Electron Induced Processing at the Molecular Level (EIPAM)

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1. Summary; Electron induced processing at the molecular level

The ability to understand, manipulate and control physico-chemical processes at the molecular level is one of the great challenges of modern research and underpins the development of vibrant new technologies of the 21st century, for example the development of nanolithography. Such *single molecule engineering* requires selective bond cleavage in target molecules to allow subsequent management of the local site chemistry. Recent research has revealed that it is possible to influence the excitation and dissociation of molecules through the manipulation of electron interactions at the individual molecular level. Since electrons are ubiquitous in nature and electron induced reactions (in the gaseous phase, on surfaces and in the condensed phase) initiate and drive the basic physical-chemical processes in many areas of science and technology from industrial plasmas to living tissues our ability to control electron interactions provides exciting new opportunities that can now be exploited by both the research and technological communities. For example, the development of the Scanning Tunnel Microscope (STM) -an electron emitter- has introduced the capability of atomic-scale imaging, analysis and individual atomic/molecular manipulation providing a new technology that has the opportunity to revolutionize the scientific approach in many aspects of both the material and life sciences.

Currently several European groups are at the forefront of such pioneering research but, in contrast to the USA and Japan, the European research effort is fragmented and coordination is rudimentary or absent. The proposed programme will bring together Europe´s leading experimental and theoretical groups in a large-scale, multidisciplinary and collaborative research programme that will both maintain its international excellence and establish Europe as the centre for investigations of molecular control through electron processing with direct relevance in many areas from the basic sciences to industrial applications.

Keywords Single-molecule engineering, molecular selectivity, surfaces, radiation chemistry, plasmas.

2. Current research on molecular processing:

The ability to understand, manipulate and control physico-chemical processes at the molecular level is one of the great challenges of modern research and underpins the development of what are envisaged to be the vibrant new technologies of the 21st century. Such *single molecule engineering* requires selective bond cleavage in target molecules to allow subsequent management of the local site chemistry. Recent research has revealed that it is possible to influence the excitation and dissociation of molecules through the manipulation of electron interactions at the individual molecular level. Since electrons are ubiquitous in nature and electron induced reactions (in the gaseous phase, on surfaces and in the condensed phase) initiate and drive the basic physical-chemical processes in many areas of science and technology our ability to control electron interactions provides exciting new opportunities that can now be exploited by both the research and technological communities. Some examples of areas of current research in which the ability to utilise electrons to manipulate molecular processes will be now be briefly discussed.

Nanotechnology and surface engineering: Attempts to control chemical processes at the fundamental level using electronic excitations are now possible by combining the Scanning Tunnelling Microscope (STM) with an understanding of dynamics of electron-molecule interactions. For example, one of the most exciting developments in the area of surface modification is the use of STM to cleave specific bonds on surfaces and adsorbates. Many of these unimolecular reactions are mediated by vibrational coupling of electronic energy into vibrational motion, placing energy into *specific reaction coordinates.* These "molecular surgery" techniques allow control of local phenomena introducing the prospect of *designer synthesis on the nanoscale*.

As an exciting example of achieving the goal of controlled chemical synthesis consider one of the simplest and most well-studied reactions, oxidation of CO to CO_2, an archetypal reaction in heterogeneous catalysis and an elementary reaction that is central to automobile emissions control, air purification, and chemical sensing. Using a STM Ho and Hahn [*Phys. Rev. Lett.,* 87, 166102 (2001)] gently coaxed a CO molecule towards a pair of closely spaced oxygen atoms on a 10K silver surface. At such low temperatures molecular vibrations are minimized confining reactants and intermediates to specific sites on the surface. As the CO molecule is moved to within 2 Å of the oxygen atoms, the atoms and molecule form an O-CO-O complex. Then, by applying a brief electron pulse from the STM the complex is excited to form CO_2, which desorbs from the surface, leaving behind a lone oxygen atom (figure 1).

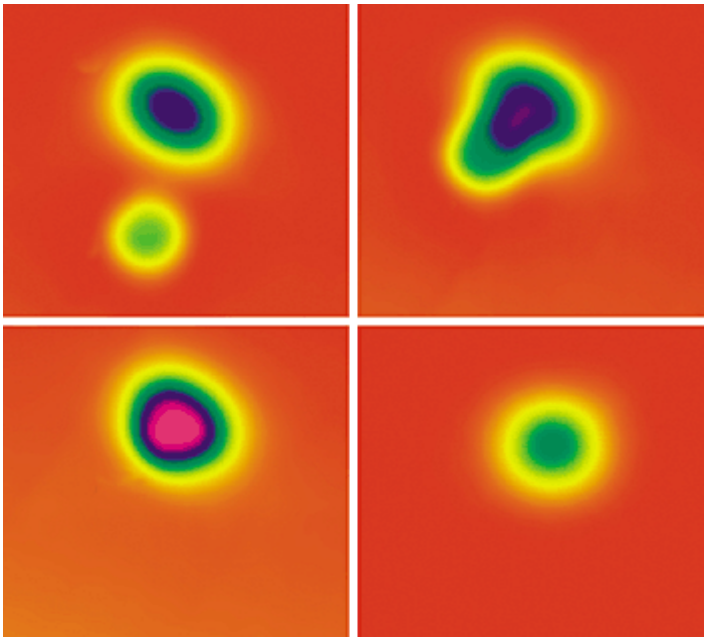

Figure 1. A pair of oxygen atoms (oblong) and a CO molecule (circular) appear as distinct features in an STM image (top left). As the species are brought closer together (top right), the image changes until, at less than 2 Å separation, an O–CO–O complex forms (bottom left). Exciting the complex causes CO_2 to form and desorb, leaving behind a lone O atom (bottom right).

