First Workshop of the
ESF Programme

Electron Induced Processing at the Molecular Level (EIPAM)

The Open University, Milton Keynes, UK
19th – 20th April 2005

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Welcome to the Open University!

Welcome to this the first workshop of the ESF Programme on Electron Induced Processing at the Molecular Level (EIPAM). The Programme has been active since July 2004 with the first EIPAM Fellows being appointed in September and the first short exchange visits having taken place. However this workshop is the first opportunity to bring together the major partners involved in the programme to discuss the scientific policy of the programme (the initial meeting of the Steering group held in Lyons in June 2004 being a purely administrative action). Each of the main partners will present a review of their research and discuss its future direction. The meeting will also provide the opportunity for discussing which EU research groups that would benefit from being invited to participate in the programme.

The Workshop is arranged in sessions which reflect the scope of the programme including both experimental and theoretical research. *The meeting will conclude with my own Professorial inaugural lecture to which I am delighted to welcome colleagues and friends !*

The meeting will also include the Second meeting of the Steering Committee at which our ESF co-ordinator Ms Chantal Durant will be present to discuss administrative arrangements and budgetary issues.

Scientific Summary;

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 present ESF programme **Electron Induced Processing at the Molecular Level (EIPAM)** has been designed to 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.

Nigel Mason Chair EIPAM Programme

Programme

Monday April 18th 2005

Participants arrive

Tuesday April 19th 2005

All talks to be held in the Systems Seminar Room, Venables Building.

	Title	
09.00	Opening	Professor Nigel Mason
09.10 to 09.50	Low Energy Electron Induced Processes in Dielectrics, Icy Satellites, Stratosperic Clouds, Nanolithography and Radiotherapy	Professor Léon Sanche
09.50 to 10.20	Electron Processing at Sub-Excitation Energies	Professor Eugen Illenberger
10.20 to 10.40	*Coffee*	
10.40 to 11.10	Low Energy Electron Interactions with Biologically Relevant Molecules	Professor Paul Scheier
11.10 to 11.40	Probing Molecules with Slow Electrons and Positrons Impacting on Gaseous Targets	Professor F Gianturco
11.40 to 12.10	R-matrix Calculations of Electron-Molecule Collisions at Low and Intermediate Energies	Prof. Jonathan Tennyson
12.10 to 12.40	Long-lived Hydrogen Molecular Anions	Professor Jiri Horacek
12.40 to 14.00	*Lunch – EIPAM Steering Group Meeting*	ESF Representative Attending Ms Chantal Durant

Tuesday April 19th 2005 continued

14.00 to 14.30	Coupled Electron-ion Dynamics	Professor Andrew Fisher
14.30 to 15.00	Electron and Force Induced Molecular Manipulations: Molecular Engines and Switches	Prof. Karl-Heinz Reider/ Dr J Pascual
15.00 to 15.30	Simulation of High-Resolution Scanning Tunneling Microscopy and Spectroscopy: Present State of the Art and Comparison with Experiments	Dr Werner A Hofer
15.30 to 16.00	Electron-Induced Processes in Single Atoms and Molecules on Surfaces	Professor M Persson
16.00 to 16.30	*Tea*	
16.30 to 17.00	Modification of Thin Molecular Films by Low-Energy Electrons	Prof. Dr. Petra Swiderek
17.00 to 17.30	Electron Induced Functionalization of Semiconductors: the Case of Polycrystalline Diamond	Professor Roger Azria
17.30 to 18.00	Single Molecule Desorption and Dissociation at Room Temperature	Prof. Dr. Richard Palmer
19.00	*Dinner at MacDonald Parkside Hotel*	

