules planned for year 2 was organized by the co-ordinator as part of the new UK National Quantum, Atomic and Molecular Physics meeting in September 2003 and Master class in UHV techniques was held in Liege, Bel.gium in December 2003 while a Master class in 'Theory of Molecular dynamics and symmetry' is now planned for autumn in 2004 (delayed until appointment of young theoretical researchers, some of whom do not start until January 2004). Those young researchers in post by July 2003 presented their work at a formal session of the Network meeting held in Prague on July 30, 2003. All researchers in post will present their work at the mid-term review. Annual presentations by younger researchers are an essential requirement for their training in communication and presentation skills.

In summary we have met and exceeded the scientific milestones set for the mid-term of the network.

#### **B5** Organisation and Management

Management Committee. A Management Committee was established at the initial Network Meeting held in the UK in February 2003. The management team is comprised of the leaders of each of the 8 partners and two co-opted members elected by the Network participants (Professor Tennyson from UCL and Professor A Zecca, ULRS). Professor N J Mason chairs the committee. Professor E Illenberger acts as Secretary with special responsibility for ensuring training of the younger members is reviewed. Minutes of the Committee meetings are recorded and are available for scrutiny by the Commission. Each partner nominates a member of their research group as mentor for the Young Researchers employed by them in the Network. At the annual meeting all younger researchers will be interviewed by a mentor (from a different partner) and questioned as to their progress and upon the training received, these comments will be examined by the management committee and where appropriate, action taken. In order to have an unbiased review of the research and training of the Network the Management Committee invited Professor Loucas Christophorou to act as external assessor of the Network. Professor Christophorou is an internationally acclaimed researcher who, having spent many years in the USA as a leader of the electron scattering community, has recently returned to Europe to the National Academy in Athens. His reports on the Initial Network meeting and first annual meeting are available in the meeting minutes.

**Research strand leaders.** To maintain focus the research programme has been divided into three inter-linked scientific strands each reviewed by task leaders.

Task 1; Electron and positron induced reactions in the gaseous phase

**Strand Leader:** Experimental Professor D A Field (UAR)

Task 2. Reactions in clusters and aggregates Strand leader; Professor T Märk, (UIBK)
Task 3. Reactions in the condensed phase

**Strand Leader:** Dr R Azria (UPSO)

Research teams working on each strand meet at least once annually to discuss progress and plan future work. The meetings are chaired by the strand leader. As some strands obviously overlap, joint task meetings will be organised as appropriate at the annual meeting. Between meetings informal contacts are maintained by email and through the Network electronic Newsletter (See below).

Annual Scientific Meetings. An annual scientific meeting is held. In July 2003 the first network meeting was held in Prague July 30 to August 1. The first day of the meeting was a closed meeting of the network at which the younger members of the network presented their work. The remainder of the Network meeting reviewed scientific progress in the three strands and held a general discussion allowing new results to be reviewed and new research avenues to be debated. Part of this meeting was held jointly with the Electron molecule and Swarms meeting allowing international colleagues to learn of the Network research programme. This was particularly useful as it has enabled the network to establish research links with US, Australian, Japanese, Indian and Brazilian research groups, making it a catalyst for international research in electron and positron induced chemistry. The second annual meeting will include the Mid-term review and will be held at Obergurgl in June 2004. Further network meetings are planned in collaboration with ESF networks on Radiation damage (COST P9) to be held in Lyons in June 2004, Collisions in Atom Traps (CATS) – first meeting held in Durham UK March 2004 and the ESF Programme Electron Induced Processing of Atoms and Molecules (EIPAM) the first meeting of which is planned as

part of the 332nd Wilhelm and Else Heraeus Seminar, "Processes Driven by Low Energy Electron-Molecule Interactions" 1st-4th September, 2004 at Bad Honnef, Germany. The network will also have a major presence at the Eighth European Conference of Atomic and Molecular Physics (ECAMP) to be held in Rennes, France July 6-10 2004 and for which N J Mason is the Chairman.

Network Newsletter and Communications. Communications between the Network is enhanced through a Newsletter. This is circulated electronically and will include updated reports by each of the partners (and their sub nodes), abstracts of papers submitted for publication, meeting information and reports, adverts for postdoctoral positions, news of visits between nodes and a monthly review of latest international research papers in the electron/positron induced chemistry scattering (drawn from Web of science database). An abbreviated version of the Newsletter will be available to all international researchers upon registration with the Network. The Newsletter is placed on the Network's WWW site which will also include full details of the partners, their research interests, ongoing research, personal profiles etc. Interim reports and pre-prints of publications will be available electronically from the Network web pages. <a href="http://physics.open.ac.uk/epic/EPIC%20home.html">http://physics.open.ac.uk/epic/EPIC%20home.html</a>

#### **B6** Cohesion with Less Favoured Regions and Associate members

The Network has sought to make major interaction with the newly joined EU countries with many of the young researchers coming from new accession countries. This is to be expected since it is the students from those countries that would require the most training in the new techniques and skills. In addition one node (Prague) is based in Eastern Europe and a sub-node of Austria is based in Commenius University in Bratislava, Slovakia. We have in addition sought to acquire additional resources to allow members of these communities to attend Network meetings (e.g EPS and ESF funds). In the new Networks discussed above there are representations and partners from most of the new EU members in Eastern Europe.

**B7 Connections with industry** A major result of the Network has been to develop contacts with the Semiconductor industry in Japan (see discussion above). These contacts provide further scientific and funding opportunities (including the prospect of some of the young research fellows visiting Japan for joint research projects and obtaining postdoctoral support after the end of their contracts). Such collaboration also ensures that the scientific output of the EPIC network is swiftly put to practical use. Therefore we wish to develop these links in the latter stages of the Network developing a joint EU Japan research programme in electron induced chemistry.

#### C1 Training

#### C1 Appointment of Younger researchers

<u>Recruitment:</u> Research positions available under the Network were widely advertised using electronic media, at conferences and by mail shots to major laboratories. The response was good but many of the applicants were not eligible for EU awards (being from non EU states such as the Former Soviet Union). However by January 2003 all the partners had filled their posts. Some candidates were still completing their PhD and therefore did not join their partners until later in the year or at the beginning of year 2. No Postdoctoral candidate was allowed to take up the post until they had definitively completed their Phd thesis. We therefore have a complete cohort of young researchers in post in year 2. However due to the late start of some posts we have postponed some of the training courses planned in year 1 year 2.

The following table compares the current status of young researchers (Pre-Doc and Post-Doc) as of June 2002 with the plan in the contract.

| Participant   | Contract deliverable of Young<br>Researchers to be financed by the<br>contract (person- months) |              |                | Young Researchers financed by the contract so far (person-months) |              |                                      |
|---------------|---|--------------|----------------|---|--------------|--------------------------------------|
|               | Pre-doc (a)   | Post-doc (b) | Total<br>(a+b) | Pre-doc (c)   | Post-doc (d) | <i>Total</i> ( <i>c</i> + <i>d</i> ) |
| OU<br>(UCLE)  | 0   | 36           | 36             | 0   | 17           | 17                                   |
| UCL<br>(UCLP) | 0   | 24           | 24             | 9   | 5            | 14                                   |
| UIBK          | 36  | 8            | 44             | 22  | 0            | 22                                   |
| FUB           | 12  | 18           | 30             | 0   | 16           | 16                                   |
| ULRS          | 0   | 36           | 36             | 0   | 11           | 11                                   |
| UAR           | 0   | 24           | 24             | 0   | 21           | 21                                   |
| IPC           | 38  | 6            | 44             | 26  | 0            | 26                                   |
| UPSO          | 0   | 30           | 30             | 0   | 14           | 14                                   |
| TOTAL         | 86  | 182          | 268            | 57  | 84           | 141                                  |

Notes on recruitment:

- 1. OU A Postdoc has been appointed (D Mayr from Austria) from 1/7/2003 to work on experimental programme at the OU. A theoretical postdoc (Dr Simone Taioli) has been appointed from 1/1/2004. This post will be shared with UCL as computational facilities are at UCL. The movement of the Co-ordinator from UCL to the OU in October 2002 has necessitated some organisational changes in training between UCL and OU not foreseen when Annex was drawn up since the Co-ordinator was at UCL. All months now allocated
- 2. UCL. Ms Cristiana Arcidiacono pre-doc 1/9/03 24 months (appointed after node experienced difficulties finding an elegible post-doc). Dr Zoran Pesic post-doc 12/1/2004 16 months.

- 3. UIBK. The first Predoc was appointed from September 2002 Ms Sylwia Ptasinska and will continue in year 2 a second has been appointed from September 2003.
- 4. FUB The Postdoc was appointed in January 2003 and will continue in year 2 instead of predoc post.
- 5. ULRS This node was the slowest to recruit its young researchers due to loss of the candidate in 2002 following late transfer of funds from EU in fall of 2002. Dr S.Telega (from Poland) was in Rome for three months during 2003 and will return in 2004. Dr Damian Pliszka (from Poland) has been in post since December 2003. Dr. Jan Franz (from Germany) will spend six months in Rome from Sept 2004 till April 2005. Dr Kai Willner (from France) will come in 2004 *All months now allocated*
- 6. UAR a Postdoc was in place from 1 September 2002 and will be employed for the 24 months allocated to this partner. *All months now allocated*
- 7. ICP have appointed Peter Papp ( 4.11.2002 4.5.2003); Peter Hrušč (4.11.2002 4.5.2003) Vincent Brems (1.5.2004 -31.10. 2004) and Barbara Pezler (1.5.2004- 31.10. 2004)
- 8. UPSO The first postdoctoral post was filled in March 2003 for an 12 month period. A second appointment will be made later in 2004 for 12 months.

<u>Integration of Young researchers</u>; All the young researchers are provided with a detailed description of the aims and objectives of the EPIC network upon commencing their studies. Attendance at the network meetings is compulsory and all in post in July 2003 were required to give a presentation of their work by that date. All in post in June 2004 will present their work at the Midterm review. Exchange of younger members between the research teams is recommended and has been enacted by most partners in year 1 (see joint publications arising from these actions) with the expectation of more intense exchanges in year 2 and 3 as the younger have become more active.

C2 <u>Training</u>: A Master class in preparation and synthesis of bio-molecules planned for year 2 was organized by the co-ordinator as part of the new UK National Quantum, Atomic and Molecular physics meeting in September 2003 and Master class in surface preparation and UHV techniques was held in December 2003 while the Master class in 'Theory of Molecular dynamics and symmetry' is now planned for later in 2004 (delayed until appointment of young theoretical researchers some of whom did not start until January 2004). Those young researchers in post by July 2003 presented their work at a formal session of the Network meeting held in Prague on July 30, 2003. This was an essential requirement for their training in communication and presentation skills. In each partner laboratory the young researchers have been encouraged to make use of the institutes's own training programmes for young researchers. These include career instruction, project management and timekeeping courses. In addition several have made use of specialized language courses to allow them to integrate with the country in which they are undertaking training.

<u>Equal opportunities:</u> 4 of the younger researchers employed to date under the network are women and have been advised of specialized training courses at their host institutions.

<u>Interdisciplinary Aspects:</u> The nature of the network makes the training necessarily interdisciplinary with aspects of physics, chemistry and biology being employed in the research studies as well as some aspects of technology and computer science and IT.

#### C3 Factual information on the Young researchers

Host; Open University; United Kingdom

**Dr D Mayr :** Nationality Austrian; Age at appointment 27; Start date July 2003 End Date December 2004; Employment as Post-doc; Previous contact PhD University of Innsbruck

Host; Open University; United Kingdom and University College London

**Dr Simone Taoli** Nationality Italian; Age at appointment 30; Start date January 2004 End Date July 2005; Employment as Post-doc; NO Previous contact with nodes

Host; University College London

**Ms** Cristiana Arcidiacono Nationality Italian; Age at appointment 27; Start date September 2003 End Date December 2005; Employment as Pre-doc; NO Previous contact with nodes

**Dr Zoran Pesic** Nationality Serbian; Age at appointment 33; Start date January 2004 End Date May 2005; Employment as Post-doc; NO Previous contact with nodes

Host; Free University Berlin

**Dr Hassan Abdoul-Carime** Nationality French; Age at appointment 35; Start date November 2003 End Date August/September 2005; Employment as Post-doc; NO Previous contact with nodes.

Host; University of Innsbruck

**Ms Sylwia Ptasinska** Nationality Polish; Age at appointment 35; Start date January 2003 End Date August/September 2005; Employment as Pre-doc; NO Previous contact with nodes.

Host; University of Rome

**Dr S.Telega** Nationality Polish; Age at appointment 33; Start date August 2003 End Date October 2003; returning in 2004 Employment as Post-doc; NO Previous contact with nodes

**Dr Damian Pliszka** Nationality Polish; Age at appointment 31; Start date December 2003 End Date December 2004; Employment as Post-doc; NO Previous contact with nodes

Host; University of Aarhus

**Dr Nykola Jones** Nationality British; Age at appointment 25; Start date September 2002 End Date August 2004; Employment as Post-doc; Previous contact with nodes PhD student UCL.

Host; ICP Prague

**Peter Papp** Nationality Age at appointment; Start date November 2002 End Date May 2003; Employment as Post-doc; NO Previous contact with nodes

**Peter Hrušč** Nationality Slovakian Age at appointment; Start date November 2002 End Date May 2003; Employment as Post-doc; NO Previous contact with nodes

**Dr Vincent Brems** Nationality German Age at appointment; Start date may 2004 End Date October 2004; Employment as Post-doc; NO Previous contact with nodes

**Barbara Pezler** Nationality Polish Age at appointment 39; Start date May 2004 End Date October 2004; Employment as Post-doc; NO Previous contact with other nodes

**Host: University of Paris-Sud:** 

**Dr Daniel Caceres** Nationality Spanish Age at appointment 30; Start date March 2003 End Date March 2004; Employment as Post-doc; NO Previous contact with nodes

### **Part D Sketches of The Young Researchers**

#### Dagmar Mayr Employed as Postdoc at the OU

My background is in Ion physics. I did trace gas analysis of volatile organic compounds for my diploma and PhD thesis for four years. My thesis dealt with the development of quality control methods of food based on headspace measurements by Proton-Transfer-Reaction Mass-Spectrometry (PTR-MS) and with aroma analysis of food using PTR-MS and Gas Chromatography-Olfactometry (GC-O).

After finishing my PhD I started working with Prof. Nigel Mason in the Epic Network. I am investigating radiation damage of biomolecules on a molecular level to find the molecular pathways that lead from initial deposition of radiative energy to the formation of double strand breaks and lesions in DNA. Damaged DNA, if not repaired, can lead to mutation and hence the development of cancers, however, the well controlled and selective destruction of DNA can also be used as a means to kill cancerous cells. The approaches currently used in radiotherapy cannot well distinguish between different DNA. They destroy all biomolecules and are not very efficient in targeting DNA bases that encode the genetic information causing cancer. Therefore a low-energy method to achieve selective DNA base damage is certainly desirable. We recently got an Atomic Force Microscope (AFM) and are now about to apply it to observe and quantify DNA damage caused by UV and low-energy electron impact. We work together with the Chemistry Department here at the Open University as well as with other Network members. I recently visited the group of Prof. David Field in Aarhus/Denmark and collaborated with Prof. Tilmann Maerk's group in Innsbruck/Austria on electron attachment to some biomolecules (5-Bromouridine and 5-Bromo-2'-deoxyuridine) and to water.