Chemical reactions may also be induced by low lying transient anion states formed by the attachment of electrons to the parent molecule. Such quasi-bound states form since molecules are very ready to accept electrons into vacant molecular orbitals. In the case of dissociative electron attachment (DEA) in many systems a 100 % selectivity with respect to the cleavage of a particular bond can be obtained with a high cross section. This opens interesting prospects for selective chemistry induced by electrons. For example thermal electrons with CCl_4 react to yield exclusively Cl^- and CCl_3. The reactive (radical) CCl_3 may then be transported by the STM tip to another part of the surface where it may react at a specified chemical site. Such **Single Molecule STM Chemistry** has already been demonstrated for the idobenzene molecule C_6H_5I (figure 2)

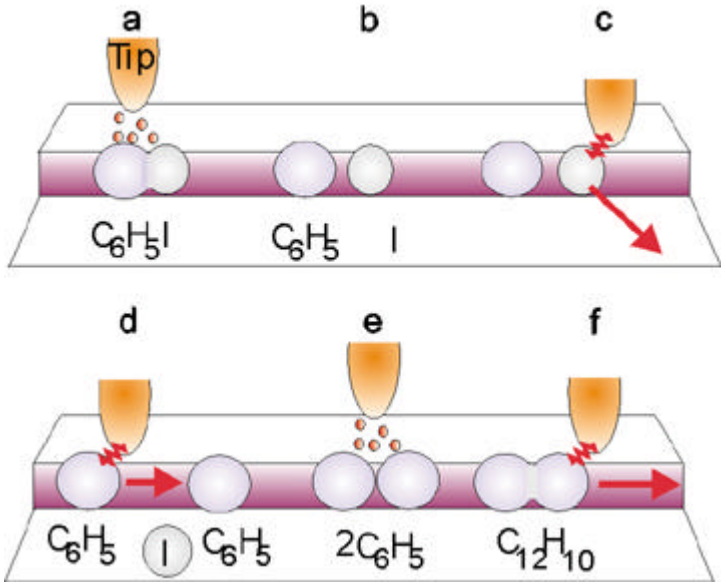

Figure 2: Schematic drawing of the sequence of steps by which an STM probe can (a) dissociate a C6H5I molecule on a terrace; (b and c) draw the iodine atom away; (d) pull one C6H5 (phenyl) molecule toward another; (e) weld them together; (f) pull one phenyl to confirm the association. Hla et al, *Physical Review Letters* **85** 2777 (2000).

Thus our understanding of the interaction and manipulation of molecules by electron processing is of key importance to the development of nanoscale processing. This in turn requires closer co-operation (co-ordination) of research in fundamental atomic, molecular physics and surface sciences communities .

Radiation damage, a new understanding : In the life sciences the role of electron-driven processes is being recognized as crucial to our understanding of radiation damage of cellular material. The mechanisms by which such degradation occurs have been the subject of considerable research effort with genotoxic effects of ionizing radiation in living cells being commonly attributed to direct impact of high-energy quanta or by complex radical chemistry (triggered by production of OH species by primary ionizing radiation). However recently this explanation has recently been questioned by the pioneering work of Sanche and co-workers who suggest that DNA lesions are induced by the *lower energy, secondary electrons* generated by the primary ionizing radiation. Data of Sanche and co-workers (figure3) revealed that :

- low energy electron irradiation directly induces both single and double strand breaks at energies well below the ionization limit of DNA (7.5eV) and
- that the probability of strand breaks are one to two orders of magnitude larger for electrons than for photons of corresponding energy.

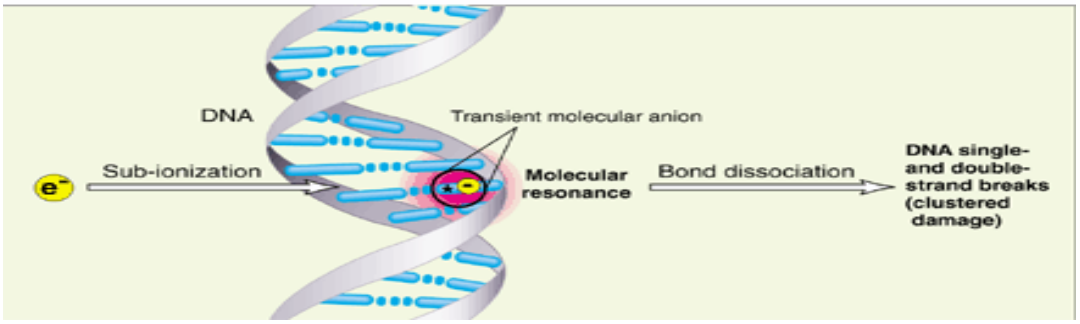

Figure 3: Most energy deposited in cells by ionizing radiation is channelled into free secondary electrons with energies between 1 eV and 20 eV
(B. Boudaïffa et al., Science **287** (2000) 1658)

The majority of the copious secondary electrons (~ 5 x 10^4 per MeV) created within 10^{-15}s along the radiation track have energies below 20eV (Figure 4) . These low-energy electrons must undergo multiple inelastic scattering events as they thermalise. The primary energy-loss channels for electrons with energies typical of the secondary distribution are ionization, direct electronic excitation and most important (but until recently little studied) ***resonance scattering***. The latter results in the formation of Temporary Negative Ions (TNIs), which decay via electron autodetachment and dissociative electron attachment (DEA) the latter process leading to direct dissociation of the parent molecule as noted above. This process may be summarised in the two step 'reaction';

$$e + M\text{-}ABC \dashrightarrow (M\text{-}ABC)^- \qquad (1)$$

$$(M\text{-}ABC)^- \dashrightarrow M^- + ABC \qquad (2)$$

where $(M\text{-}ABC)^-$ is the temporary negative ion which decays to a residual anion (M^-) and a (reactive) molecular fragment ABC, for example this may be the case in the STM experiment mentioned above where $e + C_6H_5I \rightarrow C_6H_5 + I^-$.