Wednesday 20th April 2005

	Title	
09.00 to 09.30	Cold Electron Chemistry in the Gas Phase: Benchmark Experiments	Professor David Field
09.30 to 10.00	Benchmark Cross Sections for Low-Energy Electron Attachment to Molecules with Well-Defined Internal Temperature	Professor H Hotop
10.00 to 10.30	Elastic and Vibrational Excitation Cross Sections in Methane and Cyclopropane	Professor M Allan
10.30 to 11.00	*Coffee*	
11.00 to 11.30	Electron Scattering by DNA Bases at Intermediate and High Energies	Dr Gustavo Garcia
11.30 to 12.00	Synchrotron Radiation as a Tool for Probing the VUV Spectroscopy of Biomolecules	Dr Paulo Limao-Vieira
12.00 to 12.30	Temperature Dependence of Electron-Induced Reactions	Dr Stefan Matejcik
12.30 to 14.00	*Lunch*	
14.00 to 14.30	Electron Scattering by THF Molecule	Dr. Bratislav P Marinkovic
14.30 to 15.00	Electron-Molecule Interactions Studied in Electron Backscattering Experiments	Professor Mariusz Zubek
15.00 to 15.30	Lab Opening/Tour	
15.30 to16.00	*Tea*	
16.00	Inaugural Lecture – Probing the Molecular world; Adventures with Electrons and Light *To be held in the Berrill Lecture Theatre*	Professor Nigel Mason
17.00	*Reception/Buffet*	

Low Energy Electron Induced Processes in Dielectrics, Icy Satellites, Stratosperic Clouds, Nanolithography and Radiotherapy.

Léon Sanche

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Electrons with energies in the range 0-30 eV can induce at interfaces and within condensed matter specific reactions which are of relevance to applied fields such as nanolithography, dielectric aging, radiation waste management, radiation processing, astrobiology, planetary and atmospheric chemistry, surface photochemistry, radiobiology, radiotherapy and ballistic electronics. The action of low energy electrons (LEEs) in materials of relevance to five of these fields has been investigated with model systems consisting of pure or doped thin molecular films. The target film is deposited on a metal or semi-conductor substrate and bombarded by a LEE beam (0-30 eV) under ultra high vacuum (UHV) conditions. Neutral fragments and ions emanating from these films are analysed by mass spectrometry. The products remaining in the films are analyzed *in situ* by X-ray photoelectron and electron energy loss spectroscopies; they can also be removed from the UHV system and analyzed by HPLC and LC/MS.

By comparing the results of the theory and different experiments, it is possible to determine fundamental mechanisms that are involved in the chemical reactions induced by LEEs. Such mechanisms involve (1) the formation of transient anions which play a dominant role in the fragmentation of all molecules investigated; (2) dipolar dissociation which produces an anion and a cation and (3) reactive scattering, which induces non-thermal reactions. The transient anions fragment the parent molecules by decaying into dissociative electronically excited states or by dissociating into a stable anion and a neutral radical. These fragments usually initiate other reactions with nearby molecules, causing further chemical damage. The damage caused by transient anions is dependent on the molecular environment. This research is financed by the CIHR, NSERC and the NCIC.

Electron Processing at Sub-Excitation Energies

Eugen Illenberger

Physical and Theoretical Chemistry, Freie Universitaet Berlin

We report on chemical reactions initiated by free electrons at energies below the level of electronic excitation for the respective molecules (< 3 eV). Most photochemically initiated reactions involve excited species where an electron is promoted, e. g., from the highest *occupied* molecular orbital (MO) to the lowest *unoccupied* orbital (LUMO) associated with an energy supply in the range of several eV. In contrast, the addition of an excess electron into the LUMO (generating a molecular negative ion) is often possible at very low energies, i. e., below the threshold for electronic excitation and often close to zero eV. The negative ion resonance thereby formed can be very reactive in that it dissociates by selective bond cleavage at remarkably high cross sections.

We have applied these peculiar properties of dissociative electron attachment (DEA) to explore some interesting and fascinating problems in different areas of fundamental and applied science.
We demonstrate

- that DEA is a very convenient method to study charge and energy distributions in unimolecular reactions [1]
- the potential of slow electrons as a soft and effective tool for surface modification [2], and
- the role of sub-ionisation electrons to the problem of radiation damage and the operation of radiosensitisers used in radiotherapy [3].

References
[1] *Energy Balance in Dissociative Attachment to* C_2F_5I
Judith Langer, Stefan Matejcik, Eugen Illenberger
Phys. Chem. Chem. Phys. **4** (2002) 5105.
[2] *Complete Chemical Transformation of a Molecular Film by Subexcitation Electrons*
Richard Balog and Eugen Illenberger
Phys. Rev. Letters **91** (2003) 213201.
[3] *Site-Specific Dissociation of DNA Bases by Slow Electrons at Early Stages of Irradiation*
Hassan Abdoul-Carime, Sascha Gohlke and Eugen Illenberger
Phys. Rev. Letters **92** (2004) 168103.