#### Simone TAIOLI Employed Postdoc UCL/OU

My higher education started with my attending "Liceo Classico" where I defended my final matriculation exam in Jul. 2000, with a 60/60 graduation mark. After that I attended the university in Bologna, in which I studied the basics of nuclear physics and neutronics applied to

the study of flux in a nuclear power fission reactor, and concepts about plasma instabilities and turbulence and its application to fusion reactors. I defended my degree thesis on "Quantum mechanical calculations of Auger spectra of silicon clusters" on October 2000 receiving a summa cum laude graduation mark. After, in January 2001, I became a PhD Student in the same university in the Nuclear Science and Technology Department, which is an interdepartmental institution of the university of Bologna. The laboratory has an active nuclear research reactor and a plasma focus machine. My first activity was devoted to the study of the basics physics of both fusion and fission nuclear reactors. Since 2001 I split my activity between Bologna and Pisa, where I also became a research student in Scuola Normale Superiore in the physics division. I have a position in this institution to pursue a second PhD. These studies formed my Phd degree thesis, whose title is "Inner shell photoionization and non-radiative decay processes in molecules: theory and calculations", which was defended in May 2004 and which is based on formal scattering theory, as applied to the interactions of photons with atoms and molecules, developing a new quantum-mechanical method based on the Fano's formulation of the continuum-discrete interaction. Since January 2004 I'm working within the TAMPA group at University College London for postdoctoral studies, involving me in the EPIC network, in order to solve the electron-water molecule scattering trough R-matrix type theories and to develop a method for taking into account the interplay between multiple nuclear degrees of freedom of the system and the open off-resonance decay processes that give a dominant contribution to the dynamics. During the project, I'm receiving extensive training in developing a new computer program, that will form an integrated part of the UK molecular R-matrix package, using C++ programming language. I'm learning about time-dependent quantum mechanics and interaction with experiment. Indeed the opportunity to work on a project closely with an experimental group is one aspect that particularly appeals to me as this is a new opportunity for me. I will be able to participate in the training (and other) activities of the Electron and Positron Initiated Chemistry (EPIC) network and other congresses and schools such as MOLEC 2004. I believe that collaboration with internationally leading research groups will help me make important contacts for my future career. Experimental groups include those involved in EPIC network such as that of Prof NJ Mason (Open University) with whom the host has extensive collaborations, and that of Prof L Sanche (Sherbrooke, Canada) who is working on electron collisions with biologically important molecules. The main feature I like is that of a multidisciplinary project using techniques on the borders of physics and chemistry and with application to the life sciences, astronomy, aeronomy and, given the importance of water, most likely to other areas too. I'd like to broaden the application of my work to such areas that are strategic and relevant for the community.

#### **Dr PESIC Employed PostDosc UCL**

During my PhD studies at Stockholm University (Sweden) I have studied the interaction of highly charged ions with surfaces, with focus to the relaxation of hollow atoms above and below metal surfaces. I have continued these studies at Hahn-Meitner Institute (Berlin, Germany) as post-doc. In addition, I have studied basic processes in ion-molecule collision.

I have joined the positron group at UCL 5 months ago. As part of the EPIC network, I am participating in the measurements of direct and total ionization cross sections of water molecule induced by positrons. In particular, I am responsible for managing one of the experimental setups of UCL positron physics group. I have developed the inlet gas line for water introduction in the chamber and have familiarized myself with the positron beamline.

After testing the system, with argon and obtained good agreement with previous results, we have already obtained some preliminary result for direct ionization cross sections of water. To the best of our knowledge, these are the first results for positron impact ionization of water. Further measurements are in progress to improve the statistical accuracy of the data and possibly of the mass spectrometer. I plan to present these data at forthcoming international conferences (EPIC Network meeting, Austria and SPIG2004, Serbia). Further test measurements for the total ionization cross-section are also in progress.

From an academic professional development point of view, I am assisting in the supervision of one PhD student and, from September, I will assist in the undergraduate laboratory for student exercises. I also delivered an invited talk as part of the Departmental Seminar series.

Therefore, I can say that the research fellow position within EPIC Network is providing me with excellent training on collisional physics of positrons with atomic species as well as new experimental techniques (e.g. coincidence techniques) and, not less importantly, an opportunity to develop professionally.

#### Ms C ARCIDIACONO Employed PreDoc UCL

I am a PhD student at University College of London. I got my degree "Laurea in Physics and Environmental Physics" at University of Catania, Italy. As a holder of the INFN scholarship during my thesis work, I was trained at South National Laboratory (LNS) of the National Institute of Nuclear Physics (INFN) for two years (2000/2001). There, I was mainly concerned in vivo Dosimetry and tissue inhomogeneity study at the Garibaldi Hospital and Policlinic of Catania and the treatment of critical organs (the eye) through adrotherapy at INFN-LNS (Catana Project).

I came to UCL at the end of September 2002 and begun working on positron impact differential ionization studies as MPhil student. Since August 2003, I have been involved in the EPIC project at UCL as a PhD student and participated in the Vacuum Physics and Techniques course at Louvain-la-Neuve in Belgium. Upon my return, I gave an oral presentation on the course to the whole group. Under the supervision of Professor Gaetana Laricchia, Dr Akos Kover and Dr Zoran Pesic, I am being trained on experimental methods about collision physics (positron-atom/molecules) with particular attention to positron induced (direct and total) ionization. I have also attended three English Language courses at the Language Centre sponsored by the Graduate School at UCL.

As part of my duties, I am responsible for the daily running of one of the electrostatic beamlines at UCL, to perform data analysis and simulations. Since January this year, I have been working closely with Dr Pesic and have assisted in the assembly of another apparatus. Until now, we have tested the system and preliminary measurements have been conducted. Measurements of direct ionization cross section with Ar were performed as a test. A good agreement with previous measurements has been found. Thereafter, first direct ionization cross-section for water have been obtained. These data will be presented at the next EPIC satellite meeting, Austria. New tests are in progress to enable measurement of the total ionization cross section for  $H_2O$ .

In conclusion, my PhD position inside the EPIC network at UCL provides me with a great opportunity for learning about the low-energy collision of antimatter with gaseous species and, hopefully in the future, with further biologically important molecules.

#### Dr H. Abdoul-Carime (Freie Universität, Berlin, Germany)

I graduated from Paris-Nord University (France) in 1996 where I have been investigating electron transfer occurring during collision between a highly excited atoms (i.e., Rydberg atoms) and

polar molecules and molecular clusters. It was during my Ph.D. times that I have had my first experience with the interaction of electrons with biologically relevant molecules. Indeed, I have performed the first measurements of electron attachment to nucleobases in the gas phase. After being graduated, I have had a one year contract as lecturer at the same University, continuing my Ph.D. work. Then, I went to Japan (Tsukuba) as a post-doctoral fellow to work on a different field: solution chemistry. However, I have been involved in the development of a home-built experimental apparatus to put large molecules in vacuum (electrospray - coupled to mass spectrometry technique). After my Japanese experience, I went back to the electron-molecule interaction problems at Prof. L. Sanche group (Canada) for more than 3 years, as a post-doctoral fellow. I have started investigation on how low energy electron can damage at the molecular level biological molecules (short strand DNA, DNA bases and amino acids) in condensed phase. I also have explored how low-energy electrons can induce radio-sensitization in nucleic acids containing halogenated-modified nucleobases. My background is nevertheless not restricted to biological molecules, also they represent the main part of my work since 1998. Indeed, I have had some contribution on potential sulfur contained atmospheric pollutants. Then I have taken a one year and half sabbatical to perform a real biological experiment (her name is Adele).

By 2002, Prof. Illenberger proposed me to join his group to work on biologically relevant molecules in the gas phase and cluster, under the contract with the EPIC network. At the beginning, I have planned to perform some measurements on amino-acids (cystein, tryptophan, proline) and proteins (N-acetyl-tryptophan). Those points are completed by now. In the gas phase, probing biologically relevant molecules were restricted to isolated nucleobases. I have shown for instance that electrons with energies below 3 eV can induce a loss of hydrogen at the specific nitrogen sites of DNA bases. In fact within DNA, nucleobases are bound to sugar molecules, via a chemical bond at one of the nitrogen sites. Therefore, I have suggested and then investigated how interaction of low electrons can be modified when the DNA bases (thymidine, bromouridine) are bound to sugar molecules which represent more closely DNA sub-units. I appreciate Prof. Illenberger to let me free for doing any experiments that I wanted to do, this way of our collaboration appears to be quite fruitful. I also have the opportunity to supervise (although not officially) the Ph.D. work of Sascha Golke.

# Ms Sylwia Ptasinska employed University of Innsbruck

In 2001 I was graduated as a Master of Science in Physics at Maria Curie-Skłodowska University of Lublin in Poland. The title of my master thesis is "Mass spectrometry of gaseous clusters", for which I have gotten the awards of Polish Vacuum Society for the best thesis of year. After my study I was during one year PhD student at the same university, where I continued the studies of small protonated clusters obtained from ammonia and water. I also started new topic of researches, where I used MALDI (Matrix Assisted Laser Desorption/Ionization) method for study of big biomolecules like hemoglobin, insulin and cytochrome. Since October in 2002 I have started PhD study in Institute of Ion Physics at the Innsbruck University and I have been employed there like an EPIC young researcher in Prof. Tilmann D. Märk's group. The topic of my present studies is inelastic electron interaction (attachment/ionization) with biomolecule (particularly DNA and RNA components, but also amino acids and sugars) in the gas phase. For my studies I use high resolution crossed beams machine, consisting of hemispherical electron monochromator in combination with quadrupole mass spectrometer. From these measurements we can determinate the ionization energies, cross section and also production and decay mechanisms of parent and fragment cations and anions. Also from results obtained from partially deuterated thymine it is observed that deuterium abstracted from the carbon site can be the initial

step toward strands breaks in DNA. Last time I got opportunity to involve to Prof. E. Illenberger's group (which is also the team of the EPIC network), where I studied electron attachment to clusters of propanionic acid.

# Dr S.Telega employed University of Rome

I've been employed as a predoctoral fellow under the EPIC network for three months period (from November 2003 to January 2004) in the Roman node of the network (Group of Theoretical Chemical Physics led by Prof. F.A.Gianturco, Departament of Chemistry, University of Rome "La Sapienza"). It was my third visit to this group. My first contact with the group led by Professor Gianturco was established via the European Students Exchange Program "Erasmus" in which I participated as a student.

Since my first visit I've been studying the electron - molecule scattering formalism developed in the Roman group. After obtaining M. Sc. degree I decided to start Ph. D. studies. The subject of my thesis is "Low energy electron scattering from H2 and N2". During my employment under the EPIC network I was working on application of Laboratory Frame formulation of electron - molecule scattering. We've managed to perform calculations for the case of rotational excitation of H2 and N2, which were published in a paper. Later we started calculations of ro-vibrational excitations of the mentioned molecules. We've already got results for the case of H2 molecular target, which I'm going to present at EPIC 2004 meeting. At the very moment we're calculating the cross sections for vibrational excitation of N2.

I consider the period of work under the EPIC network as an extremally valuable experience, which has helped me a lot in developing skills and exchanging ideas with other European scientists.

# Dr Damian Pliszka employed University of Rome

During my stay in Trento I'm working on positron scattering apparatus in gases. I have found very nice and helpful collegues in Trento laboratory, which helped me with some administrative things and Italy. Laboratory in itself is very well equipped and makes a very good impression. Also it creates very good conditions to work. Uding the work with PAIS apparatus I teach a lot about vacuum techniques, about electron optics techniques. We found some technical problems with the apparatus what gave me a very interesting experiences for my future works. After overcome technical problems, I have started testing of the apparatus, first with electrons and then with positrons achieving more and more experience in settings of the electron optics and in optimizing of the positrons beam. Simoultaneously I was involved in work to prepare remoderator for the PAIS apparatus. It is very difficult to obtain very thin monocrystal film of the cooper. Difficulties made that inserting of the remoderator is delayed (in nearest time it should be finished). Meantime during the tests it becames clear that apparatus can be set in deaccelerating mode, what allowed to measure cross sections of the several gases in energy range from 0.5 up to 20 eV. In that mode there are still performed measurements until remoderator stage will be ready for testing. My work in Trento laboratory is very interesting and made, that I'm going to follow that thematics in my future works. It gave ma a lot of practical and theoretical experiencies in different fields of the modern physics, which in Trento is at really high level. I'm planning two short-time visits to other laboratories involved in EPIC program. First is Innsbruck University, second - London laboratory

# Dr Nykola Jones: employed University of Aarhus

In 1996 I graduated from the Chemistry department at University College London with a BSc. From there I moved to the Physics department at UCL for postgraduate studies in the Molecular Physics Laboratory, under the supervision of Prof. Nigel Mason. I was awarded a PhD in Physics by the University of London in March 2000. Under EPIC, I have been working in the Department of Physics and Astronomy, University of Aarhus in a postdoc position. Throughout the course of my studies and employment I have been involved in a variety of experiments in the area of molecular physics (physical chemistry), investigating atoms and molecules which are relevant to the physics and chemistry of natural and man-made plasmas. These experiments include: Timeof-flight mass spectrometry used in electron-impact ionisation studies to investigate the fragmentation of dications, Electron energy loss spectroscopy, Detection of metastable neutral species in excited states, VUV Photoabsorption spectroscopy using synchrotron radiation, performed on the 3.1 station at Daresbury Laboratory, UK and at UV1 on ASTRID, Denmark. Under EPIC, I currently work on an experiment which involves low energy electron scattering from molecules. The experiment uses synchrotron radiation from the undulator in ASTRID to photoionise argon, producing low energy electrons with high resolution. These electrons, formed into a beam, are used in a transmission experiment, from which absolute total integral and backward scattering cross-sections are obtained. During the period of the network, data for a large number of molecules have been obtained and the results are published or will be published in the near future. Also a new apparatus has been designed and is currently under construction which will allow the study of low energy electron interactions with solids. In September 2003 as part of the EPIC network I attended a workshop on preparing and analysing DNA damage at the Open University, UK. In December 2003 I visited the laboratories of Dr Bratislav Marinkovic, at the Institute of Physics, Belgrade, where I also gave a seminar pertaining to my current research. I have attended/will attend the following conferences (\* indicates poster(s) presented at the meeting)

1st EPIC Network Meeting, Saturday 8th/Sunday 9th February 2003

\*EPIC Meeting, 29 July- 2 August, 2003, Pruhonice, near Prague, Czech Republic

\*ICPEACXXIII, 23-29 July 2003, Stockholm, Sweden

QuAMP Combined UK Meeting and Summer School, September 8-12 2003, Milton Keynes, UK

\*EPIC Meeting, 19-23 June 2004, Obergurgl, Austria

\*COST/RADAM Meeting, 24-27 June 2004, Lyon, France

\*ECAMP8, 6-10 July 2004, Rennes, France.

I also designed and constructed the website for the network. I have become closely integrated into the department here, especially with respect to computing, meeting organisation (for ESF and EU networks) and it has been an excellent experience.

# Peter Hrušč and Peter Papp employed J Heyrovsky Institute of Physical Chemistry

These two predoctoral EPIC Fellows were gradute students from the Faculty of Mathematics and Physics at the Comenius University in Bratislava, Slovakia. They stayed with us in Prague six months (4.11.2002 – 4.5.2003). Upon their coming to Prague, they had only a basic knowledge of the theory of electron scattering as it corresponds to the curriculum of the Comenius University. Therefore the main purpose of their visit was to improve their education and training for their future research work, and we believe that this objective was met. They could not be charged with a highly demanding project (as it was in case of postdoctoral Fellows). Instead, they joined an already running project of DMR calculations on the electron energy loss spectrum of methane. Their task was to test the performance of the DMR method, as Čársky and Čurík did it already

for propane. Unfortunately, their work remained largely unfinished and it had to be completed after their departure by R. Čurík. This project is already in the stage of writing a paper and we believe that it will bring useful new information.

# Dr Vincent Brems employed J Heyrovsky Institute of Physical Chemistry

Since 2001 up to now he has been a postdoctoral fellow working for Prof. Nestmann in Bonn. He acquired there good knowledge of the R-matrix method and theory of electron scattering in general, and he is therefore a profitable acquisition for Prague group. He started in Prague on May 1, 2004 and he wants to stay with us a year. His experience, knowledge and his calculations on resonances in Cl<sub>2</sub>(-) done in Bonn permitted Jiří Horáček to formulate a project of common interest. Collaboration of Vincent Brems with P.Kolorenc and J.Horáček already started and it concerns the use of Feshbach-Fano-R-matrix approach to the calculation of resonance parameters. The objective is to use the computed terms for investigation of low energy resonant attachment processes such as dissociation electron attachment and electron collision induced vibrational excitation. The second project of V. Brems in Prague is done in collaboration with P.Čársky and R.Čurík. The aim of this project is to run in parallel Discrete Momentum Representation (DMR) and R-matrix calculations on propane to see merits and shortcomings of the approximate DMR method (developed in Prague) when compared with accurate R-matrix calculations (to be done in Bonn).