Hence the process of DEA provides a direct low energy process for the degradation of DNA (and other key cellular material) by resonant electron attachment to basic molecular components (base, deoxyribose, phosphate, or hydration H_2O). Recent data suggest that single strand damage is *site specific* and proceeds through *discrete molecular bond rupture*. This in turn suggests that double strand breakage is simply induced through local chemical reactivity. The DEA fragments produced within the cellular DNA subsequently reacts with adjacent bases (at 3.4Å), or close-lying the phosphate-sugar backbone (at < 5Å) leading to clustered damage within the DNA strand.

Hence in contrast to traditional models of radiation chemistry which are based upon statistical modelling it would appear that cellular damage may be based upon single collisional phenomena involving transient molecular resonances localised on DNA basic components.

In this project we wish to explore this hypothesis through an intercomparison of the TNI formed from nucleotide bases and damage in DNA (and RNA) during low energy electron irradiation.

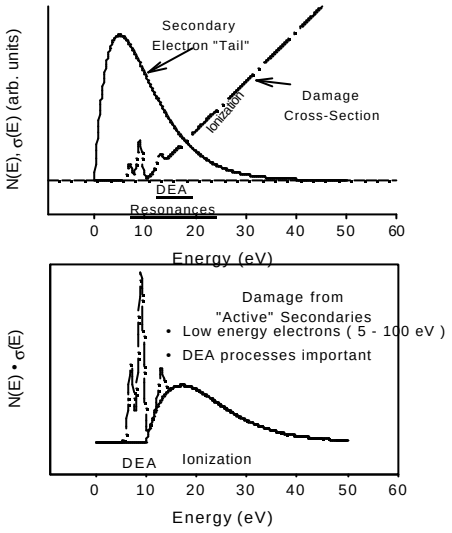

Figure 4: Top Frame: Typical energy distribution of secondary electrons emitted during a primary ionizing event. Also shown are the estimated relative cross-sections for some of the main inelastic electron energy-loss channels that the secondaries undergo as they traverse the interface. Lower Frame: Estimate of the effective "damage" probability obtained by convoluting the energy-loss cross sections with the secondary electron energy distribution.

Technological Applications: Electron induced reactions in both gaseous and condensed phases underpin many areas of applied and industrial research, and are fundamental to the operation of all plasma-based processing. For example, secondary electron cascades in mixed radioactive/chemical waste drive much of the chemistry that determines how those materials age, change, and interact with the natural environment. Electron collisions create the reactive molecular fragments in the plasma devices being used in clean technology e.g. for environmental remediation of NO_x emission of combustion exhausts and the development of ozone generators to control bacterial growth in water treatment plants and retail food outlets.

Electron induced reactions also underpin the multibillion dollar modern semiconductor industry since it is the *reactive fragments* produced by *electron impact of etchant gases* that react with the silicon substrate rather than the parent compound. However despite its high costs (>$1 billion a plant) and technological importance most of the plasma processing protocols and equipment have been designed empirically. Indeed the 1996 US National Research Council Board report on plasma processing stated that 'plasma process control remains largely rudimentary and is performed predominantly by trial and error', an expensive procedure which limits growth and innovation of the industry. In the last eight years US and Japanese research communities (supported by their manufacturing industry) have been developing research programmes to understand properties and mechanisms of technological plasmas.

Major research effort has been directed towards (i) developing new techniques for in situ plasma diagnosis and (ii) employing large scale computer modelling to simulate conditions within such plasmas. Studies aim to elucidate the plasma characteristics through an understanding of the fundamental atomic and molecular physics and place this technology on a firm theoretical basis. The ultimate goal being to advance our understanding of plasma characteristics to such a level that it will be possible to custom design, through computer models plasma reactors for any specified commercial requirement (the 'virtual factory'). To date these goals have only been partially met. While the diagnostics of such plasmas are increasingly well established, computer simulations remain inadequate and are unable to provide the technologist with any realistic predictions as to the operation of new reactor designs and processes.

Growing environmental concerns on the climatic effect of emissions of current plasma reactants (most of the compounds being strong greenhouse gases and/or ozone depletion compounds) have forced the industry to seek replacement etching gases, requiring the design of new reactors. The plasma industry has recently reinforced its call to the academic community to develop its 'virtual factory' programme

allowing new reactors/plants to be developed computationally prior to the construction of commercial plants.

Models of technological plasmas require **quantitative data** on the reactions of all the constituent neutral species and ions. The 1996 US report stated ' The main road block to the development of plasma models is the lack of fundamental data on collisional, reactive processes occurring in the plasma. Among the most important missing data are the identities of key chemical species and the dominant kinetic pathways that determine the concentrations and reactivates of these key species, especially for the complex gas mixtures commonly used in industry'. *Electron collisions initiate almost all of the relevant chemistry associated with the technology of plasma processing*. Electron collision processes involving all possible reactants, products, and intermediates must be investigated. Dissociation, ionisation and attachment cross sections are of particular importance since they determine the ionisation balance within the plasma and thus influence plasma properties such as the electron energy distribution, which in turn influences etch and deposition characteristics of plasmas. Therefore an important part of this programme will be to study electron induced processes pertinent to the modern plasma processing industry in both the gaseous and condensed phase.