Low Energy Electron Interactions with Biologically Relevant Molecules

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The interaction of highly mono energetic electrons with molecules such as DNA and RNA bases, water, glycine, deoxyribose, glycol-aldehyde and various organic acids has been studied. Experimentally the formation of both positively and negatively charged product ions has been investigated and complementary quantum chemical calculations were performed. The aim of these studies is to understand the basic processes that lead finally to the damage of living cells upon exposure to ionizing radiation (α, β, γ, ions). Sanche and co-workers [1] recently demonstrated that potentially lethal DNA damage (double strand breaks) can be induced by low energy electrons. They observed a well pronounced maximum in the yield of single and double strand breaks at electron energies of 10 eV. Such resonances are typical for the formation of fragment anions.

In the present experiment gas phase biomolecules that were vaporized in an oven are crossed with an electron beam with narrow energy spread (~100meV). The dominant negative ions formed via free electron attachment reactions to most of the molecules M studies so far (exceptions are halogenated uracil, water and sugar) are the closed shell anions $(M-H)^-$ [2] The attachment cross sections of these anions have a maximum value between 1 eV and 1.5 eV and in several cases we observed a series of narrow peaks. In the case of thymine (T) we could identify experimentally the position of the molecule where the hydrogen atoms were removed by using partially deuterated molecules. For three different reaction channels, i.e. $(T-H)^-$, $(T-2H)^-$ and H^- we could observe characteristic bond selectivity for several resonances.

The next step towards more complex biomolecules has already been taken. We investigated electron impact ionization and dissociative electron attachment of thymidine and uridine. These molecules consist of a base and a sugar molecule. Using a two sector field mass spectrometer we recently started to investigate delayed unimolecular decomposition of product ions formed via inelastic interactions of electrons with biomolecules.

Work partially supported by the FWF, ÖAW and ÖNB, Wien, Austria and the European Commission, Brussels.

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Probing Molecules with Slow Electrons and Positrons Impacting on Gaseous Targets

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Electron beams have been used over the years for the study of a very broad variety of molecular properties, ranging from the fundamental study of low-energy resonances, electron-induced molecular fragmentation, excitation, dissociative attachment and recombination to the analysis of plasma production by electrons and of chemical vapour deposition initiated by electron impact [1].

Likewise, positrons have been widely used both for probing gas properties at the molecular level [2] and for their use in several applied field related, for example, to defects in solids and to polymer formation [3].

In the present talk I shall endeavour to show that the theoretical understanding of such processes and the computational modelling of the relevant observables has also made good progress in recent years and that we are now able to gather a great deal of data which pertain to simple systems and also to analyse with good reliability the behaviour of complex gases like fullerenes or biomolecular targets [4,5].

References

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R-matrix Calculations of Electron-Molecule Collisions at Low and Intermediate Energies

Jonathan Tennyson

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University College London

The R-matrix method is now well-established as a reliable and flexible procedure for treating electron collision problems. In particular the UK molecular R-matrix codes have been applied to an increasing variety of electron molecule collision problems. Recent calculations on low-energy electron collisions with water have found outstandingly good agreement with published measurements of differential and momentum transfer cross sections. However the calculated elastic cross sections differ significantly from those inferred from experiment, suggesting that the published data still does not correctly measure the strong forward peak for this process. New calculations have been performed on the 13-atom organic ring molecule tetrahydrofuran with the aim of identifying low-lying resonances in this system.

A new molecular R-matrix with pseudo-states (MRMPS) procedure has been developed which allows the correct ab initio treatment of electron collision processes, including ionisation, above the molecular ionization threshold. Initial studies on benchmark systems suggest that this method works well.