Only six weeks elapsed from the beginning of the visit of V.Brems in Prague. In spite of this short time a remarkable progress has been done in the above-mentioned projects and it is every reason to believe that this one-year visit will be productive and profitable for both the Fellow and the Prague EPIC group.

# Barbara Pezler employed J Heyrovsky Institute of Physical Chemistry

Barbara's field of specialization is theoretical chemistry: kinetics of ion-molecule and electron-molecule reactions. Her Ph.D. thesis concerned the classical and quantum transition state theory for the ion - linear quadrupole molecule capture. Recently she has investigated the geometry and energy changes in halocarbons after the electron capture.

Under EPIC she is working on the investigation of spatial differential cross-section maps for the vibrational excitation of some molecules (nonpolar and polar) using Discrete Momentum Representation method to find the correlation between electron energy loss intensities and chemical structure of the molecule.

This is her first appointment within a Research Training Network.

# Dr Daniel Caceres employed University Paris Sud

# Appendix 1

CVs of

# Young Researchers employed

under EPIC

# **Curriculum Vitae Dr Dagmar Mayr**

# PERSONAL DATA

NAME: Dagmar MAYR

ADDRESS: Department of Physics and Astronomy

The Open University

Walton Hall

Milton Keynes MK7 6AA, UK

EMAIL: d.mayr@open.ac.uk

DATE OF BIRTH: May 19, 1975

BIRTH PLACE: Innsbruck (Austria)

NATIONALITY: Austrian

# **EDUCATION**

09/81-07/85 primary school in Wilten/Innsbruck

09/85-06/93 grammar school in Innsbruck 06/93 school leaving examination

10/93-05/00 studies in physics at the Leopold-Franzens-University Innsbruck,

obtained Mag. rer. nat. (MSc)

03/99-05/00 **diploma thesis** at the Institute for Ion Physics, *title*: "Volatile Organic Compounds

in Human Breath: Measurements Using Proton-Transfer-Reaction Mass-

Spectrometry with High Time Resolution", supervisor: Univ. Prof. Dr. Lindinger,

grade: excellent.

06/00-03/03 **PhD**. studies in physics at the Institute for Ion Physics, Leopold-Franzens-

University Innsbruck, title: "Aroma Analysis and Quality Control of Food Using

Highly Sensitive Analytical Methods", *supervisor*: Univ. Prof. Dr. Lindinger (†),

Univ. Prof. Dr. Märk, grade: excellent, obtained Dr. rer. nat.

# ADDITIONAL EDUCATION

12/03 **Vacuum physics and techniques**, SOCRATES Intensive Program

(http://www.fyam.ucl.ac.be/enseignement/Vide/Vacuum03.html), Catholic

University of Louvain, Louvain-la-Neuve, Belgium, 1 - 11 December 2003.

# PROFESSIONAL EXPERIENCE

Positions held

- 06/00-07/03 Employment as a **research assistant** at the Institute for Ion Physics, Leopold-Franzens-University Innsbruck
- 07/03-present Employment as a **research fellow** at the Department of Physics and Astronomy,
  The Open University, Milton Keynes

# Research visits

| 05/02-08/02 | Department of Food Sciences and Technology, University College Cork             |
|-------------|---|
|             | (http://www.ucc.ie/acad/departments/foodtech/), Ireland: Marie Curie Fellowship |
| 10/03       | University of Innsbruck, Institute for Ion Physics                              |
|             | (http://www.uibk.ac.at/c/c7/c722)   |
| 10/03       | Rutherford Appleton Laboratory (http://www.cclrc.ac.uk/Activity/RAL)            |
| 11/03       | University of Innsbruck, Institute for Ion Physics                              |
|             | (http://www.uibk.ac.at/c/c7/c722)   |
| 02/04       | Rutherford Appleton Laboratory (http://www.cclrc.ac.uk/Activity/RAL)            |
| 04/04       | Institute for Storage Ring Facilities ISA (http://www.isa.au.dk), University of |
|             | Aarhus, Denmark   |
| 06/04       | University of Innsbruck, Institute for Ion Physics                              |
|             | (http://www.uibk.ac.at/c/c7/c722)   |
|             |   |

# **Curriculum vitae: Simone Taioli**

Surname TAIOLI First name SIMONE

Date of birth 27th September 1974

Home address: Via Serraglio 7 CESENA (FC)

Post Code 47023

personal e-mail: simone@theory.phys.ucl.ac.uk

# **EDUCATION**

# LICEO CLASSICO, V.Monti, Cesena, Italy

Matriculation exam. Jul. 1994

Graduation Mark: 60/60.

# UNIVERSITY OF BOLOGNA, Bologna, ITALY

Degree: Nuclear Science and Technology (Neutronic and plasma Section)

Sept 1994 -Oct 2000

Final thesis: Quantum mechanical calculation of Auger spectra of silicon

clusters. Graduation Mark: first-class degree (summa cum laude).

MILITARY SERVICE: June 2000-May 2001.

# PHD STUDENT, BOLOGNA, ITALY

Nuclear Science and Technology Jan 2001-May2004

# RESEARCHER STUDENT IN SCUOLA NORMALE SUPERIORE, PISA, ITALY

Chemical Physics

September 2001 – December 2004

# **EDUCATIONAL EXPERIENCE:**

**National School on parallel calculation** 

Bologna, ITALY, 3-14 July 2001.

**National School on Synchrotron Radiation** 

S.Margherita di Pula, Cagliari, ITALY, 17-28 September 2001.

Second European Summer School on microscopic quantum many-body theories and their applications

ICTP, Trieste, ITALY, 3-14 September 2001.

National School on condensed matter physics

Torino, ITALY, 19-25 September 2003.

First national Summer School on computational chemistry: excited states, spectroscopy and photochemical processes

Pisa, ITALY, 25-31 August 2002.

**European Summer school in Quantum Chemistry (ESQC-03)** 

Lund, Sweden, August 17-30 August 2003.

**Course on solid state theory (prof. Giuseppe Grosso)** 

Pisa, ITALY, 6 January to 15 December 2001.

Course on theoretical physics (prof. Adriano Di Giacomo)

Pisa, ITALY, 6 January to 15 December 2001.

Course on superconductivity (prof. Rosario Fazio)

Pisa, ITALY, 6 January to 30 March 2003.

Course on quantum many-body (prof. Mario Tosi)

Pisa, ITALY, 6 January to 30 March 2002.

# **PUBLICATIONS:**

- 1) On the angular dependence of L x-ray production cross sections following photoionization at an energy of 59.54 keV: Agostino Tartari, Claudio Baraldi, Ernesto Casnati, Andrea Da Re, Jorge E Fernandez and Simone Taioli
- J. Phys. B: At. Mol. Opt. Phys. 36 No 5 (March 2003) 843-851
- 2) Ab-initio calculation of the C1s photoelectron spectrum of C2H2: R.Colle, S.Taioli, D.Embriaco, M.Massini, S.Simonucci

Nucl. Inst. and Meth. in Phys. Res. Journal (Section B) (January 2004) Vol.213, 65-70

3)Ab initio calculation of the normal Auger spectrum of C2H2: R.Colle, S.Taioli, D.Embriaco, M.Massini, S.Simonucci

J.Phys.B.: At.Mol.Opt.Phys. (March 2004) Vol.37, 1-8.

4) Auger electrons angular distribution calculated without two-step approximation: angle-resolved Auger spectra of the C2H2 molecule.

Accepted in Phys.Rev.A

5) Photoelectrons angular distributions of fixed in space CO.

**Submitted to Phys.Rev.Lett.** 

#### **CONGRESSES:**

5th International Topical Meeting on Industrial Radiation and

**Radioisotope Measurement Applications** 

IRRMA V ,Bologna, ITALY

Local Organizing Committee, 9-14 June 2002 and oral talk

**XXXII Italian Meeting of Physical Chemistry** 

Ferrara, ITALY

Poster presentation, 23-28 June 2002.

XIII International conference on photonic electronic and atomic collision, ICPEAC Stockholm, 23-29 July, 2003

Poster session.

International Symposium on (e,2e), Double Photoionization and Related Topics Frankfurt, July 30-August 2 2003

## WORK EXPERIENCE:

July 2000-March 2001

NMR technician in the M.Bufalini hospital of the national sanitary service.

# **COMPUTER EXPERIENCE**

Operating systems: UNIX BSD, IBM AIX, LINUX DEBIAN, MICROSOFT WINDOWS 2000, NT4.0.

Programming skills: C, C++(STL), FORTRAN, ACCESS, MATLAB.

LANGUAGES: -Italian (mother-tongue), -English (good). -French (beginner).

HOBBIES: Philosophy; Italian Literature; Running; Scuba Diving, Sailing, Volleyball and football. I was an active member of a professional football team.

REFERENCES AND DETAILS: Available upon request. According to the privacy laws, I authorize the processing of my personal data.

# Cristiana Arcidiacono

First name: Cristiana Family name: Arcidiacono

Place and date of birth: Catania (Italy), July 7th, 1975

Nationality: Italian

*Term-Address:* 76 Musbury street

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**Tel.:** *020 7679 2133 Mob.* : 07985075443

*E-mail:* c.arcidiacono@ucl.ac.ucl

National Insurance Number: SC 45 54 11 D

#### Education:

Dec. 2003: Vacuum Physics and Techniques course at Louvain-la-Neuve (Belgium).

Feb. 2003: Radiation Protection course (UCL), UK

Nov. 2001: Theoretical study on the Pamela Project (Astroparticle group at the University of Rome2, Italy)

Sept. 2001: European Summer School on Experimental Nuclear Astrophysics (ENA), Sicily, Italy

Oct. 1994 – Apr. 2001: University of Catania, Italy

Degree title: Laurea in Fisica e Fisica dell'Ambiente (BSc in Physics)

Final grade: graduating marks (108/110)

Dissertation: "Dosimetry in vivo in treatment of radiotherapy with photon

beams"

March 1996 – July 1996: Diploma at the Course for Social, Tourist-Cultural Animator (F.S.E.)

Sept. 1989 – July 1994: Liceo "Archimede" specializing in scientific studies, Acireale (C.T:) Diploma di Maturita' Scientifica (Upper school leaving certificate) with marks 58/60

Informatics skills: Fortran, Window, Word, Works, Excel, Power Point, Sigma Plot, SIMION, Macintosh

# Language skills:

Italian: mother tongue

English: fluent Hungarian: fluent French: good

Spanish: basic knowledge

# Employment history:

October 2002 - April 2004: Teaching Assistant in the Physics & Astronomy Department, University College London (UCL), UK January 2000 - September 2002: Journalist assistant and photographer for the journalist of the Sicilian daily news: "La Sicilia"

January 2002 – June 2002: irregular work as a Mathematics and Physics teacher, Italy

April 2002 - May 2002: social work for elderly, Stella Polare cooperative, Italy

October 2000: Hostess and conference coordinator in International Congresses, Italy

July 2000: Volunteer as a tourist guide, interpreter and gallery assistant, Rome, Italy

July 1997: Animator and director of a children's summer group (GREST), Santa Venerina, Italy

# Experiences abroad and language courses:

October 2003 – December 2003: Public speaking and pronunciation Course, Language Centre, University College London (UCL).

January 2002 – March 2003: In Sessional English Course (Advanced Level), Language Centre, University College London (UCL).

November 2002-March 2003: English Lesson Courses (Advanced Intermediate Level) at the University College London (UCL).

March 15, 2002: TOEFL test Computer Based version, Rome.

Score report 230. Essay score report in the Toefl test 5.0

December 2001 - February 2002: Part - Time Course in English at the Science Politics Department of the University of Catania, Italy.

July1998: English course at the Stanton School in England (3-weeks), London.

# **Grants and Scholarships**

2003: EPIC maintenance grant

2002: Contribute by "Fondazione Angelo della Riccia"

2002-2005: The Engineering and Physical Sciences Research Council Scholarships (EPSRC), Government's leading funding agency for research and training in engineering and the physical sciences, for the Mphil/Phd fees in Physics, University College London (UCL), London.

2000-2001: Scholarships of the National Institute of Nuclear Physics (INFN) for final-year undergraduate at the South National Laboratory (L.N.S.)

#### **Publications and Posters**

Differential ionization experiments on positron – atom scattering Á. Kövér, C. Arcidiacono and G. Laricchia

Nucl. Instr. Meth. B221 (2004) 56-59

Ionisation and fragmentation of H<sub>2</sub>O molecule in the interaction with positrons and ions Z. D. Pešić\*\*, C. Arcidiacono\*\*, R. Hellhammer, N. Stolterfoht and G. Laricchia to be published in AIP conference series (2004)

Electron Ejection from Collisions of Positrons with Helium Atoms

C. Arcidiacono, Á. Kövér, and G. Laricchia

Abstract published on "XII International Workshop on Positron and Positronium Physics

Sandbjerg, Denmark 19-21 July (2003) Poster presented.

"Utilization of Thermoluminescent detectors for *in vivo* dosimetry

C. Arcidiacono, G. Cuttone, L. Valastro, G. Lo Nigro

Acts of 2<sup>nd</sup> National Congress AISM - Brescia 12-16 June (2001). Poster presented.

# Dr. Zoran Pešić

Dept. of Physics & Astronomy University College London Gower Street London WC1E 6BT, UK

tel.: (+44) 0207 6792380 fax.:(+44) 0207 6797145 E-mail: z.pesic@ucl.ac.uk

Curriculum vitae
Date of Birth: 6<sup>th</sup> May 1970

1989–1996: I studied experimental physics and received a **Bachelor of Science** diploma at the University for Mathematics and Natural Sciences, Belgrade, Yugoslavia. The title of my diploma work was "Using a Diode Laser in the Atomic Collision Physics".

1996–1998: After my diploma work, I have started Master degree studies in the Electron Atom Collision Group, in the Institute of Physics, Belgrade, Yugoslavia. The project "Stepwise electron laser excitation of the atoms" under the supervision of Dr. B. Marinković has had a goal to develop one completely new experimental set-up. Due to the fact that my experimental set-up was in development phase, I took part in the experiments in the field of electron spectroscopy at an existing set-up.

1998-2002: I moved to Sweden, where I have continued my PhD studies at Stockholm University. Professor Reinhold Schuch was my supervisor. The subject of my PhD work was the interaction of highly charged ions with crystal surfaces. The investigated phenomena were the neutralization and the energy loss of incident ions, as well as the relaxation of hollow atom formed in the interaction. I have used electrostatical and time-of-flight spectrometers, as well as x-ray detectors (Si(Li) detector) in my investigations. In order to explain experimental results, I used a neutralization model and classical trajectory simulations (MARLOWE code and SIMKIT). I was also involved in recombination measurements with Prof. R. Schuch at the heavy ion storage ring (CRYRING) at Stockholm.

I passed the Licentiat exam in June 2000 (At the Stockholm University, Licentiat exam should be performed after 50 % of full PhD studies is accomplished, it has analogy with the Master degree). The title was "Energy Dependence of Neutralization in Scattering of Slow Highly Charged Ar Ions from a Au Surface".

I defended PhD degree with the title "Relaxation of Hollow Atoms Above and Below Metal Surfaces" in May 2002.

2002-2003: I spent 1.5 years as postdoc position in the group of Prof. Nikolaus Stolterfoht in Hanh-Meitner Institute in Berlin where I took part in several research programs. As the continuation of the investigation of the interaction of slow, highly charged ions with crystal surface, we did experiments with insulators (collaboration with Rossendorf, Germany). I was also actively involved in studies of nanostructures produced at surface and in solids. Besides my active role in all phases of the experiment and data analysis, I was particularly responsible for the

AFM/STM imaging of the samples. Finally, I was responsible for experimental studies of the fragmentation of molecules following the interaction with slow HCI.

It should be also mentioned that part of my work was to manage the ion source, i.e. to provide the ion beam from the ECR ion source for guest groups (Stockholm University - Sweden, ATOMKI –Hungary, GANIL – France, Rossendorf – Germany). In the collaboration with Stockholm University and Rossendorf Institute I am actively involved in data analysis and writing of papers.

#### Present status and work:

I have got the research fellow position in the Positron Physics Group, University College London, under the supervision of Prof Gaetana Laricchia. The position has been opened within the European network Electron and Positron Induced Chemistry (EPIC), and it is limited until the end of 2004. The goal of the project is investigation of single and multiply charged ionization (with and without positronium formation) including the first near-threshold measurements. Until now, the positron beam line has been set and detection system (TOF) has been tested, which makes available first test measurements.