Future research: A research imperative in the next decade will be to increase our knowledge of the interaction of electrons with more complex targets and in all phases of matter. This is widely recognized in many national and international research reviews but perhaps most strongly by the 2000 USA DOE 'Atomic, Molecular and Optical Science' report which concluded that 'It is apparent from this report that major progress in the future in the area of electron-driven processes must include interdisciplinary research between different communities such as atomic, molecular, and optical physics, surface physics and chemistry and the physics and chemistry that is concerned with the interaction of radiation with matter. It is also apparent from this report that significant future progress can only be achieved if experiment, theory, computation, and simulation work hand in hand and coordinate their respective efforts'. ***The primary objective of this proposed programme is to initiate such a strategy and develop a large-scale, multidisciplinary and collaborative effort that will implement a research strategy to develop 'Electron Induced Processing at the Molecular Level '.***

3. The European dimension:

The study of electron interactions with molecular targets is a field of research in which Europe is currently at the forefront. This is supported by a review of publications in major international journals and the number of European researchers invited to give presentations at relevant international conferences. All the above processes are currently being studied, both theoretically and experimentally, by European groups who will participate in the proposed programme. Indeed these European groups have developed many of the new experimental techniques and theoretical codes that are driving forward the international programme and therefore are well placed to exploit the scientific and latterly commercial benefits of this research.

However to date there have been few opportunities to co-ordinate such research within the Europe. Activities under the EU Framework V programme have had more limited objectives[1], in part due to the restriction of the number of partners (8) allowed under these Networking activities. Similarly the research objectives of Framework VI are concentrated upon narrower areas of more applied research and there are fewer opportunities for co-ordination of research that requires study of more fundamental investigation prior to the commercial application. This is in notable contrast to comparable research programmes in both the USA and Japan which are co-ordinated by their National funding agencies. For example in the USA the Department of Energy (DOE) recently organised major reviews of such research and thus ensured that a more structured *interdisciplinary* research programme can be developed. Similarly in Japan research into processes related to technology have been co-ordinated for nearly ten years by a joint academic/industry forum (ASSET). In this ESF Programme we therefore propose to bring together the leading European groups in this field to develop a coordinated international research programme that will

[1] The co-ordinator is PI of a current FPV Network entitled Electron and Positron Induced Chemistry (EPIC) and a COST programme on Radiation Damage (Programme P9 under Physics) programmes that have some limited overlap with the proposed ESF programme

provide a breadth and depth of research that will consolidate European strengths in this area. The programme will;

- Allow transfer of staff between European research groups to allow transfer of knowledge and techniques
- Train new and younger researchers in the techniques and applications of electron interactions with molecules in all phases of matter
- Further European research integration through hosting of workshops and conferences to develop and execute co-ordinated research plans
- Bring together applied and fundamental research communities to investigate applications of fundamental studies and develop commercial/industrial spin-offs of such research and
- Communicate outcomes of such research to global audiences and form links with other international partners e.g . the US and Japanese research communities.

Such a programme will lead to a major advances in our understanding of how to manipulate molecular processes using electrons. It will no longer then be fanciful to speculate that, within a decade, we will be able to accurately model a whole range of electron driven processes and understand their intricate dynamics and evolution allowing the dream of engineering at the single molecule level to be successfully developed across a range of fundamental and applied sciences.

4. Work programme:

In this ESF programme we will bring European research teams together to develop an integrated collaborative research programme to perform systematic investigations of how electron induced processes may be used to manipulate molecular formation and reactions as one makes the transition from isolated particle behaviour in a low pressure gas to many body interactions in the condensed phase.

The work programme will comprise of a ***scientific programme*** dedicated to co-ordinating research in participating laboratories and research institutes, this will primarily be performed by exchange of personnel and thus conducted through joint research projects in the gas phase. Experimental research will include studies of the collisions of electrons with molecules held on surfaces in mono- or multilayers, with bulk material, and within with clusters. The study of electron interactions with clusters is seen to be of particular significance since this provides the opportunity for investigating *binary collisions* which are expected to be important in nanoscale chemistry and provide a bridge between single molecule reactions and bulk phenomena. *Each of the experimental studies is supported by theoretical studies*.

The target molecules will be largely chosen for their applications and will include a variety of atmospherically, industrially and biologically important molecules. For example the bond cleavage of halocarbons is pivotal to the plasma etching industry and therefore studies will concentrate upon investigating new 'environmentally friendly' halocarbon compounds that may be adopted by the industry to fulfil the requirements of the Montreal Treaty. For the life sciences amino acids, of the bases of DNA and strands of DNA itself, will be studied to extend and refine present knowledge of the mechanisms of single and double strand breaks of DNA induced by secondary electrons, in particular down to thermal energies where cross-sections may be very high.

In the study of how the elementary processes involving electrons change during the transition from isolated particle behaviour in a low pressure gas to many body interactions in the condensed phase two complimentary approaches exist : (i) interphase and (ii) cluster physics and chemistry. In the former approach, a given reaction or property is studied as a function of the density and nature of the medium in which it occurs from the low-pressure gas to the liquid or solid. Traditionally, such studies begin at either end of the density range: from the solid (liquid) density to progressively lower densities and from a low-density gas (binary collisions) to progressively higher densities (multiple scattering regime). In the latter approach, the properties and reactions of a given species (atom or molecule) are studied as a function of its size (increased gradually by clustering), cluster shape and cluster composition. A unique feature of clusters is that they allow studies of the transition from large finite clusters to the bulk. Thus, one can determine the minimum cluster size beyond which properties are essentially those of the bulk material**. *In***

this programme specific molecules and electron processes will be studied as a function of phase by combining complementary research techniques from different European research groups.