Long-Lived Hydrogen Molecular Anions

Jiri Horacek

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Charles University in Prague, Czech Republic

The existence of (metastable) molecular hydrogen anions H2- and D2- is uncertain despite intensive experimental search. Here we present a definitive experimental demonstration of their existence and discuss theoretically their formation. These anion species were produced by sputtering of TiH2 and TiD2 targets with Cs and were identified unambiguously by accelerator mass spectrometry. From the respective flight times through the spectrometer, lifetimes for H2 and D2 of at least 2.7 µs and 3.9 µs, respectively, can be inferred. Theoretical calculations within the non-local resonance model predict the existence of highly rotationally excited anions with lifetimes in the µs range. It is proposed that in sputtering molecular hydrogen species with high rotational and vibrational excitation are formed that are stable on the time scale of the experiment.

Coupled Electron-ion Dynamics

A.J. Fisher (1), A.P. Horsfield (1), T.N. Todorov (2), C. Sanchez (2)
and D.R. Bowler (1,3)

(1) Department of Physics and Astronomy and London Centre for
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(2) Atomistic Simulation Group, Queen's University Belfast
(3) International Centre for Young Scientists, NIMS, Tsukuba, Japan

Coupled dynamics of electrons and ions is important throughout the physical sciences, in phenomena as diverse as desorption-induced electronic transitions (DIET), electron-induced amnd photo-induced chemical reactions, local heating in nanostructures, radiation damage, and molecular electronics.

I will describe a new approach to simulating these processes, which focuses on retaining just enough of the crucial correlations between electrons and ions as the system evolves to describe energy transfer between them correctly. I will give a status report on the development and applications of this new technique, known as CEID (Coupled Electron-Ion Dynamics).

Electron and Force Induced Molecular Manipulations: Molecular engines and Switches

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Several novel effects upon electron and force induced processes on single molecules on Cu(111) surfaces are presented. Topics include:

- Molecular "shooting" upon lateral manipulation of sexiphenyl molecules. A possible relation to the engines on atomic scale as proposed by Porto et al. is discussed.
- Various electron induced reversible isomerization reactions of azobenzene (Disperse Orange 3) single molecules and dimers opening routes towards molecular switches.
- Identification of Chlorine-Nitrobenzene and electron induced isomerization.
- Manipulation of and surface structuring with Hexabenzocoronene Derivatives.

* In collaboration with:
Francesca Moresco, Karina Morgenstern (Univ. of Hannover),
Micol Alemani, Leonhard Grill, Leo Gross, Saw-Wai Hla (Ohio State Univ.),
Michael Mehlhorn, Heiko Gawronski, Violeta Simic-Milosevich, Jörg Henzl

Simulation of High-Resolution Scanning Tunneling Microscopy and Spectroscopy: Present State of the Art and Comparison with Experiments.

Dr Werner A Hofer

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The aim of the talk is to give an overview over the current state of theoretical research in scanning tunnelling microscopy. I shall introduce the basic theoretical concept, which unifies existing models of scattering (Landauer-Buttiker approach) and perturbation (Bardeen approach) in a common framework based on non-equilibrium Green's functions and discuss its limitations with respect to achievable currents and minimum distances [1,2].

The precision of the method is illustrated by recent simulations of oxygen covered ruthenium surfaces and detailed comparisons with experiment [3]. Interactions between STM tip and surface will be highlighted for close packed metal surfaces like gold, copper, or aluminium [4]; the method of inferring interaction energies and forces from the simulation of electron transitions, and the high elasticity of aluminum is shown to fully account for the observed giant corrugations.

The second half of the talk will be devoted to recently developed spectroscopic tools. We show that direct simulation of differential contributions to a spectrum leads to the correct behaviour also for demanding problems like the surface states on close packed noble metal surfaces [5]. It is pointed out that the resolution of the simulations accounts only for experimental data above 100K; for very low temperature experiments new interpolation schemes need to be developed for the bandstructure map. As a final example I shall talk about recent experiments and simulations on ferromagnetic surfaces, where the spin-state of a single atomic impurity can be measured and changed by STM tips.

References
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Electron-Induced Processes in Single Atoms and Molecules on Surfaces

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In this talk I will present some highlights of our on-going theoretical work concerning atomic processes induced by inelastic electron tunnelling from a scanning tunnelling microscope (STM) tip through single atoms and molecules adsorbed on a metal surface. These processes include single molecule vibrational spectroscopy and microscopy [1,2] and chemistry [3], and charge state control of single adatoms on thin insulating films supported by a metal substrate [4]. Our theoretical approach is based on density functional theory of the electronic structure and a many body extension of Tersoff-Hamann theory to vibrational inelastic tunnelling.