# Achieved experience during my research work:

I made a lot of hardware development. I have very good knowledge of the modern electronic devices, particle and x-ray detectors, UH Vacuum technique, electron optics and spectrometers, time-of-flight spectrometers, ion sources (EBIS, ECR) and beam transport. I have learned to use the OMICRON UHV AFM /STM system.

I worked with operational systems: **MicrosoftWindows, UNIX**, and **DOS**, with programming languages: **FORTRAN**, **C** and **C**++, and programs: Microsoft Office, SigmaPlot, Origin, Simion, MARLOWE, SIMKIT.

# **Knowledge of languages:**

English (good), Serbocroatian (mother tongue), Swedish (beginner).

# Realized visits to other laboratories achieved within collaboration:

- -3 x 3 weeks measurement in Hahn-Meitner Institute, Berlin, Germany (in 1998, 1999 and 2000).
- -1 week at Queens University, Belfast, N. Ireland (2003)
- -1 week in Manne Seighban Laboratory, Stockholm, Sweden (2003)
- -1 week in measurement in Hahn-Meitner Institute in Berlin, Germany (2004)

I have published 15 articles in the most acknowledged international journals for physics. Same data are still in processing and that will be published in near future. I had 4 talks at International Conferences: 1.) The Third Balkan Physical Union BPU-3 Conference, 1997, Cluj-Napoca, Romania, 2.) 4<sup>th</sup> LEIF (Low Energy Ion Facility) Annual Meeting 2003, Belfast, N. Irelandand 3.) ISIAC 2003 (International Symposium on Ion-Atom Collisions), Helsinki, Finland 4.) Austrian - Hungarian Workshop on Charged - Particle Transport Through Nanostructures and Solids 2003, Debrecen, Hungary

During the last year I gave a talk in AMOP seminar at UCL. I have also invited to present my recent data (concerning positron physics) at 22nd Summer School and International Symposium on the Physics of Ionized Gases (SPIG 2004) in Tara, Serbia.

# **Hassan Abdoul-Carime**

Educational and Professional Background

#### Assistant Researcher

Institut für Physikalische und Theoretische Chemie der Freien Universität Berlin, Takustrass 3, D-14195 Berlin, Germany

Phone: +49-30-838-55353 Fax: +49-30-838-56612 E-Mail: hcarime@chemie.fu-berlin.de

**Marital Status:** Single, 2 children

Date and

**Place of Birth:** 15<sup>th</sup> of November 1967, Phnom-Penh (Cambodia)

Citizenship: French

**Education: Habilitation** *May 2003* Université Paris-Nord

**Ph.D. Physics** (Atomic, Molecular and Optics)

January 1996

Laboratoire de Physique des Lasers

Université Paris Nord, Institut Galilée, Villetaneuse 93430, France

Thesis Advisor: Prof. Jean Pierre Schermann

Thesis Title: Dipole Bound Anions: Applications to the study of electron attachment to biological molecules and to separation of geometrical

isomers of weakly bound molecular complexes

M.Sc. Physics (Lasers and Applications)
Université Paris Nord, Institut Galilée, Villetaneuse 93430, France
M.Sc. Physics (Optical Engineering)
June 1991

Université Jussieu-Paris 7, Paris 75005, France

**B.Sc. Physics** June 1990

Université Jussieu-Paris 7, Paris 75005, France

**Specialties:** *Experimental atomic and molecular physics*:

effusive, supersonic and liquid molecular beam, atomic and molecular clusters, surface analysis techniques (LEED, XPS), laser excited Rydberg atoms; low energy electron (0-30eV), trochoidal monochromator, thin physisorbed or chemisorbed films; ultra-high vacuum technology, mass spectrometry analysis (time of flight, Q-mass), Infra-red spectroscopy, simulation of molecular structures and molecular dynamics with commercial (CHARMM) or self-written

codes

# Research Experience:

# 1. Freie Universität

**Assistant Researcher** Jan.2003-present

Investigation of molecular dissociation induced by sub-excitation electrons in gas phase and in clusters.

# 2. Université de Sherbrooke

# **Post-doctoral Fellow**

Sept.1998-2001

Investigation of damages to bio-molecules physisorbed and chemisorbed (self assembled monolayer) onto a surface induced by low energy electrons (<30eV)

# 3. National Institute for Advanced Interdisciplinary Research

# **Post-doctoral Fellow**

1997-to 1998

Investigation of intermolecular interaction in electrolyte and non-electrolyte solutions, using thermospray and electrospray coupled to mass spectrometer. Molecular simulation with commercial code Quanta-Charmm

# 4. Université Paris-Nord

# Attache de Recherche – Lecturer

1996 to 1997

Investigation of subthermal-electron attachment to bio-molecules produced via supersonic beam.

# 5. Graduate Research Assistant

1993 to 1996

Experimental investigation of dipole bound anions. Simulation of a potential energy surface of small molecular clusters, using empirical force field and genetic algorithm coupled to the steepest descent method.

# **Teaching**

# **Experience: Teaching Assistant**

Sept. 1993 to June 1996

Laboratoire de Physique des Lasers Université Paris Nord, Institut Galilée, Villetaneuse 93430, France

**Instructor** Sept. 1996 to June 1997

Laboratoire de Physique des Lasers

Université Paris Nord, Institut Galilée, Villetaneuse 93430, France

#### **Honors & Awards:**

- 1) *Invited Speaker* at the 13 th International Symposium on Electron-Molecule Collision and Swarm, Prag, Czech Republic (2003)
- 2) *Invited Speaker*, Travel Award for the 48<sup>th</sup> Radiation Reserch Annual Meeting, Puerto-Rico, (2001)
- 3) Award for the Euresco Conference on "Molecules of Biological Interest in the Gas Phase", Euresco Conference on Experimental Tools and Quantum Chemistry, Les Houches, France, (2000)
- 4) *Invited Speaker* at the 8<sup>th</sup> International Workshop on Desorption Induced by Electronic Transitions, New Jersey, USA, (1999)
- 5) *Invited Speaker* at the 20<sup>th</sup> Symposium on Solution Chemistry, Kyoto, Japan, (1998)
- 6) *Invited Speaker* at the 4<sup>th</sup> Workshop on Dynamic of Ions Atoms and Molecules, Bourges, France, 1996

#### **Grants:**

1) Grant from the European Electron and Positron Induced Chemistry (EPIC) Network (January 2003 – July 2004)

# Prof. Eugen Illenberger

Institut für Chemie – Physikalische und Theoretische Chemie, Takustrasse 3, D-14195 Berlin Phone: +49-30-838 55350/52096, Fax: +49-30-838 56612/527177 email: <u>iln@chemie.fu-berlin.de</u>

2) Fellow from the Medical Research Council of Canada (September 1998 to August 2001) **Prof. Léon Sanche** 

Département de médecine nucléaire et de radiobiologie, Faculte de médecine, Université de Sherbrooke, 3001,12e ave nord,Sherbrooke, QC,Canada J1H5N4

Tel: (1)819-346-1110 ext.14678, Fax: (1)819-564-5442 e mail lsanche@courrier.usherb.ca

3) STA-Japan Science and Technology Corporation *Fellowship*, (February 1997 – February 1998)

# Dr. Akihiro Wakisaka

(moved from NAIR-Tsukuba. Present adress unkown)

4) Attaché Temporaire de Recherche (September 1996 – January 1997)

Prof. Jean-Pierre Schermann

Laboratoire de Physique des Lasers, Institut Galilee, Villetaneuse 93430, France Tel: (33) 01 4940 3816 fax (33) 014940 3200 e mail scherman@galilee.univ-paris13.fr

**Referees:** (see addresses above)

- 1) **Prof. Eugen Illenberger**
- 2) Prof. Léon Sanche
- 3) Prof. Jean-Pierre Schermann

## Other:

Languages: French, English and Cambodian (mother tongue) *Hobbies*: Go game, Cooking and "Triumph" Motorbikes

**Publications:** (\* corresponding author)

- 1 Dipole binding to a strongly polar molecule and its homogeneous clusters: Magic distribution of acetonitrile cluster anions.
- C. Desfrançois, **H. Abdoul-Carime**, C. Adjouri, N. Khelifa and J.P. Schermann *Europhys. Lett.* **26** 25 (1994)
- $2\ \text{From}\ 1/r\ \text{to}\ 1/r^2$  potentials: electron exchange between Rydberg atoms and polar molecules
- C. Desfrançois, **H. Abdoul-Carime**, N. Khelifa and J.P. Schermann *Phys.Rev.Lett.* **73** 2436 (1994)

- **3** Electron attachment to closed-shell polar molecule assemblies: from dipole-bound anions to solvated electrons
- C. Desfrançois, **H. Abdoul-Carime**, N. Khelifa and J.P. Schermann

Journal de Chimie-Physique **92**, 409 (1995)

- **4** Dipole binding: an experimental test for small polar cluster cluster calculations
- C. Desfrançois, **H. Abdoul-Carime**, N. Khelifa, J.P. Schermann, V.Brenner, P.Millié *J.Chem.Phys* **102** 4952 (1995)
- **5** Laser separation of geometrical isomers of weakly bound molecular complexes
- C. Desfrançois, **H. Abdoul-Carime**, C.P.Schulz and J.P. Schermann

Science **269**, 1707 (1995)

**6** Ground state dipole-bound anions

C. Desfrançois, **H.Abdoul-Carime** and J.P. Schermann

Int. Journ. Mod. Phys. B 10, 1339 (1996) Invited Review article

7 Electron attachment to isolated nucleic acid bases

C. Desfrançois, H. Abdoul-Carime and J.P. Schermann

J.Chem.Phys. 104, 19, 7792 (1996)

**8** On the binding of electrons to nitromethane:dipole and valence bound electrons

R.N.Compton, H.S.Carman, C. Desfrançois, H. Abdoul-Carime, J.P.Schermann,

J.Hendricks, S.A.Lyapustina, K.H.Bowen

J.Chem.Phys. 105, 3472 (1996)

**9** Structure and intermolecular motions of the water dimer anion

Y.Bouteiller, C. Desfrançois, H. Abdoul-Carime and J.P. Schermann

J.Chem.Phys. **105**, 6420 (1996)

10 Non destructive isomer selection of some small van der Waals clusters.

C. Defrançois, **H. Abdoul-Carime**, J.P. Schermann

Frontiers Science Series 16 (Structures and Dynamics of Clusters) 311-319 (1996)

11 Excess electrons in polar cluster anions

H. Abdoul-Carime, Y.Bouteiller, C. Desfrançois, L.Philippe and J.P. Schermann

Acta Chemica Scandinavica, vol.51, 145 (1997) Review article

12 Rigid or floppy water-containing dipole-bound anions

H. Abdoul-Carime, A.Wakisaka, Y.Bouteiller, C. Desfrançois, J.P. Schermann

Z. Phys. D, 40, 55 (1997)

13 Non-covalent binary interaction between some organic acids and bases

H. Abdoul-Carime, A. Wakisaka, H. Takeo, V. Périquet, J. P. Schermann, C. Desfrançois

J. Chem. Soc. Faraday Trans., 93, 4289 (1997)

**14** Non-ideality of Binary Mixtures: water-methanol ans water acetonitrile from the view point of clustering structure

A. Wakisaka, H. Abdoul-Carime, Y. Yamamoto, Y. Kiyozumi

J. Chem. Soc. Faraday Trans. 94, 369 (1998)

\* 15 Alkali metal cations and Chorand crown ether complexes:"Best fit" concept investigated by Electrospray Mass Spectrometer

# H. Abdoul-Carime

J. Chem. Soc. Faraday Trans. **94**, 2407 (1998)

16 Electron weakly bound to molecules by dipolar, quadrupolar or polarization forces

H. Abdoul-Carime, C.Desfrançois

Eur. Phys. J. D 2, 149 (1998)

17 Experimental and Theoritical ab-initio study of the influence of N-methylation on the dipole-bound electron affinities of thymine and uracil

C.Desfrançois, H. Abdoul-Carime, S.Carles, V.Periquet and J.P. Schermann

*J.Chem.Phys.* **110**, 24, 11876 (1999)

**18** Damage induced by 0-30eV electrons on thymine and bromouracil substituted oligonucleotides

H. Abdoul-Carime, P.C. Dugal, L.Sanche

Radiat. Research, 153, 23, (2000)

19 DIET of Neutral Fragments from Chemisorbed Biological Molecular Systems

H. Abdoul-Carime, P.C. Dugal, L.Sanche

*Surface Science*, **451**, 102, (2000)

**20** Mechanism for low energy (1-30eV) electron induced pyrimidine ring fragmentation within thymine and halogen substituted single strands of DNA

P.C.Dugal, H. Abdoul-Carime, L.Sanche

J. Phys. Chem. B, 104, 5610 (2000)

21 Dissociative Electron Attachment to Gas Phase BromoUracil

H. Abdoul-Carime, M.A.Huels, F..Brüning, E.Illenberger, L.Sanche

*J.Chem.Phys.*, communication, **113**, 2517, (2000)

**22** Low Energy (5-40 eV) Electron Stimulated Desorption of Anions from Physisorbed DNA bases

H. Abdoul-Carime, P.Cloutier, L.Sanche

*Radiat.Res.*, **155**, 625 (2001)

23 Sequence Specific DNA Damage Induced by Very Low Energy (1-30 eV) Electrons

H. Abdoul-Carime and L. Sanche

Radiat. Res. 156, 151 (2001)

**24** Sensitizing DNA to secondary electron damage: Resonant formation of oxidative radicals from 5-halouracils

H. Abdoul-Carime, M.A. Huels, E. Illenberger, L. Sanche

J. Am. Chem. Soc. 123, 5354 (2001)

25 Fragmentation of short single DNA strands by 1-30 eV electrons: dependence on base identity and sequence

H. Abdoul-Carime and L. Sanche

Int. J. of Radiat. Biol.. **78**, 89 (2002)

26 Alteration of the Protein Structure Induced by Low-Energy (0-18 eV) Electrons: I - *Investigation of Model Systems: Acetamide and Dimethyl Disulfide* 

H. Abdoul-Carime, S. Cecchini, L.Sanche

Radiat. Research. 158 23 (2002)

27 Mechanism for sulfur-radical production by low-energy (1-18eV) electron impact on Dimethyl Disulfide adsorbed on ice

H. Abdoul-Carime, L. Sanche

J. Phys. Chem. B, 106 12186 (2002)

28 Multipole-bound molecular negative ions.

H. Abdoul-Carime, J.P. Schermann, C. Desfrançois

Few-Body Systems 31(2-4), 183 (2002)

29 Alteration of the Protein Constituents Induced by Low-Energy (0-18 eV) Electrons: II - Dissociative Electron Attachment to Amino Acids Containing Cyclic Groups

H. Abdoul-Carime. L.Sanche

Radiat.Res. 160 86 (2003)

**30** Fragmentation of Gas Phase HaloUracils Induced by Low-Energy (0-18eV) Electron Impact

H. Abdoul-Carime, M.A.Huels, E.Illenberger, L.Sanche

Int.J. Mass Spectrom. 228 703 (2003)

- \* 31 Dehydrogenation of Adenine Induced by Slow (<3 eV) Electrons
  - S. Gohlke, H. Abdoul-Carime, E. Illenberger,

Chem.Phys.Lett. 380 595 (2003)

32 Alteration of Protein Constituents Induced by Low-Energy (< 35 eV) Electrons: III. *The aliphatic amino-acids* 

# H. Abdoul-Carime and L.Sanche

J.Phys.Chem. 108 457 (2004)

\* 33 Conversion of Amino-Acids by Electrons at Subexcitation Energies

# H. Abdoul-Carime, S. Gohlke, E. Illenberger

*PCCP* **6** 161 (2004)

34 Dissociation of Dimethyl Sulfide on Amorphous Ice Initiated by Low-Energy (< 20 eV) Electrons

H. Abdoul-Carime, L. Sanche

*PCCP* **6** 1043 (2004)