Of particular importance will be the transfer of knowledge from the study of single gas phase collisions to the use of STM technology to manipulate individual molecules on selected surfaces, and control chemical reactions with sub-Ångstrom resolution, for example chiral recognition in cysteine. STM provides a very powerful and direct method of detecting and creating bond cleavage and vibrational excitation at the single molecule level for surface adsorbed species and STM prepared single site chemistry is now being developed (see above). ***This programme will be the first forum for the European STM and the molecular physics/physical chemistry communities to interact and collaborate in a substantive way.***

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

1. The study of electron induced reactions in the gaseous phase to determine single electron/isolated molecule interactions (co-ordinator N J Mason)

2. The study of electron induced reactions as a function of phase including study of molecular clusters to investigate binary collisions (co-ordinator E Illenberger) and

3. The application of STM technology to electron induced manipulation of single molecules on surfaces (co-ordinator J Pascual)

4. Since the above are primarily experimental strands a fourth strand that coordinates theoretical and modelling of these processes will be developed (co-ordinator F Gianturco)

In the latter part of the programme (years 3-5) a fifth strand is envisaged being dedicated to **the application of such research to technology and industry.** The steering committee of the fourth strand will therefore *latterly in the project* include industrial/commercial partners. Workshops in each of these areas are planned with two conferences being arranged to bring together all partners. Such conferences may be arranged as part of Eurocore/EU conference series.

In addition to the scientific work programme it is a vital part of the proposal to arrange a **training and knowledge transfer programme.** These will be aimed at providing training for postgraduate and younger researchers and are expected to be a mixture of formal lectures, tutorials and laboratory exercises. Initial topics include; Molecular structure and dynamics; Surface science; biomolecular chemistry and scattering theory.

Results from the programme will be reported in formal research publications. However the Programme will also publish its formal conference proceedings (it is anticipated that this will be in collaboration with a European Journal). Reports on workshops and notes for participants in the training schools associated with the proposed programme will also be produced as will the customary webpage which will provide details of the research teams taking part in the research programmes and encourage other researchers in Europe to contact participants for further research collaboration and integration.

5. Duration :The proposed programme is planned to run for a period of 5 years commensurate with research strategy outlined above. Although this period is not expected to see a complete understanding of electron induced processes at the molecular level. This is the timescale over which it is envisaged that a co-ordinated research programme could be developed by bringing researchers together from what are currently disparate research communities, and make significant advances in understanding electron-induced processes at the molecular level.

6. Budget Estimate: The programme will comprise of exchanges of scientific staff, hosting workshops and conferences and establishing training schools for research students. **Budget 150,000 Euro per year**. Steering committee meetings 10000pa; Workshops (2 per year) 30000pa; Conferences (year 3,5) and Training schools (years 1,2,4) 30000pa; Grants for exchanges between research groups 60000pa(envisaged at some 40 months of mobility per annum); administration of communications and databases etc (5000pa) and ESF Administration fee 7500pa, External administration costs 7500pa.

Year 1 (2004) ; Initial meeting of Steering committee 10000 Euros
Workshops on Electron induced reactions in the gaseous phase to determine single electron/isolated molecule interactions (co-ordinator N J Mason) to be held as satellite of ECAMP VIII July 2004 and The application of STM technology to electron induced manipulation of single molecules on surfaces (co-ordinator J Pascual) to be held in Barcelona 2 x 15000 Euros
Training school on Molecular structure and dynamics and scattering theory September 2004 30000Euros
Year 2 (2005) ; Workshops on Electron induced reactions as a function of phase including study of molecular clusters to investigate binary collisions (co-ordinator E Illenberger) February 2005 including meeting of steering committee(10000 Euros) and a workshop on Modelling of Collisional phenomena on surfaces (to be held April) 2 x 15000 Euros
Training school on surface science and application of single molecule techniques September 2005 30000Euros
Year 3 (2006) ; Workshops on Electron induced reactions with biomolecules (co-ordinator N J Mason) February and Surface engineering (co-ordinator J Pascual)September 2 x 15000 Euros
First conference on Electron Induced Molecular Processing (**EIPAM 1**) 30000 Euros (July) to include steering committee meeting (10000 Euros).
Year 4 (2007) ; Workshop on the applications of Single molecule engineering (perhaps pertinent to the in plasma industry and radiation chemistry) to include meeting of steering committee (10000 Euros) and Electron induced reactions as a function of phase (co-ordinator E Illenberger) to be held as satellite of ECAMP IX July 2 x 15000 Euros and Training school (topic to be chosen at EIPAM1) September 30000 Euros
Year 5 (2008) ; 2 Workshops to be developed from topics arising form earlier meetings one of which is expected to be related to applications 2 x 15000 Euros
Second conference on Electron Induced Molecular Processing (**EIPAM 2**) 30000 Euros (July) to include steering committee meeting (10000 Euros).

Annex 1. CVs of the Principal Applicants

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Professor N J Mason has managed a number of collaborative projects within the UK, throughout Europe and in India. He is chair of the European Physical Society Atomic, Molecular and Optical Physics Division (AMPD) hence serving on the EPS Council. He is also Secretary of UK Institute of Physics Division of Atomic, Molecular and Plasma Physics and Recorder of the Physics Section of the British Association. He was Secretary of the successful Fifth European Conference of Atomic and Molecular Physics (ECAMP V) held in Edinburgh in 1995, and was a Member of the Organisational Committees for ECAMP VI, 1998, ECAMP VII 2001 and will be Chair of ECAMP VIII in 2004. In 2001 in recognition of his standing in this field, he was elected chair of the European Physics Society Atomic and Molecular Physics Division. Subsequently he was invited to act as an external expert in the US DOE review of the future of radiation physics, in 1997 and US DOE review of electron scattering in 2000. He was co-chair of a 1998 CECAM/EPS meeting on 'Data for modelling and simulation of plasma processing' and was International Chair of Low Energy Electron Molecule Interactions (LEEMI) conference in 2002. He is also a Board member of several prestigious journals. He was elected a Fellow of the Institute of Physics in 1998, Member of the European Physical Society and EurPhys 1998. Formally Head of the Molecular Physics Laboratory at University College London in 2002 he was appointed Director of the new Centre of Molecular and Optical Physics at the Open University. Co-author of over 100 publications in refereed journals and over 300 conference papers, he is author of a major text book on 'Environmental Physics'. He receives funding from a number of UK grant awarding panels including EPSRC, NERC and PPARC and the Royal Society. International funding includes the EU, NATO and the British Council.