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Modification Of Thin Molecular Films By Low-Energy Electrons

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Interest in the chemical modification of adsorbates and thin molecular films at surfaces by exposure to low-energy electrons is increasing. This concerns not only the curing of coatings and lithographic techniques such as proximity printing, i.e. exposure of a surface to lowenergy electrons through a mask [1], but also reactions induced by the current under the tip of the scanning tunneling microscope (STM) [2]. Examples have shown that products are sometimes formed with surprising selectivity [3]. On the other hand, the underlying elementary reaction steps are often not well established. This, on the other hand, is essential to achieve reaction control using low-energy electron beams. Therefore, basic mechanistic studies are needed to complement present and to form a foundation for future technical developments.

This contribution will present recent work in this direction concerning the identification of products and reaction sequences and the measurement of reactive cross sections [4] in thin molecular films exposed to low-energy electrons.

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Electron Induced Functionalization of Semiconductors: the case of polycrystalline Diamond

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Organic modification of semiconductors or functionalization is a fast growing field due to the need to create devices, exploiting the properties of organic and inorganic materials, capable of molecular recognition and chemical or biological sensing.

Different methods in wet or dry environment have been developed some of them photo assisted.

Silicon substrates have been widely used for these studies [1] and only recently Diamond substrates have been considered.[2]

In this talk I will present electron induced functionalization method of Diamond substrates which consists in depositing few layers of organic compounds on non-reactive hydrogenated surface and irradiating this film with low energy electrons.

Results on hydrogenated diamond/CH_3CN system will shown.

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Single Molecule Desorption and Dissociation at Room Temperature

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Bond-selective molecular manipulation is one of the frontiers of atomic manipulation with the STM. Traditionally such experiments are conducted in the stable, low temperature regime; room temperature manipulation is much more challenging. Here we demonstrate room temperature, bond selective manipulation (“molecular dissection”) in a polyatomic molecule - chlorobenzene (C_6H_5Cl) anchored to the Si(111)-7x7 surface by chemisorption. Recently we showed that the mechanism of electron (or hole) injection from the STM tip into the □* LUMO (or □ HOMO) orbitals of the benzene ring leads to controlled molecular desorption beyond a threshold voltage of +2.5V (-1.5V) [1]. The desorption yield is linearly proportional to the STM junction current, indicating a one electron process. In this work we explore C-Cl bond dissociation in the chemisorbed chlorobenzene molecule. Detailed STM images allow us to identify the azimuthal orientation of the individual chlorobenzene molecules on the surface and thus to correlate the final location of the liberated chlorine “daughter” atom with the position and orientation of the parent molecule [2]. We identify Cl atoms up to 50Å from the parent molecules. We find that both the radial and azimuthal distributions of Cl atoms depend sensitively on the tunnelling current [3] and that a wide range of surface sites is populated by the (energetic) Cl atoms (probably anions). This behaviour can be explained in terms of an energetic, two-electron dissociation process, as implied by the measured quadratic dependence of the dissociation rate on tunnelling current. We propose a mechanism based on dissociative electron attachment (DA) of the “second” electron to a molecule vibrationally excited by the “first” electron [3]. Such a mechanism explains how one can overcome the symmetry barrier to C-Cl dissociation via electron attachment to the ring states.

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Cold Electron Chemistry in the Gas Phase: Benchmark Experiments

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A great deal of interest is focussed at present on cold scattering encounters, in which the wavelength of the projectile is very much greater than the physical dimensions of the target. We consider here electrons of a few to a few tens of meV (1), whose wavelengths are of the order of 10 nm, impinging on molecules whose dimensions are less than 1nm. Strong quantum effects are very apparent in the scattering.

In this presentation I concentrate upon virtual state effects in molecules such as C_6F_6 and the application to CCl_4 and SF_6 of a method which allows the determination of absolute cross-sections for attachment of cold electrons without recourse to rate constant data.

Recent experimental work has demonstrated that the phenomenon of virtual state scattering can lead to very large scattering cross-sections in very low energy encounters. These experiments will be described (1) and data shown for a number of species including C_6F_6 and other species (2,3,4). The qualitative nature of virtual state scattering will be discussed, in terms of nuclear adiabatic and diabatic channels.