- \* 35 Thymine Excision by Electrons at Subexitation Energies
  - **H. Abdoul-Carime**, S. Gohlke, E. Fischbach, J. Scheike, E. Illenberger, *Chem. Phys. Lett.* 387 267 (2004)
- \* 36 Site-Specific Dissociation of DNA Bases by Low-Energy Electrons at Early Stages of Irradiation
  - H. Abdoul-Carime, S. Gohlke, E. Illenberger,

Phys. Rev. Lett. 92 168103.1 (2004)

**37** Low Energy Electron Driven Reaction in Free and Bound Molecules: From Unimolecular Processes to Complex Reaction in a Condensed Environment

J. Langer, R. Balog, M. Stano, S. Gohlke, H. Abdoul-Carime, E. Illenberger

*Int. J. Mass Spectrom.* 233 267 (2004) – (Review Article)

\* 38 Decomposition of Vitamin C by Radiation–Induced Slow Electrons

H. Abdoul-Carime, E. Illenberger

Chem. Phys. Lett. 390 481 (2004)

- \* 39 Decomposition of Protein at the Early Time of Irradiation
  - H. Abdoul-Carime, S. Gohlke, E. Illenberger

(submitted 2004)

40 D<sup>-</sup>, O<sup>-</sup> and OD<sup>-</sup> desorption induced by low-energy (0-20 eV) electron impact on amorphous D<sub>2</sub>O films

X. Pan, H. Abdoul-Carime, P. Cloutier, A.D. Bass and L. Sanche,

(accepted Radiat. Phys. Chem. 2004)

- \* 41 5-Bromodeoxiuridine radiosensitization induced by electron at subexcitation energies H. Abdoul-Carime, P. Limao-Vieira, I. Petrushko, N.J. Mason, S. Gohlke, E. Illenberger (submitted 2004)
- \* **42** Dissociative Electron Attachment to Tryptophan
- **H. Abdoul-Carime**, S. Gohlke, E. Illenberger (submitted 2004)
- \* 43 Fragmentation of Proline by slow electrons
  - H. Abdoul-Carime, E. Illenberger

(in preparation 2004)

# **Chapter of Book:**

- **1 H.Abdoul-Carime**, P.C. Dugal, L.Sanche, "DIET of Neutral Fragments from Chemisorbed Biological Molecular Systems" publié dans Desorption Induced by Electronic Transition DIET VIII, edts. T:D Madey, A. Zimmermann, Springer–Verlag (2001)
- **2** S. Gohlke, **H. Abdoul-Carime**, E. Illenberger, "Site—specific Dehydrogenation of DNA bases Induced by Low-Energy (<3eV) Electrons: Nucleic Acid alteration at Early Stage of Radiation", (à publier dans Gaseous Dielectrics X, edt. L.G. Christophorou, Kluwer Academic / Plenum Publisher (2004))

# Sylwia Ptasińska

# **Personal Data:**

Date of Birth: 14.08.1977

Nationality: Polish

Present Address: Institute of Ion Physics

Technikerstr. 25

A-6020 Innsbruck, Austria Phone: +43 512 507 6268 Fax: +43 512 507 2932

Email: Sylwia.Ptasinska@uibk.ac.at



# **Education:**

1984-1992 Primary school, Lublin, Poland 1992-1996 High school, Lublin, Poland

1996-2001 Maria Curie-Skłodowsa University, Lublin, Poland

Master of Science (physics), diploma thesis: "Mass spectrometry of gaseous

clusters"

2001-2002 Maria Curie-Skłodowsa University, Lublin, Poland

PhD student

Leopold-Franzens-University, Innsbruck, Institute of Ion Physics

PhD student

# **Achievement:**

Award of Polish Vacuum Society for the best master thesis." Mass spectrometry of gaseous clusters", 2002.

# **Publications:**

#### 2003:

- 1. S. Ptasińska, J. Dąbek, L.Michalak Formation of water dimers in expanding air flows. Vacuum, Volume 70, Issues 2-3. 2003, 403-409
- 2. S. Ptasińska, A. Bajuk, L.Michalak *Influence of potassium chloride on the MALDI detection process*. Vacuum, Volume 70, Issues 2-3. 2003, 439-445
- 3. S. Ptasińska, L.Michalak, M. Smolira *Some aspects of the stability of ion current in a matrix-assisted laser desorption/ionisation source*. Rapid Communication in Mass Spectrometry, Volume 17, Issue 9, 2003, 917-923
- 4. S. Denifl, S. Ptasinska, M. Cingel, S. Matejcik, P. Scheier, T.D. Märk *Electron attachment to the DNA bases thymine and cytosine*. Chem. Phys. Letters 377, 2003, 74-80
- 5. S.Denifl, S.Ptasinska, G.Hanel, B.Gstir, P.Scheier, M.Probst, B.Farizon, M.Farizon, S.Matejcik, E.Illenberger, T.D.Märk *Electron attachment to uracil, Thymine and cytosine*, Physica Scripta, in print (2003)
- 6. S. Ptasinska, S. Denifl, A. Abedi, P. Scheier, T.D. Märk- *Dissociative electron attachment to gas-phase glycine*. Analytical and Bioanlytical Chemistry 377, (7-

#### 2004:

- 7. S. Denifl, S. Matejcik, S. Ptasinska, B. Gstir, M. Probst, P. Scheier, E. Illenberger and T.D. Märk *Electron attachment to chlorouracil: a comparison between 6-ClU and 5-ClU*. J. Chem. Phys. 120 (2004) 704-709
- 8. S. Denifl, S. Ptasinska, P. Scheier and T.D. Märk- *Electron impact ionization of 5-and 6-chlorouracil: appearance energies.* Int. J. Mass Spectrom. 232 (2004) 99-105
- 9. S. Denifl, S. Ptasinska, G. Hanel, B. Gstir, M. Probst, P. Scheier and T.D. Märk *Electron attachment to gas-phase uracil.* J. Chem. Phys. 120 (2004) 6557-6565
- 10. S. Ptasinska, S. Denifl, P. Scheier and T.D. Märk *Inelastic electron interaction (attachment/ionization) with deoxyribose*. J. Chem. Phys. 120 (2004) 8505-8511; and
  - Virtual Journal of Biological Physics Research 7 (2004) issue 9
- 11. S. Denifl, S. Ptasińska, M. Probst, J. Hrusak, P. Scheier and T. D. Märk-*Electron* attachment to the gas phase DNA bases cytosine andthymine. J. Phys. Chem. (accepted)
- 12. S. Ptasińska, S. Denifl, T. D. Märk, P. Scheier, S. Gohlke, M. A. Huels and E. Illenberg *Site selective H<sup>-</sup> abstraction from Thymine*. Phys. Rev. Lett. (submitted)

# **Lectures:**

- 1. S. Ptasińska *Mass spectrometry of gaseous clusters* . VI National Vacuum Conference, Korbielów, Polska 2002.
- 2. S. Ptasińska *Mass spectrometry of gaseous clusters*. (invited lecture) Technical University of Gdańsk, Poland 2002.
- 3. S. Ptasińska *MALDI method for biomolecules*. (invited lecture) Technical University of Gdańsk, Poland 2002.
- S. Ptasińska, S. Denifl, A. Abedi, P. Scheier, T. Märk Dissociative electron attachment to glycine by low energy electron impact.
   EPIC Network Meeting, Pruhonice near Prague, Czech Republic 2003
- S. Ptasińska, S. Denifl, A. Abedi, P. Scheier, T. Märk Electron attachment to biological relevant molecules.
   53.ÖPG-Jahrestagung, Salzburg, Austria 2003
- S. Ptasińska- Radiation damage of biomolecules.
   Schwerpunktseminar Ionen- Plasmaphysik, Leopold-Franzens-University, Innsbruck, Austria 2004
- 7. S. Ptasińska, S. Denifl, E. Illenberger, T. D. Märk, and P. Scheier *Site selective electron at tachment to the partially deuterated thymine* EPIC Network Meeting, Obergurgl, Austria 2004

# **Conference Contributions:**

## 2002:

1. S. Ptasińska, J. Dabek, L.Michalak - Some aspects of formation of ammonia micro-

- *clusters*. IV International Symposium Ion Implantation and other Application of ions and electrons, Kazimerz Dolny, Poland 2002
- 2. S. Ptasińska, J. Dąbek, L.Michalak *Formation of water dimers in expanding air flows*. IV International Symposium Ion Implantation and other Application of ions and electrons, Kazimerz Dolny, Poland 2002
- 3. S. Ptasińska, A. Bajuk, L.Michalak *Influence of potassium chloride on the MALDI detection process*. IV International Symposium Ion Implantation and other Application of ions and electrons, Kazimerz Dolny, Poland 2002

#### 2003:

- 4. S.Denifl, S.Matejcik, S.Ptasińska, G.Hanel, B.Gstir, A.Stamatovic, P.Scheier, T.D.Märk *Electron attachment and electron impact ionization of biomolecules*. Deutsche Gesellschaft für Massenspektromtrie-meeting (DGMS 2003), Munich, Germany 2003
- 5. S. Denifl, G. Hanel, B. Gstir, S. Ptasińska P. Scheier, M. Probs, B. Farizon, M. Farizon, S. Matejcik, E. Illenberg, T.D. Märk *Site selctive electron attachment to RNA and DNA bases*. XXIII International Conference on Photonic, Electronic, and Atomic Collisions (XXII ICPEAC), Stockholm, Sweden 2003
- 6. E. T.M. Selim, L. Michalak, S. Ptasińska *Study of manganese chloride and its reactivity in the negative ion mode using laser desorption/ionization (LDI) TOF-mass spectrometer.* 16<sup>th</sup> International Mass Spectrometry Conference (IMSC-16), Edinburg 2003
- 7. S. Ptasińska, S. Denifl, A. Abedi, P. Scheier, T. Märk *Dissociative electron attachment to glycine by low energy electron impact*. 13th International Symposium on Electron-Molecule Collisions and Swarms July (EMS 2003 Prague), Pruhonice near Prague, Czech Republic 2003
- 8. S.Denifl, G.Hanel, S.Ptasinska, B.Gstir, S. Matejcik, A.Stamatovic, P.Scheier, T.D.Märk *Electron impact and attachment studies of biomolecules*.
  - 13th International Symposium on Electron-Molecule Collisions and Swarms (EMS 2003 Prague), Pruhonice near Prague, Czech Republic 2003
- 9. S. Ptasińska, S. Denifl, A. Abedi, P. Scheier, T. Märk *Electron attachment to biological relevant molecules*. 53.ÖPG-Jahrestagung, Salzburg, Austria 2003
- 10. S. Denifl, S. Ptasinska, G. Hanel, M. Probst, P. Scheier, T.D. Märk *Radiation damage in molecules of biological relevance*. Austrian- Hungarian workshop on charged-particle transport through nanostructures an solids; Debrecen, Hungary 2003

#### 2004:

- 11. S. Ptasińska, S. Denifl, P. Candori, P. Limão-Vieira, P. Scheier and T. D. Märk *Inealastic electron interaction (attachment/ionization) with sugar moleculs and amino acids* V -th International Conference Ion Implantation and Other Applications of Ions and Electrons, Kazimierz Dolny, Poland 2004 (ION 2004)
- 12. S. Ptasińska, P. Candori, S. Denifl, S. Yoon, P. Scheier and T. D. Märk *Electron interactions with nucleosides of dna and rna: thymidine and uridine*. RADAM Conference, Radiation Damage in Biomolecular System", Lyon, France
- 13. P. Scheier, S. Denifl, S. Ptasinska, M. Probst, S. Yoon and T.D. Märk *Dissociative electron attachment to biologically relevant molecule*. 8th European Conference on Atomic and Molecular Physics, Rennes, France 2004 (ECAMP8)
- 14. S. Ptasińska, S. P. Denifl, P. Limão-Vieira, P. Scheier and T. D. Märk Damage of

*DNA sugar and its moiety by electron impact.* 8th European Conference on Atomic and Molecular Physics, Rennes, France 2004 (ECAMP8

# Slawomir Telega

Born: 12. 12. 1977 in Gdynia (Poland)

Nationality: Polish

Employment in the Network: Predoctoral fellow under the EPIC network Period of Employment: November 2003 - January 2004 (three months)

Present position: Assistant and Ph. D. Student, Departament of Theoretical Physics and Mathematical Methods, Faculty of Applied Physics and Mathematics, Gdansk University of Technology

- \* Ro-vibrationally inelastic electron scattering from diatomic molecules
- \* Critical minima in relativistic electron scattering from rare gas atoms
- \* Dynamic distortion effects in the relativistic version of polarized orbital method

\*\*\*\*\*\*\*\* Colaboration \*\*\*\*\*\*\*

- \* Group of Theoretical Chemical Physics led by prof. F.A. Gianturco, Departament of Chemistry, University of Rome "La Sapienza"
- \* Prof. B. Marinkovic, A. Milosavljevic, Institute of Physics, Belgrade, Serbia and Montenegro

\*\*\*\*\*\*\*\*\*\*\*\*\*\* CV \*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*

- \* 1992 1996 XII LO Gdañsk (Secondary School)
- \* 1996 2001 Faculty of Technical Physics ans Applied Mathematics, Gdañsk University of Technology
- \* 2001 M.Sc. Thesis with Honours entitled Solving Schrodinger equation for scattering states using T-matrix method
- \* 2001 Ph. D. student in the Departament of Theoretical Physics and Mathematical Methods, working on the Ph. D. thesis entitled Low energy electron scattering from H2 and N2 molecules

\*\*\*\*\*\*\*\*\*\*\*\*\*\* Visits \*

Spring 2001 - European Student Exchange Programme Erasmus, Group of Theoretical Chemical Physics led by prof. F. A. Gianturco, Departament of Chemistry, University of Rome "La Sapienza"

Spring/Summer/Fall 2002 - Group of Theoretical Chemical Physics led by prof. F. A. Gianturco, Departament of Chemistry, University of Rome "La Sapienza"

Fall/Winter 2003/2004 - Group of Theoretical Chemical Physics led by prof. F. A. Gianturco, Departament of Chemistry, University of Rome "La Sapienza"

\*\*\*\*\*\*\* Meetings attended \*\*\*\*\*\*\*\*

RMK I (conference on the relativistic quantum mechanics), Warsaw 2002

XXIII International Conference on Photonic, Electronic and Atomic Collisions ICPEAC XXIII, Stockholm 2003

XXXVII Zjazd Fizyków Polskich (XXVII Meeting of the Polish Physicists), Gdañsk 2003

RMK II (conference on the relativistic quantum mechanics), Olsztyn 2002

\*\*\*\*\*\* Papers \*\*\*\*\*\*\*\*\*\*\*

# published:

1. Konopiñska V., Telega S., Sienkiewicz J. E.,

Electron-argon scattering: a high minimum in differential cross sections,

Task Quarterly, vol.5, no.1, Jan. 2001, pp.13-16. Publisher: TASK Publishing, Poland.

2. Sienkiewicz JE, Konopinska V, Telega S, Syty P.

Critical minima in elastic electron scattering from argon,

Journal of Physics B-Atomic Molecular & Optical Physics, vol.34, no.13, 14 July 2001, pp.L409-18. Publisher: IOP Publishing, UK. (1 citation)

3. Sienkiewicz JE, Telega S, Syty P, Fritzsche S.

Differential cross section minima in elastic scattering of electrons from zinc,

Physics Letters A, vol.293, no.3-4, 28 Jan. 2002, pp.183-7. Publisher: Elsevier, Netherlands

4. Sienkiewicz JE, Telega S, Syty P, Fritzsche S.

Critical minima in elastic scattering of electrons from Ar and Zn. Elsevier.

Radiation Physics and Chemistry, vol.68, no.1-2, Sept. 2003, pp.285-9. UK.