Publications:

1.Electron scattering in chlorine dioxide D Field, N C Jones, J M Gingell, N J Mason, S L: Lunt and JP Ziesel (2000) J Phys B **33** 1039
2.Enhanced electron capture by metallic clusters S Senturk, J P Connerade, D D Burgess and N J Mason J. Phys. B **33** 2763-74 (2000)
3.Electron stimulated desorption of O^- and O_2^- from condensed ozone P Tegeder, P A Kendall, M Penno, N J Mason and E Illenberger Phys.Chem. Chem. Phys. **3** 2625-29 (2001)
4.Dissociation pathways in low energy (0-2 eV) electron attachment to Cl_2O W Sailer, P Tegeder, M Probst, H Drexel, V Grill, P Scheier, N J Mason,E Illenberger and T D Maerk Chemical Physics Letters **344** 471-78 (2001)
5.Electron impact ionisation studies for SF_5CF_3 G Hanel, B Gstir, M Probst, P Scheier, N J Mason and T D Maerk J. Phys B **35** 2567-74 (2002)

Prof. F.A. Gianturco (Strand leader for Theoretical & Computational modelling)

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Professor F.A. Gianturco received his D Phil in Applied Mathematics from the University of Oxford (UK) and his Habilitation in Theoretical Physical Chemistry from the University of Pisa (Italy). He has worked at the Theoretical Physics Division of the Atomic Energy Research Establishment at Harwell (UK), at the Dept. of Applied Matematics of Queen's University Belfast (UK), at the Max Planck Institut für Strömungsforschung, Göttingen (Germany) and at the Institute for Theoretical Atomic and Molecular Physics (ITAMP), Harward University (USA). He has been professor of Chemical Physics at the Universities of Pisa, of Bari and, since 1979, at the University of Roma "La Sapienza". He is the author of nearly 400 publications in International Scientific Journals, editor of six specialists' Volumes and author of one book. Has been Editor in Chief of the leading European Physics publication, Europhysics Letters, and is currently on the Editorial Board of Comp. Phys. Comm., of Eur. Phys. J. D and of Europhys. Lett. His research interests have focussed on the theoretical and computational aspects of a broad variety of elementary processes involving electrons, positrons, atoms and ions interacting with molecules in the gas phase, at low and ultralow temperatures and in cluster aggregates. He has been chief coordinator of

Italian National Research Collaborative Projects, and has taken part in several European Research Networks as leader of a Research Unit and as Strand Coordinator within the Networks.

Publications

1) M. Satta, E. Bodo, R. Martinazzo, F.A. Gianturco *Photoexcitation of LiH^+_2 from selected initial states: a time dependent model* J. Chem. Phys. 117 (2002) 2587
2) E. Bodo, F.A. Gianturco, A. *DalgarnoThe reaction of $F+D_2$ at ultracold temperatures: the effect of rotational excitation* J. Phys. B 35 (2002) 4075
3) T. Nishimura and F.A. Gianturco *Threshold efficiency of vibrational excitation of methane by electron/positron impact: a comparison* Europhys. Lett. 59 (2002) 674
4) M. Satta, F. Sebastianelli and F.A. Gianturco *Nucleation dynamics in Neon trimer photoionization: a time-dependent modelling* Mol. Phys. 100 (2002) 3699
5) E. Bodo, F. Sebastianelli, E. Scifoni, F.A. Gianturco, A. Dalgarno *Rotational quenching of ionic systems at ultracold temperatures* Phys. Rev. Lett. 89 (2002) 283201

Professor Dr. Eugen Illenberger (Strand leader clusters and aggregates)

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Professor Eugen Illenberger received his PhD in Atomic and Molecular Physics from the University of Freiburg (Germany) and his Habilitation in Physical Chemistry from the Freie Universität Berlin. He spent a year as visiting Professor at the Chemistry Department at Stanford University and several one month periods as invited Professor at the Université Paris Sud and the Universität of Innsbruck. He has managed a number of national and international collaborative projects, and has chaired or co-chaired several international conferences. His publication list includes over 130 original articles in refereed journals and several review articles. He is the author of the textbook *Gaseous Ions. An Introduction to Elementary Processes Induced by Ionization* and the co-editor of the book *Linking the Gaseous and Condensed Phases of Matter. The behaviour of Slow Electrons*. The research interests are focused on elementary reactions of molecules in the gas phase in liquids and at surfaces. Research funding has been obtained through Deutsche Forschungsgemeinschaft (DFG), Volkswagen Stiftung, Humboldt-Stiftung, Fonds der Chemischen Industrie, Deutscher Akademischer Austauschdienst (DAAD), Heraeus Stiftung, EU and NATO.