Implications of results for both industrial and naturally occurring plasmas, such as the interstellar medium, will be discussed.

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Benchmark Cross Sections for Low-Energy Electron Attachment to Molecules with Well-Defined Internal Temperature

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Using two variants of the laser photoelectron attachment method [1] we have measured (relative) cross sections for low-energy electron attachment to the molecules SF_6 (formation of SF_6^-, SF_5^-,and F^-), CCl_4 (Cl^- formation) and CF_3I (I^- formation) in a diffuse gas target with well-defined temperature ($T_G = 300$ K) from 0 eV up to 2 eV (electron energy width 1 – 2 meV for $E < 200$ meV and about 30 meV for $E > 200$ meV). Absolute cross sections have been established with reference to reliable rate coefficients, obtained consistently by several groups at equal electron and gas temperature ($T_e = T_G = 300$ K) [2]. At energies above 0.2 eV, our cross sections exhibit substantial deviations from recommended values [3-5]. For SF_6 and CCl_4 these differences can be attributed to the fact that in most of the earlier electron beam experiments the gas temperature was higher than 300 K. For CF_3I the previously recommended attachment cross sections are too high by at least a factor of five for energies above 0.1 eV.

This work has been supported by the Deutsche Forschungsgemeinschaft and by Forschungszentrum *Optische Technologien und Lasergesteuerte Prozesse*.

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Elastic and Vibrational Excitation Cross Sections in Methane and Cyclopropane

Michael Allan

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Elastic and vibrational excitation cross sections in methane and cyclopropane have been measured from threshold to 20 eV. The Ramsauer-Townsend minimum, the presence/absence of threshold peaks, and shape resonances will be discussed.

Electron Scattering by DNA Bases at Intermediate and High Energies

G. García

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In this talk we will present an adaptation of our experimental system to the study of electron interactions with molecular basis of DNA in the gas phase. For this purpose, we have arranged and indirect heated oven to vaporise the target with a temperature controlled electron bombardment system. The effusive molecular beam is then crossed with an electron beam to analyse the energy loss of electrons after the interaction. Ion fragments induced by electron impact can be extracted from the collision region and analysed in a time of flight mass spectrometer.

Experimental results will be complemented with our electron scattering cross section data calculated with an optical potential method in an independent atom representation.
The reliability of this model potential calculation to study DNA strings formed by base sequences will be discussed.

Synchrotron Radiation as a Tool for Probing the VUV Spectroscopy of Biomolecules

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Despite the fact that, after formic acid (HCOOH), acetic acid is the second simplest organic acid, and therefore component of biological molecules, we are particularly interested on its electronic state spectroscopy by means of VUV photo-absorption, as important route to understand the effects of direct energy deposition by radiation that can lead to damage. The electronic state spectroscopy of acetic acid has been studied by VUV photo-absorption measurements in the energy range 3.5 – 11.0 eV. The high-resolution photon beam (~ 0.075 nm) has made possible the detailed analysis of the vibrational progressions, new assignments for the Rydberg series, where some new assignments are proposed for the first time. The result is compared with electron energy loss spectra (EELS).

Temperature Dependence of Electron-Induced Reactions

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The electron induced reactions depend on the energy of the electrons and on the initial state of the molecules [1]. The initial state of the molecules can be described by the electronic, vibrational and rotational excitation. In many cases, especially polyatomic molecules, it is very difficult or even impossible to prepare molecule in well defined excited state (vibrational, rotational excitation) in the time window necessary for the experiments with the electrons. Another possibility is to study electron interaction with molecules with well defined temperature (vibrational and rotational excitation). The studies of gas temperature dependencies for electron induced reaction are of practical importance as many media (discharges, plasmas) where these reactions take place are at elevated temperatures. The crossed electron molecule beams apparatus at the department of Plasma physics in Bratislava has been designed for studies of ionization reactions of the electrons with the molecules at elevated temperatures.