# in print:

1. S. Telega, E. Bodo, F.A. Gianturco

Rotationally inelastic collisions of electrons with H 2 and N 2 molecules: A close-coupling calculations in space frame

Eur. Phys. J. D (2004)

2. Marinkoviæ B, Sienkiewicz JE, Milosavljeviæ A, Telega S.

Elastic electron scattering by argon in the vicinity of the high-energy critical minimum Radiation Physics and Chemistry (2004)

3. Sienkiewicz JE, Marinkoviæ B, Milosavljeviæ A, Telega S.

The high-energy critical minimum in elastic electron scattering by argon

Eur. Phys. J. D (2004)

# **Damian Pliszka**

# PERSONAL DATA

Name: Damian Pliszka

Passport No: BM 1222244

Fiscale code (NIP) 839-202-25-25, (italian) PLSDMN71A08Z127M

Address and telephone: ul. Witosa 98, 76-251 Kobylnica, Poland

tel. (0-59) 84-15-333

Date and place of birth: 08.01.1971; Słupsk, Poland

# **EDUCATION**

1990 - 1995 – Pomeranian Pedagogical Academy in Słupsk, master of science degree in physics,

MSc thesis: "Energy transfer between 6<sup>3</sup>P<sub>0.1,2</sub> states in Hg-N<sub>2</sub> ring discharge plasma",

supervisor prof. H. Wrembel

1999 - 2003 – Gdańsk University PhD studies, PhD thesis: "Application of positron spectroscopy in

solid state physics"

PhD Thesis "Applications of positron annihilation techniques in Solid State spectroscopy" Presented 24.04.2003, Gdańsk University

# WORK

1995- – Pomeranian Pedagogical Academy in Słupsk, assistant

**SKILLS** – Languages: English – good, Russian – good, German – intermediate

# **SCIENTIFIC INTERESTS**

Optical molecular spectroscopy

Structural research in solids, especially semiconductor materials.

Positron annihilation techniques

Optical Solid State spectroscopy (Photoluminescence, IR spectroscopy).

# **DIDACTICS**

**Physics** 

Informatics

# **PUBLICATIONS:**

6 articles

11 conference rapports3 internal rapports

# Dr Nykola Jones

## Personal Information

Current Work Address: Institute of Physics & Astronomy, University of Aarhus, Ny

Munkegade, Building 520, DK- 8000 Aarhus C, DENMARK

Nationality: British

# Education & Qualifications

University College London, Dept of Chemistry

1993 - 1996

B.Sc.- Upper Second class Honours degree in Chemistry

University College London, Dept of Physics & Astronomy

1996 - 2000

PhD Post Graduate Studies in Molecular Physics Supervisor: Dr N. J. Mason,

Spectroscopy and Dissociation Dynamics of Simple Polyatomic Molecules

PhD in Physics from the University of London Awarded 31<sup>st</sup> March 2000

# Employment

# Institute of Physics and Astronomy, University of Aarhus,

Post-doctoral research assistant- Low energy electron-molecule scattering experiments.

# Experimental Experience

Experience gained in experimental physical chemistry

# • Low Energy Electron Scattering from Molecules

Low energy electrons (a few meV) with high resolution (~1 meV FWHM) are produced via the photoionisation of argon, using monochormatised light from the ASTRID synchrotron storage ring in Aarhus. An electrostatic lens system focuses these electrons into a beam, which is used in a transmission experiment to determine total integral scattering cross-sections for molecules. Further information regarding the processes occurring between molecules and low energy electrons is gained through the measurement of cross-sections in the presence of a magnetic field, whereby phenomena such as virtual state scattering, electron attachment and angular distribution of scattering processes can be observed. A large number of molecules have been investigated using this method, many of which are of reactive plasma, atmospheric and astrophysical interest: CO<sub>2</sub>, CS<sub>2</sub>, OCS, N<sub>2</sub>O, CF<sub>4</sub>, C<sub>2</sub>F<sub>4</sub>, C<sub>4</sub>F<sub>8</sub>, CF<sub>3</sub>Cl, CF<sub>2</sub>Cl<sub>2</sub>, CFCl<sub>3</sub>, CF<sub>3</sub>I, CF<sub>3</sub>Br, CCl<sub>4</sub>, C<sub>6</sub>F<sub>6</sub>, OClO, Cl<sub>2</sub>O, MeNO<sub>2</sub>, HCOOH and CH<sub>3</sub>COOH, CH<sub>3</sub>I, CH<sub>3</sub>Cl, CH<sub>3</sub>Br, SF<sub>6</sub>, SF<sub>5</sub>CF<sub>3</sub>, CH<sub>3</sub>CN, CHCl<sub>3</sub>, p-xylene, p-C<sub>6</sub>F<sub>2</sub>H<sub>4</sub>, THF, N<sub>2</sub>.

# • VUV Photo-absorption spectroscopy using synchrotron radiation

Daresbury Laboratory - The absorption spectra for many compounds of atmospheric and astrophysical interest have been recorded including OCl,  $N_2O$ ,  $SO_2$ ,  $N_2O_5$  and several PAH's Physikalisches Institute, University of Bonn - High resolution photoabsorption experiments concentrating on the investigation of Rydberg states of molecules e.g. vinyl bromide.

#### • Electron/molecule collisions -

Electron energy loss spectroscopy – EELS for  $N_2O$  (and  $N_2$  for calibration) have been recorded and analysed.

Detection of metastable neutral species in excited sates. - Metastable excited state neutrals have been detected using (1) a time-of-flight technique and (2) observation of resonance structure.

Coincidence studies of the dissociation of highly excited states of neutral molecules - The development of a coincidence experiment to look at the fragmentation dynamics of the highly excited electronic states of neutral molecules.

#### • Photoionisation

The high resolution He(I) photoelectron spectrum of Cl<sub>2</sub>O has been recorded, working with Prof. J Delwiche at the University of Liege, Belgium

# • Electron-Impact Ionisation of Reactive Molecules Involved in Ozone Depletion

Third year research project for degree studying the fragmentation of the dications of dinitrogen pentoxide and nitric acid using time-of-flight mass spectrometry.

#### Publications

# Electron-impact ionisation of dinitrogen pentoxide

C. S. S. O'Connor, N. C. Jones, K. O'Neale, S. D. Price,

Int. J. of Mass Spec. & Ion Proc., vol.154, no.3, pp.203-211 (1996)

# The formation and dissociation of the dinitrogen pentoxide dication

C. S. S. O'Connor, N. C. Jones, S. D. Price,

Chemical Physics, vol. 214, No.1, pp.131-141 (1997)

# Electron-impact ionisation of nitric acid

C. S. S. O'Connor, N. C. Jones, S. D. Price,

Int. J. Of Mass Spec. & Ion Proc., vol.163, No.1-2, pp.131-139 (1997)

# On the high resolution He(I) photoelectron spectrum of Cl<sub>2</sub>O

F. Motte-Tollet, J. Delwiche, J. Heinesch, M.-J. Hubin Franskin, J. M. Gingell, N. C. Jones, N. J. Mason, & G. Marston.

Chem. Phys. Lett vol. 284, p452-458 (1998)

# Electronic excitation and oscillator strength of ethyl iodide by VUV photoabsorption and electron energy loss spectroscopy

A. Guiliani, F. Motte-Tollet, J. Delwiche, J. Heinesch, N. J. Mason, J. M. Gingell, I. C. Walker, N. C. Jones, M.-J. Hubin-Franskin.

Chem. Phys, Vol.110, No.21, pp.10307-10315 (1999)

# Experimental studies on electron scattering from atoms and molecules: the state of the art.

N. J. Mason, J. M. Gingell, N. C. Jones and L. Kaminski,

Phil. Trans. Roy. Soc. Series A, Vol.357, No.1755, pp.1175-1200 (1999)

# Vacuum ultraviolet spectrum of dinitrogen pentoxide

B. A. Osborne, G. Marston, J. M. Gingell, N. C. Jones, L. Kaminski, N. J. Mason, I. C. Walker, J. Delwiche and M.-J. Hubin-Franskin,

J. Quant. Spec. and Radiat. Transfer, Vol. 64, No. 6, p67-74. (2000)

# Electronic excitation and oscillator strengths of ethyl bromide by vacuum ultraviolet photoabsorption and electron energy loss spectroscopy.

A. Guiliani, F. Motte-Tollet, J. Delwiche, I. C. Walker, N. J. Mason, J. M. Gingell, N. C. Jones, M.-J. Hubin-Franskin,

J. Chem. Phys., Vol.112, No.14, pp.6285-6292 (2000)

# **Electron scattering in chlorine dioxide**

D. Field, N. C. Jones, J. M. Gingell, N. J. Mason, S. L. Lunt, J.-P. Ziesel,

J. Phys. B, vol. 33, No.5, pp.1039-1046 (2000)

# VUV optical absorption and energy loss spectroscopy of chlorine nitrate

N. J. Mason, N. C. Jones, L. Kaminski, B. A. Osborne, G. Marston, M. A. Fernandez, I. C. Walker and E. A. Seddon,

Int. J Mass Spec. Vol.205, No.(1-3), pp.183-196, (2001)

# Very low energy electron scattering in nitromethane, nitroethane and nitrobenzene.

S. L. Lunt, D. Field, J.-P. Ziesel, N. C. Jones, R. J. Gulley,

Int. J. Mass. Spect. Vol.205, No.(1-3), pp. 197-208, (2001)

# Experimental evidence for a virtual state in a cold collision: Electrons and carbon dioxide

D. Field, N. C. Jones, S. L. Lunt & J.-P. Ziesel,

Phys. Rev. A., vol. 64, 022708, (2001)

# Low energy electron scattering in CF<sub>2</sub>Cl<sub>2</sub> and CF<sub>3</sub>Cl

D. Field, N. C. Jones, S. L. Lunt, J.-P. Ziesel & R. J. Gulley,

J. Chem. Phys., Vol. 115, No. 7, p3045, (2001)

# **Cold collisions of electrons with molecules**

D. Field, N. C. Jones & J.-P. Ziesel

Few Body Systems, Vol. 31, , p1-7, (2002)

# Cold collisions of electrons with Molecules: virtual state scattering in CO<sub>2</sub>.

S. L. Lunt, N.C. Jones, J.-P. Ziesel and D. Field

In: Photonic, Electronic and Atomic Collisions XXII ICPEAC Santa Fe, New Mexico, July 18 24. Burgdorfer, J.; Cohen, J.S.; Datz, S.; Vane, C.R. (Eds.), (2002)

# Collisions froides electron molecule: etats virtuels et resonances

*J.-P. Ziesel, N.C. Jones, S. L. Lunt, and D. Field* In: PAMO 2002. French Physical Society (Atomic, Molecular and Optical Physics Division) Symposium, Bourges, (2002).

# Giant Resonances in cold electron scattering by CS<sub>2</sub>

N. C. Jones, D. Field; J.-P. Ziesel, T.A. Field,

Physical Review Letters; 89: 93201 93204, (2002).

# Very low energy encounters: cold electrons and molecules

D. Field, N. C. Jones, J.-P. Ziesel,

Europhys. News, 33/6, 196-197, (2002)

# An undulator based spherical grating monochromator beamline optimised for low energy electron-molecule scattering experiments

S. V. Hoffmann, N. C. Jones, D. Field and J.-P. Ziesel

Rev. Sci. Inst. 73; 73: 4157 4163, (2002)

# **Reaction and Scattering in Cold Electron Collisions**

J. P. Ziesel, N. C. Jones, D. Field, and L. B. Madsen,

Phys. Rev. Lett., **90**, 083201, (2003)

# Cold electron scattering in SF6 and C6F6: bound and virtual state channels

D. Field, N.C. Jones, and J.-P. Ziesel, Phys. Rev. A, 69, 052716-1, 2004

# Abstracts/Reports

# Low energy electron scattering from halogenated hydrocarbons

N. C. Jones Talk presented at EPIC Network meeting, Obergurgl, Austria, Monday 21 June 2004

# Low energy electron-molecule scattering experiments

N. C. Jones Talk presented at EPIC Network meeting, Pruhonice, Near Prague, Wednesday 30 July 2003

# Very low energy electron scattering in nitromethane, nitroethane and nitrobenzene

N. C. Jones Talk presented at 1<sup>st</sup> International Symposium on Low energy electron-molecule scattering (LEEMI), March 2001, Austria.

# New results in cold electron-molecule scattering experiments

N. C. Jones Talk presented at the Institute of Physics and Astronomy (IFA) November 2000, Denmark.

# Low energy electron scattering from halogenated hydrocarbons

D. Field, N. C. Jones, I. Struve, S. V. Hoffmann and J.-P. Ziesel.

Poster presented at EPIC2004, Obergurgl, June 2004

# The determination of absolute electron attachment cross-sections from beam scattering data

D. Field, J.-P. Ziesel, N. C. Jones, S. V. Hoffmann and L. B. Madsen

Poster presented at EPIC2004, Obergurgl, June 2004, COST/RADAM meeting, Lyon, June 2004 and ECAMP8, Rennes, July 2004

# Cold electron scattering by a chiral molecule.

D. Field, I. Struve, P. Cahillane, N. C. Jones, S. V. Hoffmann, L. B. Madsen, and J.-P. Ziesel

Poster presented at EPIC2004, Obergurgl, June 2004, COST/RADAM meeting, Lyon, June 2004 and ECAMP8, Rennes, July 2004

# Low energy electron-molecule scattering from CCl<sub>4</sub>, SF<sub>6</sub> and C<sub>6</sub>F<sub>6</sub>.

D. Field, N. C. Jones, L. B. Madsen, S. V. Hoffmann and J.-P. Ziesel.

Poster presented at ICPEACXXIII, Stockholm, July 2003, 13<sup>th</sup> EMS conference, Prague July 2003 and Danish Physical Society, May 2003

# Giant resonances in cold electron scattering by CS<sub>2</sub>

N. C. Jones, D. Field, S. V. Hoffmann, J.-P. Ziesel, and T. A. Field

Poster presented at ICPEACXXIII, Stockholm July 2003, 13<sup>th</sup> EMS conference, Prague July 2003

# Experimental evidence for a virtual state in a cold collision: Electrons and carbon dioxide

D. Field, N. C. Jones, S. L. Lunt & J.-P. Ziesel

Poster presented at ECAMPVII, Berlin 2001

# **VUV Photoabsorption spectroscopy of Polycyclic Aromatic Hydrocarbons (PAH's)**

J M Gingell, N J Mason, A R Birrell, N C Jones, L Kaminski, M Pontefract, D Ruffle, J Rawlings and D A Williams

Poster presented at ECAMPVI, Italy, July 1998

# Coincidence studies of the dissociation of neutral molecules in highly excited states N C Jones, N J Mason and S D Price

Poster presented at ATMOP XXIV March 1997; ICPEAC XX, Vienna, July 1997; ECAMPVI, Italy, July 1998

# Rydberg state spectroscopy of haloalkanes

F Motte-Tollet, M-P Ska, J M Gingell, N C Jones, L Kaminski, N J Mason and I C Walker Poster presented at ICPEAC XX, Vienna, July 1997

# VUV Spectroscopy of simple polyatomic aromatic hydrocarbons

N J Mason, J M Gingell, N C Jones, L Kaminski, A R Birrell, M Pontefract, D Ruffle, J Rawlings and D A Williams

Poster presented at ICPEAC XX, Vienna, July 1997

# High resolution electron spectroscopy of haloalkanes.

M-J Hubin-Franskin, F Motte-Tollet, M-P Ska, A Giuliani, J M Gingell, N C Jones, L Kaminski, N J Mason, I C Walker

Daresbury Report 1997

# UV Photoabsorption spectroscopy of organic CN substituted compounds

M-J Hubin-Franskin, J Delwiche, F Motte-Tollet, L Christiaens, J Mareque, J M Gingell, N C Jones, N J Mason, I C Walker Daresbury Report 1997

# Vacuum ultraviolet spectrum of dinitrogen pentoxide

B A Osborne, G Marston, J M Gingell, N C Jones, L Kaminski, N J Mason,
I C Walker

Daresbury Report 1997

# **VUV** Absorption spectroscopy of free radicals :OCl

I C Walker, G Marston, N J Mason, J M Gingell, N C Jones, L Kaminski

Daresbury Report 1997

# Conference Organisation

Local organiser for the ESF/PESC Exploratory Workshop 2002, 'Collisions in Atom Traps (CATS)', Sunday 7th to Thursday 11th April 2002, Sandbjerg Manor, Sønderborg, Denmark.

Assisted in the organisation of the meetings:

- ISA/ASTRID User Meeting 2003, 22<sup>nd</sup>/23rd May 2003, University of Aarhus, Denmark
- Nordic School in Atomic Physics 2001 23<sup>rd</sup>-27<sup>th</sup> August, Sandbjerg Manor, Sønderborg, Denmark.
- "Synchrotrons, Accelerators and Laboratory Astrophysics" (SALA), University of Aarhus, Denmark, 30<sup>th</sup> August 1<sup>st</sup> September 2000,

# Volunteer experience

Volunteer student tutoring at schools in London to help class teachers with pupils of varying ability and to gain experience of teaching. For several months I attended a girls secondary school helping with science lessons, organised by the North London Connection.