Publications

1. *Electron Attachment Processes in Free and Bound Molecules* Eugen Illenberger in *Photoinonization and Photodetachment*, Part II, pp 1063 – 1160. Advanced Series in Physical. Chemistry – Vol. 10B., Cheuk - Yiu Ng, ed., World Scientific, Singapore (2000).
2. *Synthesis of Cl_2 Induced by low Energy (0-18 eV) Electron Impact on Condensed 1,2-$C_2F_4Cl_2$ Molecules* Richard Balog, Negib Hedhili, Fabrice Bournel, Martin Penno, Michel Tronc, Roger Azria, Eugen Illenberger Phys. Chem. Chem Phys. **4** (2002) 3350 – 3355.
3. *Formation of Anion Fragments from Gas Phase Glycine by Low Energy (0-15 eV) Electron Impact* Sascha Gohlke, Andrzej Rosa, Frank Bruening, Michael A. Huels and Eugen Illenberger J. Chem. Phys. **116** (2002) 10164-10169.
4. *Dissociative Electron Attachment to Formic Acid (HCOOH)* Andrzej Pelc, Wolfgang Sailer, Paul Scheier, Michael Probst, Nigel J. Mason, Eugen Illenberger and Tilmann D. Märk Chem. Phys. Lett. 361 (2002) 277.
5. *Energy Balance in Dissociative Attachment to C_2F_5I* Judith Langer, Stefan Matejcik, Eugen Illenberger Chem. Phys. Phys. Chem. **4** (2002) 5105 - 5109.

Dr José I. Pascual (Strand leader Surfaces and STM processing)

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Dr. J.I. Pascual's main research topics exploit the spectroscopic capabilities of scanning tunnelling microscopy to resolve electronic and vibrational information at the local scale. He received his PhD in Physics from the Universidad Autónoma de Madrid in the year 1998. There, he co-authored significant contributions to the properties of electronic transport through atom-sized contacts, and single molecules. In 1999, he was awarded with a "Marie Curie" contract from the European Commission, and joined the

Fritz-Haber-Institut, in Berlin. He specialised on the recently initiated field of excitation of single-molecule vibrations by tunnelling electrons, and succeeded to apply mode-selective schemes to control single molecule dynamics. In 2002 he joined the Spanish research council, CSIC, with a "Ramon y Cajal" contract to develop techniques of controlling matter at the local scale using low temperature scanning tunnelling microscopy. He has co-authored 29 publications.

Publications

1. Seeing molecular orbitals. J.I. Pascual, J. Gómez-Herrero, C. Rogero, A.M. Baró, D. Sánchez-Portal, E. Artacho, P. Ordejón, and J.M. Soler. Chemical Physics Letters 321, 78 (2000).
2. Adsorbate-substrate vibrational modes of benzene on Ag(110) resolved with scanning tunneling spectroscopy. J.I. Pascual, J.J. Jackiw, Z. Song, P.S. Weiss, H. Conrad, and H.-P. Rust. Physical Review Letters 86, 1050 (2001).
3.Visualization of surface electronic structure: dispersion of surface states of Ag(110).
J.I. Pascual, Z. Song, J.J. Jackiw, K. Horn, and H.-P. Rust. Physical Review B 63, 241103(R) (2001).
4.Vibrational spectroscopy on single C_{60} molecules: The role of molecular orientation.
J.I. Pascual, J. Gómez-Herrero, D. Sánchez-Portal, and H.-P. Rust. Journal of Chemical Physics 117**,** issue 1 December (2002).
5.*Mode-selectivity in vibrationally mediated single-molecule dynamics.*
J.I. Pascual, N. Lorente, Z. Song, H. Conrad, and H.-P. Rust. Submitted (2002).

Annex 2: Steering Committee

Austria
Institut fuer Ionenphysik
University of Innsbruck
Professor T D Mark

Belgium
Department of Chemistry
University of Liege
Professor J Delwiche

Czech Republic
Department of Chemistry
Charles University
Professor J Horackek

Denmark
Department of Physics
University of Aarhus
Professor D Field

France
University of Paris-Sud
Professor Gérald Dujardin

Germany
Department of Chemistry
Freie University
Professor E Illenberger

Italy
Department of Chemistry
La Sapienza University Rome
Professor F Gianturco

Poland
Department of Physics
Gdansk University
Professor M Zubek

Portugal
Department of Physics
Universidade Nova de Lisboa
Professor A M C Moutinho

Slovak Republic
Department of Plasma Physics
Commenius university, Bratislava
Professor J D Skalny

Spain
Department of Physics
University of Barcelona
Dr J Pascual

Switzerland
Department of Chemistry
Fribourg university
Professor M Allan

United Kingdom
Centre of Molecular and Optical Sciences
The Open University
Professor N J Mason

Annex 3: Research Groups indicating a wish to participate in the programme

Austria
University of Innsbruck Institute Ionen Physik
Professor T D Mark
Professor P Scheier

Belgium
University of Liege; Dept of Chemistry
Professor J Delwiche
Professor M J Hubin-Franskin

Czech Republic
Charles University Prague, Physics
Professor J Horac ek
J Heyrovsky Institute Prague
Professor P Carsky

Denmark
University of Aarhus Dept of Physics
Professor D Field
Professor F Besenbacher

France
University of Paris, Dept of Physics
Professor R Azria *(P-Sud)*
Professor G Dujardin *(P-Sud)*
Dr Teillet-Billy (*P-Sud*)
Professor J P Schermann *(P-Nord*)
Professor C Desfrancois *(P-Nord)*
University of Rennes, Dept of Chemistry
Professor B Mitchell
Professor B Rowe
University Paul Sabatier Toulouse, IRSAMC
Dr N Lorente

Germany
Freie University Berli, Physics and Chemistry
Professor E Illenberger
Professor Martin Wolf
Professor Karl-Heinz Rieder
University of Kaiserslautern, Physics
Professor H Hotop
University of Cologne, Dept Physical Chemistry
Dr P Swiderek
University of Regensberg, Physical Chemistry
Professor P Saalfrank

Italy
La Sapienza University Rome Chemistry
Professor F A Gianturco
Department of physics
Trento university
Professor A Zecca
Dr G Karwasz

The Netherlands
Faculty of Science and Technology
University of Twente
Professor J W Zandvliet

Poland
Gdansk University of Technology
Department of Physics
Professor M Zubek
Siedlce University, Dept of Chemistry
Professor M. Forys
Professor I Szamrej-Forys,

Portugal
Universidade Nova de Lisboa Dept. Physics
Professor A M C Moutinho
Dr P Limao Vieira

Slovak Republic
Commenius University Dept of Physics
Professor J D Skalny
Dr S Matejcik

Spain
University of Barcelona, Physics
Dr J Pascual
University of San Sebastian, Physics
Professor. P.M. Echenique
Dr Andres Arnau
Universidad Autónoma de Madrid
Chemistry
F Martin

Sweden
Chalmers University, Göteborg
Dept. of Physics
Professor Mats Persson

Switzerland
Fribourg University, Dept of Chemistry
Professor M Allan

United Kingdom
The Open University
Centre for Molecular & Optical sciences
Professor N J Mason
Professor N Braithwaite
Birmingham University, Dept of Physics
Professor R Palmer
Dr C Mayhew
University of Liverpool
Dr W Hofer
Professor S Holloway
University of Manchester
Professor G Thornton
University College London Dept of Physics
Professor J Tennyson
Professor A Fisher

Links with Non European research teams

This research programme can not be developed in isolation and must take account of the progress in other major international research centres. Therefore we expect to exploit agreements with the US NSF to allow collaboration and further discussion with major US groups. Suggested participants include Professor T Madey (Rutgers University), Professor T Orlando (Atlanta), Professor Roberto Lucchese (Texas A&M), Professor W Ho (University of California, Irvine) and Professor Ilya Fabrikant (Nebraska) and Dr M Salmeron, LBNL.

We also wish to develop contacts with major Japanese research groups led by Professor Mineo Kimura (Yamaguchi University), Professor Toshiaki Makabe (Keio University) Professor Hiroshi Tanaka (Sofia University)Professor Maki Kawai, (RIKEN,Hirosawa, Wako, Saitama), Professor H. Ueba (Toyama University Gofuku), Dr H Onishi (Kanagawa Research Institute), Prof Y Iwasawa, (Univ Tokyo) and elsewhere the internationally renowned group at Sherbrooke University, Canada led by Professor L Sanche and the ANU- Australian National University, Canberra led by Professor S Buckman.

We would seek to invite key staff from these institutes to participate in the conferences and workshops and participate in discussions as to the future development of the research programme.

Annex 4: Previous applications to the ESF

In 2002 an ESF Workshop co-ordinated by Professor N J Mason was awarded and held (April 7-11 in Denmark) entitled 'Collisions in atom traps (CATS)'.

Annex 5: Framework V and COST applications pertinent to this application

Proposed members of the programme have been or are members of several EU Networks. One current Framework V Network entitled Electron and Positron Induced Chemistry (EPIC) has one sub theme that investigates electron dissociation processes. A Second Network entitled Radiation Induced Chemistry is recommended for funding as Programme P9 of Physics programme of COST . One aspect of this is to study electron induced damage on DNA and its constituents. However neither of these programmes provide the detailed investigations of *Electron Induced Processing at the Molecular Level* proposed in this programme and neither involve the nanotechnology community.

Budget Estimate revised for 120kEuro per annum

The programme will comprise of exchanges of scientific staff, hosting workshops and conferences and establishing training schools for research students. **Budget 120,000 Euro per year**.

Steering committee meetings 5000pa (These will mainly be held at workshops and conferences); Workshops (2 per year) 25000pa; Conferences (year 3,5) and Training schools (years 1,2,4) 20000pa; Grants for exchanges between research groups 50000pa(envisaged at some 40 months of mobility per annum); administration of communications and databases etc (5000pa) and ESF Administration fee 7500pa, External administration costs 7500pa.

Year 1 (2004) ; Initial meeting of Steering committee 5000 Euros
Workshops on Electron induced reactions in the gaseous phase to determine single electron/isolated molecule interactions (co-ordinator N J Mason) to be held as satellite of ECAMP VIII July 2004 and The application of STM technology to electron induced manipulation of single molecules on surfaces (co-ordinator J Pascual) to be held in Barcelona 2 x 12500 Euros
Training school on Molecular structure and dynamics and scattering theory September 2004 20000Euros

Year 2 (2005); Workshops on Electron induced reactions as a function of phase including study of molecular clusters to investigate binary collisions (co-ordinator E Illenberger) February 2005 including meeting of steering committee(5000 Euros) and a workshop on Modelling of Collisional phenomena on surfaces (to be held April) 2 x 12500 Euros
Training school on surface science and application of single molecule techniques September 2005 20000Euros

Year 3 (2006); Workshops on Electron induced reactions with biomolecules (co-ordinator N J Mason) February and Surface engineering (co-ordinator J Pascual) September 2 x 12500 Euros
First conference on Electron Induced Molecular Processing (**EIPAM 1**) 20000 Euros (July) to include steering committee meeting (5000 Euros).
Year 4 (2007) ; Workshop on the applications of Single molecule engineering (perhaps pertinent to the in plasma industry and radiation chemistry) to include meeting of steering committee (10000 Euros) and Electron induced reactions as a function of phase (co-ordinator E Illenberger) to be held as satellite of ECAMP IX July 2 x 15000 Euros and Training school (topic to be chosen at EIPAM1) September 30000 Euros
Year 5 (2008) ; 2 Workshops to be developed from topics arising form earlier meetings one of which is expected to be related to applications 2 x 15000 Euros
Second conference on Electron Induced Molecular Processing (**EIPAM 2**) 30000 Euros (July) to include steering committee meeting (10000 Euros).