#### Other skills

I have extensive experience with computers and am proficient using the windows operating system environment. I have a thorough knowledge of many packages including word-processors,

spreadsheets and databases which I have used for a number of years. I also have basic knowledge of the Unix platform and completed a basic Fortran programming course in the first year of my undergraduate degree. More recently I have been learning how to program in VB. I have also constructed and maintain several web sites for conferences and research networks.

# References

Professor D Field
Department of Physics and Astronomy
University of Aarhus
Ny Munkegade, Building 520
DK-8000, Aarhus C
DENMARK

Tel: 0045 89 42 36 50 email: dfield@phys.au.dk

Professorr N J Mason
Centre of Molecular and Optical Sciences
Department of Physics and Astronomy
The Open University,
Walton Hall,
Milton Keynes, MK7 6AA
Tel: 0044 1908 655 132

email: n.j.mason@open.ac.uk

# **Peter Papp**

Title: RNDr.

Date of birth: August 13<sup>th</sup> 1978

Place of birth: Nove Zamky, Slovak Republic

Address: Nabrezna 31

940 74 Nove Zamky Slovak Republic

Marital status: single

Education: 2001- PhD student at Department of Chemical physics, Faculty of Mathematics, Physics and Informatics Comenius University, Bratislava, Slovak Republic

Branch: Chemical physics

Supervisor: prof. Ing. Ivan Hubac, DrSc.

The topic of the dissertation thesis: The study of electron quasi-degeneracy by using

Brillouin-Wigner perturbation theory.

1996-2001 Department of Biophysics and Chemical physics, Faculty of Mathematics, Physics and Informatics, Comenius University, Bratislava, Slovak Republic

Branch: Biophysics and Molecular physics

Master examination: General physics, Basis of biophysics and molecular physics, Methods in biophysics and molecular physics.

Supervisor: prof. RNDr. Dusan Chorvat, DrSc.

The topic of the diploma thesis: Using of Raman spectroscopy for study of specifical properties of biological systems.

1992-1996 Secondary Grammar School, Nove Zamky, Slovak Republic School leaving examination: Slovak, English, Mathematics and Physics

1984-1992 Basic School in Nove Zamky, Slovak Republic

# Peter Hrušč

Born: April 5, 1977 in Michalovce, Slovak Republic

Current address: Komenského 20, 07101 Michalovce, Slovak Republic

Marital status: single

#### **Elementary education:**

1983–1991 VI. Basic school in Michalovce, Slovak Republic

#### **Secondary education:**

1991-1995 Secondary grammar school of Pavol Horov in Michalovce. School leaving

examinations in Slovak, Mathematics, Physics and Biology (1995)

#### **University education:**

1995-2001

Studies of general physics at the Faculty of Mathematics, Physics and Informatics, Comenius University in Bratislava. Studies of biophysics and molecular physics at the Department of Biophysic and Chemical Physics, Faculty of Mathematics, Physics and Informatics, Comenius University in Bratislava. Diploma thesis in the field of quantum chemistry, supervisor doc. RNDr. Ján Urban, CSc.

The topic of diploma thesis: Theoretical study of ground and excites states of rare gas atom clusters.

Master examination in general physics, basis of biophysics and molecular physics, methods of biophysics and molecular physics, obtained in 2001.

#### **Graduate studies:**

2001-

Graduate studies at the Department of Chemical Physics, Faculty of Mathematics, Physics and Informatics, Comenius University in Bratislava. Supervisor doc. RNDr. Ján Urban, CSc., Faculty of Mathematics, Physics and Informatics, Comenius University in Bratislava.

The topic of the dissertation thesis: Study of the dynamics of collision processes.

January 31, 2003 in Prague

# **Vincent Brems's Curriculum Vitae**

Private Address:

Tentenstraße 32, 53225 Bonn, Germany

Tel: +49 228 433 65 29

Date and place of birth:

70-9-25, Hermalle-sous-Argenteau, Belgium

Nationality: Belgian

Marital status: Married, one daughter, one son

Languages: French (mother tongue), German, English (working languages), Dutch (school level)

Computer science: Unix and Fortran programming skills

Post-doctoral positions

2001-2002 : Post-doctoral fellow, Theoretical Chemistry (Dir. H Köppel , University of Bonn ) Main research : R-matrix approach to the low-energy electron scattering on molecules in

collaboration with BM Nestmann

1999-2001 : Post-doctoral fellow, Theoretical Chemistry (Dir. LS Cederbaum , University of Heidelberg )

Main research: low-energy electron scattering on molecules in collaboration with HD Meyer 1996-1999:

Post-doctoral fellow, Theoretical Chemistry (Dir. S Peyerimhoff, University of Bonn)

Main research : core-excited molecules and their Auger decay in collaboration with BM Nestmann

Education

1992-1996: PhD in Physics (Theoretical Chemistry)

PhD thesis: Resonance Overlapping in Molecular Predissociation

Supervisor: M Desouter-Lecomte

Laboratory for Molecular Dynamics and Quantum Chemistry, Dir. J-C Lorquet,

University of Liege

1994 : Agrégation de l'Enseignement Secondaire Supérieur (examination for posts on the teaching staff of lycées), University of Liege

1988-1992 : Graduate studies in Physics, University of Liege

Honour thesis: Relativistic Quantum Mechanics: the Aharonov-Bohm Effect

Supervisor : M Bawin

Fundamental theoretical Physics, Dir. C. Mahaux, University of Liege

1982-1988 : School education at the College St Hadelin at Visé, Belgium

Pedagogical experience

1990-1991:

Practical course in Experimental Physics (37 h)

Life science students (first year university level)

Lecturers: R Evrard, M Delmelle, University of Liege

1993-1994:

Agrégation in Physics

15-Day practical training at school (30 h)

Writing of a course on Electrostatic

1997-1998:

Tutorial in Mathematics (80 h)

Chemistry students (first and second year university level)

Lecturer: BM Nestmann, University of Bonn

1999-2000:

Lecture in Theoretical Chemistry (40 h)

PhD strudents of the Graduate Program "Modelling and Scientific Computing in

Mathematics and Natural Sciences", University of Heidelberg

2001-2002:

Tutorial in Quantum Chemistry (second part) (24 h)

Chemistry students (third and fourth year university level)

Lecturer: S Peyerimhoff, University of Bonn

2002:

Tutorial in Quantum Chemistry (first part) (24 h)

Chemistry students (third and fourth year university level)

Lecturer: M Hanrath, University of Bonn

#### Awards

1996:

Award of the Science Faculty of the University of Liege dedicated to the support of Chemistry and Life Science (25 000 BEF = 620 EUR)

1998-1999:

NATO Scientific Fellowship (280 000 BEF = 7 000 EUR)

**Publications** 

# Barbara Pezler

#### Birthdate:

04-11-1963 Birthplace: Krasnik, Poland

#### Home Address:

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#### Work Address:

Faculty of Science University of Podlasie ul. 3 Maja 54, 08-110 Siedlce, Poland

Phone: +48(25)6431139(office) Email: pezler@ap.siedlce.pl

#### Education:

M.S. 1990 University of Podlasie - Chemistry Ph.D.1997 Warsaw University - Chemistry

#### Experience:

1990-1997 Research/Teaching Assistant, University of Podlasie 1997-2003 Research/Adjunct, University of Podlasie March 2001 Visiting Scientist, University of Calgary, Canada (David A. Armstrong, Professor of Chemistry)

#### Fields of Specialization:

Theorethical chemistry: kinetics of ion-molecule and electron-molecule reactions.

#### **Professional Societies:**

Polish Radiation Society

#### **Publications:**

- 1. J. Turulski, B. Pezler, J. Niedzielski, "Classical transition state theory for the ion-linear quadrupole capture", Chem. Phys., <u>166</u>, (1992), 115-121.
- 2. B. Pezler, J. Turulski, J. Niedzielski, "Quantum TST of the capture the ion by the linear quadrupole in the state of low rotational excitation", Chem. Phys., <u>166</u>, (1992), 123-129.
- 3. J. Turulski, B. Pezler, J. Niedzielski, "Is the ion-linear quadrupole capture rate constant anisotropic with respect to the sign of the charge on the ion and the quadrupole moment of the molecule?", React. Kinet. Catal. Lett., <u>47</u>, (1992), 199-205.
- 4. B. Pezler, J. Turulski, J. Niedzielski, "Effect of anisotropy of polarizibility of the linear quadrupole molecule on the rate of ion capture", J. Chem. Soc. Faraday Trans., <u>89</u>, (1993), 655-670,.
- 5. J. Turulski, J. Niedzielski, B. Pezler, "Transition-state theory treatment of capture collisions between ions and symmetric top dipolar molecules", J. Chem. Soc. Faraday

- Trans, 90, (1994), 3061-3063.
- 6. J. Turulski, J. Niedzielski, B. Pezler, "The capture rate of an ion by a symmetrical top quadrupole", Chem. Phys., 192, (1995), 319-323.
- 7. Barbara Pezler, Jan Niedzielski, Artur Ratkiewicz, Jan Turulski, *Chem Phys.*, 222, 215-221, (1997). "*Temperature denpendence of the charge- linear dipole capture rate constant*".
- 8. Barbara Pezler and Iwona Szamrej, "Geometry and energy changes in halomethanes due to electron capture", Res. Chem. Intermed., Vol. 27, No 7,8, (2001), 787-794.
- 9. J. Turulski, T. Su, J. Niedzielski, B. Pezler, "Classical theories of the ion/linear quadrupole capture", Int. J. Mass. Spectrom., 216 (2002), 115-128.

# Papers Presented at National and International Meetings:

- 1. Barbara Pezler, "Geometry and Energy Changes in Halomethanes After the Electron Capture", The 6th International Conference On Pulse Investigations in Chemistry, Biology and Physics, PULS 2000, Łeba, 2000, p 27.
- 2. W. Barszczewska, B. Pezler, I. Szamrej, M. Foryś, "Electron drift velocities in the mixtures of carbon dioxide and nitrogen", 13th Symposium on Application of Plasma Processes, Tale, Slovakia, 2001, p 71.
- 3. W. Barszczewska, B. Pezler, I. Szamrej, "Electron drift velocities in the mixtures of carbon dioxide and nitrogen", Ninth iInternational Symposium On Gaseous Dielectrics, Ellicott City USA, 2001, 30.
- 4. B. Pezler, W. Barszczewska, J. Kopyra, J. Wnorowska, I. Szamrej, "Electron attachment to halopropanes", XIVth Symposium on Application of Plasma Processes, Liptovsy Mikulas, Slovakia, 2003, p 81.

# **Daniel Cáceres Sánchez**

#### **Personal information**

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**Telephone:** +34 91 652 11 33 and +34 91 624 94 78

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**Birth date:** 17/1/74 Madrid (Spain)

Marital status: Single

#### **Education**

• Graduated in Physics. Universidad Autónoma de Madrid, June 1997.

- PhD in Physics. "Study of the mechanical properties of single-crystals and thin films of MgO by means of nanoindentation". Universidad Autónoma de Madrid. Cal. Sobresaliente CUM LAUDE.
- Studying Technical Engineering in Computer Systems. Universidad Nacional de Educación a Distancia (UNED)

#### Languages

- Good level of English.
- Learning German.

#### **Courses attended**

- Summer School (El Escorial) "Advanced materials for the micro and optoelectronics". 25 29 August 1997.
- "Mechanical testing by indentation". Fishkill, New York (USA), 3 4 August 1998.

#### **PhD Courses**

- "Chemical characterization of surfaces".
- "Physical techniques in spectroscopy".
- "Nanotecnology".
- "Fundamentals in surface analysis and epitaxial growth".
- "Transmission electron microscopy applied to the study of materials".
- "Preparation and characterization of coatings and thin films".

#### **Research Activities**

- During July 1996 stays in Instituto de Estudios de la Energía (CIEMAT) learning about dosimetry, radiation detectors, and high energy spectroscopies.
- In September 1996 incorporates as collaborator in the Laser Spectroscopy Group in the Department of Physics of Materials (Universidad Autónoma de Madrid) working in the characterization of laser materials
- Since October 1997 is working as assistant teacher at the Physics Department (Universidad Carlos III de Madrid) where studies mechanical properties of different materials by means of the nanoindentation technique, and the growing and characterization of thin films deposited by rf-sputtering.

#### Experimental techniques used

- Nanoindentation.
- Rf-sputtering
- Optical absorption techniques.
- X-ray diffraction (XRD).
- Auger Electron Spectroscopy (AES).
- X-Ray Photoelectron Spectroscopy (XPS).
- Electron Stimulated Desorption (ESD).
- Scanning Electron Microscopy (SEM).
- Profilometry.
- Ion implantation.
- Rutherford Back Scattering (RBS).

### Participation in funded scientific projects

- "Rf-Sputtering system". CAM Convocatoria de Infraestructura. Ref: 008, 1998-2001. Head of the project: Prof. Roberto González Amado.
- "Characterization of the desorbed ions from ceramic oxides' surfaces". CICYT (Acción Especial) MAT1999-1703-E, 1999-2000.
  - Head of the project: Prof. Roberto González Amado.
- "Ion implantation in ceramic oxides". Ministerio de Ciencia y Tecnología, 2001-2002. Head of the project: Prof. Roberto González Amado.

#### **Refereed publications**

- 1) "Nanoindentation on AlGaN thin films"
- **D.** Cáceres, I. Vergara, R. Gonzalez, E. Monroy, F. Calle, E. Muñoz and F. Omnès. Journal of Applied Physics. Vol. 86, n. 12 (1999) p. 6773-6778.
- 2) "Radiation damage in neutron-irradiated Ytria-Stabilized-Zirconia Single Crystals"
- B. Savoini, **D. Cáceres**, I. Vergara, R. González and J.E. Muñoz Santiuste.

Journal of Nuclear Materials. Vol. 277, n. 2-3, (2000) p. 199-203.

- 3) "Bonding and hardness in non-hydrogenated carbon films with moderate sp3 content"
- R. Gago, I. Jiménez, J.M. albella, **D. Cáceres**, I. Vergara, J.C. Blanks, B.L. Doyle and J.L. Terminello.

Journal of Applied Physics. Vol. 87, n. 11 (2000) p. 8174-8180.

- 4) "Spectroscopy of  $\pi$ -bonding in hard graphitic carbon nitride films: Superstructure of basal planes and hardening mechanisms"
- I. Jiménez, R. Gago, J.M. Albella, D. Cáceres and I. Vergara.

Physical Review B. Vol 62, n° 7 (2000) p. 4261-4264.

- 5) "Correlation between bonding structure and mechanical properties of amorphous carbon nitride thin films"
- C. Quirós, R. Núñez, P. Prieto, I. Vergara, **D. Cáceres**, L. Soriano, G.G. Fuentes, E.Elizalde and J.M. Sanz.

Surface and Coatings Technology. Vol. 125 (2000) p. 284-288.

6) "Anomalous elastic properties of Si/Ge superlattices: The role of interfaces"

A. de Bernabé, C. Prieto, **D. Cáceres**, I. Vergara, A.G. Every and H.E. Fischer.

Physica Status Solidi (a). Vol.188, n. 3, (2001) p. 1023-1040.

- 7) "Hardening mechanisms in graphitic carbon nitride films grown with N<sub>2</sub>/Ar ion assistance"
- R. Gago, I. Jiménez, **D. Cáceres**, F. Agulló-Rueda, T. Sajavaara, J.M. Albella, A. Climent-Font, I. Vergara, J. Räisänen, and E. Rauhala.

Chem. Mater. Vol. 13 (2001) p.129-135.

8) "Investigation of TiC thin films synthesised by low energy IBAD from electron evaporation of TiC powder"

J.M. López, F.J. Gordillo-Vázquez, M. Fernández, J.M. Albella, **D. Cáceres** and Vergara.

Applied Surface Science. Vol. 172 (2001) p. 110-116.

- 9) "Nanoindentation on nominally pure and doped MgO crystals"
- D. Cáceres, I. Vergara, R. González and Y. Chen.

Rad. Effects and Defects in Solids. Vol. 156 (2001) p. 39-43.

10) "Supresión of anion vacancy formation in neutron irradiated MgO:Li crystals: camouflage or fact?"

R. González, I. Vergara, **D.Cáceres** and Y. Chen.

Proceedings of the Fourth Pacific Rim International Conference on Advanced Materials and Prodessing (PRICM4) (2001) p. 1427-1430.

11) "Mechanical behaviour of the interphase between matrix and reinforcement of Al 2014 matrix composites reinforced with (Ni<sub>3</sub>Al)<sub>p</sub>"

J.M. Torralba, F. Velasco, C.E. Costa, I. Vergara and **D. Cáceres**.

Composites, partA: applied science and manufacturing. Vol. 33 (2002) p. 427-434.

- 12) "Hardness and elastic modulus from nanoindentations in nominally pure and doped MgO crystals"
- D. Cáceres, I. Vergara, R. González and Y. Chen.

Philosophical Magazine A. Vol. 82, n° 6 (2002) p. 1159-1171.

- 13) "Elastic properties of hard TiC<sub>x</sub>N<sub>y</sub> films grown by dual ion beam sputtering"
- G.G. Fuentes, **D. Cáceres**, I. Vergara, E. Elizalde and J.M. Sanz.

Surface and Coatings Technology. Vol.151-152 (2002) p. 365-369.

- 14) "Effects of the low energy-ion beam assistance in the properties of TiC<sub>x</sub>N<sub>y</sub> thin films"
- G.G. Fuentes, **D. Cáceres**, I. Vergara, E. Elizalde and J.M. Sanz.

Surface and Coatings Technology. Vol.151-152 (2002) p. 189-193.

15) "Characterization of MgO thin films grown by rf-sputtering"

D. Cáceres, I. Colera, I. Vergara, R. González and E. Román.

Accepted for publication in Vacuum.

16) "Tribological study of vanadium based alloys ion implanted at low energy – high temperature"

J.A. García, R. Rodriguez, R. Sánchez, A. Martinez, C. Ballesteros, M. Varela,

D.

Cáceres and I. Vergara.

Accepted for publication in Vacuum.

17) "Nanoindentation on MgO crystals implanted with Lithium ions"

D. Cáceres, I. Vergara, R. González, Y. Chen and E. Alves.

Nuclear Instruments and Methods B. Vol. 191 (2002) p. 154-157.

18) "Nanoindentation on neutron irradiated MgO crystals"

D. Cáceres, I. Vergara, R. González and Y. Chen.

Nuclear Instruments and Methods B. Vol. 191 (2002) p. 178-180.

19) "Role of hydrogen and lithium impurities in radiation damage in neutron-irradiated MgO single crystals"

R, González, I. Vergara, **D. Cáceres** and Y. Chen.

Physical Review B. Vol. 65 (2002) p. 224108-224114.

20) "Effect of neutron irradiation on hardening in MgO"

D. Cáceres, I. Vergara, R. González and Y. Chen.

Accepted for publication in Physical Review B.

21) "Surface mechanical effects of nitrogen ion implantation on vanadium alloys"

J.A.García, R. Sánchez, A. Martínez, A. Medrano, M. Rico, R. Rodríguez, M. Varela, I. Colera,

D. Cáceres, I. Vergara, C. Ballesteros, E. Román and J.L. de Segovia.

Accepted for publication in Surface and Coatings Technology.

22) "Study of reactive sites for D<sub>2</sub>O and <sup>18</sup>OH<sub>2</sub> on MgO (100) thin films"

I. Colera, J.L. de Segovia, E. Román, D. Cáceres, I. Vergara and R. González.

Submitted to Surface Science.

23) "Study of the interfaces between austenite and ferrite grains in P/M duplex stainless steels"

M. Campos, A. Bautista, **D. Cáceres**, J. Abenojar and J.M. Torralba.

Submitted to Journal of the European Ceramic Society.

#### **Conferences and workshops contributions**

1) "Correlation between bonding structure and mechanical properties of amorphous Carbon Nitride thin films"

C.Quiros, R. Nuñez, P. Prieto, I. Vergara, **D. Cáceres**, L. Soriano, G. García, E. Elizalde and J.M. Sanz.

E-MRS 1999 spring meeting on Protective Coatings and Thin Films-99. SymposiumB.

2) "Obtención de recubrimientos duros de compuestos de Boro, Carbono y Nitrógeno mediante evaporación asistida con iones".

R. Gago, I. Jiménez, J.M. Albella, D. Cáceres and I. Vergara.

SEMAT99, San Sebastián, 1999.

3) "An approach to the study of the interface between matrix and reinforcement in Al 2014 matrix composites reinforced with (Ni<sub>3</sub>Al)<sub>p</sub>"

J.M. Torralba, F. Velasco, C.E. Costa, I. Vergara and **D. Cáceres**.

International Materials Conference, Sevilla 1999.

- 4) "TiN films by Ion Beam Assisted Deposition"
- López, J.M., Barrena, E., Böhme, O, **D. Cáceres,** I. Vergara, E. Román and J.M. Albella. Euromat 99, Munich 27-30 September 1999.
- 5) "Nanoindentation on nominally pure and doped MgO Crystals"
- D.Cáceres, I. Vergara, R. González and Y. Chen.

International Conference on Defects in Insulating Materials (ICDIM 2000), Johannesburg (South Africa).

- 6) "Mejora de las propiedades tribológicas de aleaciones V-Ti mediante implantación iónica"
- R. Rodríguez, J. García, R. Sánchez, A. Medrano, M. Rico, C. Ballesteros, M. Varela, **D. Cáceres** and I. Vergara.
- 8º Congreso Nacional de Tratamientos Térmicos TRATERMAT-2000. (Barcelona, Spain).
- 7) "Effect of Oxigen on Ti thin films grown by IBAD"
- J.M. López, F.J. Gordillo-Vázquez, M. Fernández, **D. Cáceres**, I. Vergara and J.M. Albella.
- 19<sup>th</sup> European Conference on Surface Science (ECOSS). Madrid, September 5<sup>th</sup> 8<sup>th</sup> 2000.
- 8) "Elastic properties of hard TiC<sub>x</sub>N<sub>y</sub> films grown by dual ion beam sputtering"
- G.G. Fuentes, **D. Cáceres**, I. Vergara, E. Elizalde and J.M. Sanz.
- E-MRS, Estrasburgo. June, 2001.
- 9) "Effects of the low energy-ion beam assistance in the properties of TiC<sub>x</sub>N<sub>y</sub> thin films"
- G.G. Fuentes, **D. Cáceres**, I. Vergara, E. Elizalde and J.M. Sanz.
- E-MRS, Estrasburgo. June, 2001.
- 10) "Nanoindentation on MgO crystals implanted with Li ions"
- D. Cáceres, I. Vergara, R. González, Y. Chen and E. Alves.

Radiation Effects in insulators (REI11). Lisboa, Portugal. September 2001.

- 11) "Nanoindentation on neutron irradiated MgO crystals"
- D. Cáceres, I. Vergara, R. González and Y. Chen.

Radiation Effects in insulators (REI11). Lisboa, Portugal. September 2001.

- 12) "Characterization of MgO thin films grown by rf-sputtering"
- **D. Cáceres**, I. Colera, I. Vergara, R. González and E. Román.
- VII European Vacuum Conference (EVC-7). Madrid, Spain. September 2001.
- 13) "Tribological study of vanadium based alloys ion implanted at low energy high temperature"
- J.A. García, R. Rodriguez, R. Sánchez, A. Martinez, C. Ballesteros, M. Varela, **D. Cáceres** and I. Vergara.
- VII European Vacuum Conference (EVC-7). Madrid, Spain. September 2001.
- 14) "Water reactivity with MgO(100) thin film surfaces studied by electron stimulated desorption"
- D. Cáceres, I. Colera, I. Vergara, R. González, E.L. Román and J.L. de Segovia.
- IUVSTA 15<sup>th</sup> International Vacuum Congress, AVS 48<sup>th</sup> International Symposium. San Francisco, USA. October 2001.
- 15) "Study of reactive sites for D<sub>2</sub>O and <sup>18</sup>OH<sub>2</sub> on MgO (100) thin films"
- I. Colera, J.L. de Segovia, E. Román, **D. Cáceres**, I. Vergara and R. González.

Desorption induced by electronic transitions (DIET 9). Aussois, France. June 2002.

- 16) "Study of the interfaces between austenite and ferrite grains in P/M duplex stainless steels"
- M. Campos, A. Bautista, **D. Cáceres**, J. Abenojar and J.M. Torralba.
- International Workshop on Ceramics & Metal Interfaces. Oviedo, Spain. 23-27 June 2002.
- 17) "Radiation-damage recovery in undoped MgO crystals implanted with lithium ions"
- B. Savoini, **D. Cáceres**, I. Vergara, R. González, R.C. da Silva, E. Alves and Y. Chen.
- 13 International Conference on Ion Beam Modification of Materials (IBMM 2002). Kobe, Japan. 1-6 September 2002.

18) "Structural Characterization of low-energy high-temperature nitrogen ion implanted vanadium-titanium alloys"

M. Varela, J.A. García, **D. Cáceres**, I. Vergara, R. Rodríguez and C. Ballesteros. 2002 MRS Fall Meeting. 2-6 December 2002.

## **Teaching experience**

Oct. 97 - : Assistant teacher. Escuela Politécnica Superior (Universidad Carlos III de Madrid).

Lab. Sessions:

#### • Curso 97/98

Física I. 1º Ingeniería Técnica en Informática de Gestión.

Principios Físicos. 1º Ingeniería Técnica Industrial Mecánica.

Física I. 1º Ingeniería Industrial Superior.

Física II. 1º Ingeniería Industrial Superior.

#### • Curso 98/99

Física I. 1º Ingeniería Técnica en Informática de Gestión.

Física I. 1º Ingeniería Industrial Superior.

Física II. 1º Ingeniería Superior de Telecomunicaciones.

#### • Curso 99/00

Física I. 1ºIngeniería Superior de Telecomunicaciones.

Electromagnetismo. 2º Ingeniería Industrial Superior

#### • Curso 00/01

Física I. 1º Ingeniería Técnica Industrial Electrónica y eléctrica.

Electromagnetismo. 2º Ingeniería Industrial Superior.

Física I. 1º Ingeniería Técnica de Telecomunicación: Sistemas de Comunicación.

#### • Curso 01/02

Física I. 1º Ingeniería Técnica de Telecomunicación: Telemática.

Principios Físicos. 1º Ingeniería Técnica Industrial Mecánica.

Fudamentos Físicos de la Informática. 1º Ingeniería Informática Superior.

Física II: 1º Ingeniería Técnica Industrial en las especialidades de Electricidad y Electrónica.

#### **Other teaching merits**

- Advisor of the project "Growth and characterization of thin films obtained by rf-sputtering" presented by Manuel Jesús Tavira Manjón to obtain the Technical Industrial Engineering (Mechanics) degree (Universidad Carlos III de Madrid). (May 2000). Calification: 10.
- During September 2000 participates in the first edition of the course of introductory Physics organized by Universidad Carlos III de Madrid for the first course students.
- Board of the examiners of the project "Evaluation of the milling process in magnetic materials with stoichiometry NiFe<sub>2</sub>O<sub>4</sub>" presented in the Department of Materials Science and Metallurgy Engineering (Universidad Carlos III de Madrid) by Álvaro Santos Caballero to obtain the Technical Industrial Engineering (Mechanics) (January 2001).
- Co-advisor of the project "Characterization of ceramic fibers with composition La<sub>2/3-x</sub>Li<sub>3x</sub>TiO<sub>3</sub> grown by laser induced zonal fusion", presented by David Sanz Moreno to obtain the Industrial Engineering degree (Universidad Carlos III de Madrid). (March 2001).

Calification: 10.

- Board of the examiners of the project "Synthesis of the bioglass SiO<sub>2</sub>-Na<sub>2</sub>O-CaO by the sol-gel method. Evaluation of the bioactivity" presented in the Department of Materials Science and Metallurgy Engineering (Universidad Carlos III de Madrid) by Javier Medina Fernández to obtain the Industrial Engineering degree (April 2001).
- During September 2001 participates in the second edition of the course of introductory Physics organized by Universidad Carlos III de Madrid for the first course students.
- Board of the examiners of the project "Improvement of the behaviour of pre-alloyed steels sintered at 1120 °C. Thermal treatments" presented in the Department of Materials Science and Metallurgy Engineering (Universidad Carlos III de Madrid) by Diana Sánchez García to obtain the Industrial Engineering degree (January 2002).

#### Other merits

- Assistance to the congress "Radiation Effects in Insulators" (REI-11) Lisboa (Portugal) September 2001, presenting the oral contribution "Nanoindentation on MgO crystals implanted with Li ions".
- Assistance to the congress "7<sup>th</sup> European Vacuum Conference" (EVC-VII) Madrid (Spain) September 2001, presenting the oral contribution "Characterization of MgO thin films grown by rf-sputtering".

- Assistance to the congress "IUVSTA 15<sup>th</sup> International Vacuum Congress, AVS 48<sup>th</sup> International Symposium, 11<sup>th</sup> International Coference on Solid Surfaces" San Francisco (USA) October-November 2001, presenting the oral contribution "Water reactivity with MgO(100) thin film surfaces studied by electron stimulated desorption".
- Stay in the Instituto Tecnológico e Nuclear de Sacavem (Portugal) 11-15 March 2002. During this period is working in the implantation of MgO with Li, Co and Ni ions and the study of the samples by Rutherford Back Scattering (RBS).
- Referee for the "Journal of Materials Processing Technologies".

# Part E Financial report

The fist year financial report has only just been approved so the figures below are only an update and in severloa case are only estimates not figures approved by the partner institutes Financial offices.

The total request for EC financial support for the proposed three year period of the Contract s summarized in the Table below:

| Participant No. and name | A<br>Young     | B<br>Networking | C<br>Overheads | Totals  |
|--------------------------|----------------|-----------------|----------------|---------|
|                          | Researchers    | Costs           | 1.5            | 1.0     |
|                          | kEuro (months) | kEuro           | kEuro          | kEuro   |
|                          |                |                 |                |         |
| 1. UCLE                  | 119.1 (36)     | 57.2            | 35.3           | 211.6   |
| 2. UCLP                  | 80.7 (24)      | 37.1            | 23.6           | 141.4   |
| 3. UIBK                  | 109.2 (44)     | 40.3            | 29.9           | 179.4   |
| 4. FUB                   | 114.5 (30)     | 40.3            | 31.0           | 185.7   |
| 5. ULRS                  | 144.7 (36)     | 43.5            | 37.6           | 225.8   |
| 6. UAR                   | 110.9 (24)     | 41.3            | 30.4           | 182.6   |
| 7. ICP                   | 82.1 (44)      | 39.1            | 24.4           | 146.0   |
| 8. ULSO                  | 118.0 (30)     | 48.26           | 33.3           | 199.56  |
| TOTALS                   | 879.2 (268)    | 347.06          | 245.5          | 1472.06 |

# The estimates of costs to date is summarized in the Table below:

| Participant No. and name  | A<br>Young<br>Researchers | B<br>Networking<br>Costs | C<br>Overheads | Totals |
|---------------------------|---------------------------|--------------------------|----------------|--------|
|                           | kEuro (months)            | kEuro                    | kEuro          | kEuro  |
|                           |                           |                          |                |        |
| 1. UCLE                   | 56 (17)                   | 33                       | 17             | 106    |
| 2. UCLP                   | 18 (14)                   | 10                       | 5              | 33     |
| 3. UIBK                   | 34 (22)                   | 3                        | 2              | 39     |
| 4. FUB                    | 80 (16)                   | 20                       | 25             | 125    |
| 5. ULRS                   | 44(11)                    | 15                       | 11             | 70     |
| 6. UAR                    | 95 (21)                   | 12                       | 24             | 131    |
| 7. ICP                    | 30(26)                    | 17                       | 9.5            | 56.5   |
| 8. ULSO                   | 43 (14)                   | 9                        | 9              | 61     |
| TOTALS                    | 400 (141)                 | 119                      | 102.5          | 621.5  |
| Percentage of<br>Contract | 45 (53)                   | 34                       | 42             | 42     |
| Contract                  |                           |                          |                |        |