The temperature dependences of dissociative electron attachment (DEA) reaction to the molecules have been studied in many swarm experiments and it has been shown that the gas temperature in many cases enhance the rate coefficient for this reaction. We have studied the gas temperature dependences of the cross sections for exotherm DEA reactions (e.g. halo-derivatives of methane [2, 3, 4]). Generally, if a reaction of DEA was sensitive to the gas temperature the magnitude of the cross section has been changed only in the low electron energy range (from zero to few hundred meV).

The influence of the gas temperature on the electron impact ionization (EII) reactions has been studied for molecules C_xH_y (x=1..3, y=4..8) [5, 6, 7]. We have observed the influence of the temperature (gas temperatures 293 and 690 K) on the values of the ionization energy (IE) of the molecule and on the values of the appearance energies (AE) of the fragment ions formed via the reaction of dissociative electron impact ionization. The IE and AE values were decreasing with the increasing of the gas temperature and the shifts of the values were proportional to the rotational and vibrational excitation of the molecules.

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Electron Scattering by THF Molecule

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The backbone of the DNA molecule may be seen as a series of tetrahydrofuran (THF) molecules connected by phosphate bonds to which the bases are attached. Qualitative estimation of effects linked to chemical and structural changes of cellular DNA connected with radiation damage is performed by electron interactions with THF (C_4H_8O) sugar-like analogue molecule in gas phase. We report results for elastic scattering of electrons as a function of angle and electron impact energies. The absolute elastic differential cross section (DCS) as a function of scattering angle (10°-110°) is presented at impact electron energy range from 10 to 300 eV. Experimental set-ups used in the experiment are two electron spectrometers designed for lower and higher energy ranges, the first being of hemispherical electrostatic type and the other of double cylindrical mirror type.

Electron-Molecule Interactions Studied in Electron Backscattering Experiments

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The interaction of electrons with molecules in single-electron collision processes have been studied using experimental techniques which enable observation of scattering in the backward direction close to 180°. These techniques include applications of the magnetic angle-changing technique [1,2] and a new backscattering electron spectrometer, that is presently being developed, equipped with a hypocycloidal electron selector [3]. Up to now such investigations of elastic and inelastic processes have been limited to the noble gas atoms, Ar, Kr [4,5] and the simple molecules, O_2, N_2, H_2O [6,7]. However it is intended to extend these techniques to molecules that are of wide interest in plasma etching gases and to biological molecules such as DNA bases. Scattering in the backward direction increases the effects due to various types of interactions. In particular, polarization and exchange effects are expected to be more significant than the electric-dipole interaction.

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Inaugural Lecture
Professor Nigel Mason

Probing the Molecular World;
Adventures with Electrons and Light

We live in a molecular world; a nano-scale world in which molecules are constantly interacting with one another and external stimuli to produce physical and chemical processes that influence the macroscopic world around us. The formation of molecules in the interstellar medium; the processes that lead to the destruction of ozone in the terrestrial atmosphere; the engineering that underpins the construction of semiconductor chips and the mechanisms that lead to radiation damage of DNA – all are controlled by molecular processes. Understanding such molecular interactions and devising new techniques that allow them to be manipulated and controlled remains one of the greatest challenges for modern research and underpins the development of many of the new technologies for the 21st century.

This talk will describe how Professor Mason's research on electron and photon interactions with molecules has revealed that it is possible to control the excitation and dissociation of molecules through the adaptation of selective cleavage of chemical bonds. Such 'single molecule engineering' provides exciting new opportunities that can now be exploited by both the research and technological communities and may even help explain the origins of life itself!

Professor Nigel Mason

Nigel John Mason was born into physics, his father being Sir John Mason FRS, Director General of the Meteorological Office and a noted environmental physicist. Thus he was ‘indoctrinated’ at an early stage into recognizing physics as the premier science.

After graduating from University College London in 1983 his postgraduate studies involved the study of electron collisions with atoms and molecules in the presence of laser fields. As part of the atomic physics group at UCL he was able to demonstrate, for the first time, a prediction first made in the 1930s that in a three-body collision between an electron, atom and photon the electron may excite the atom by ‘absorbing’ the photon, even if its initial kinetic energy is less than the excitation energy of the atomic state. Awarded a SERC Postdoctoral Fellowship in 1988 and a Royal Society University Research Fellowship in 1990 he established the Molecular Physics Group in the Department of Physics and Astronomy, University College London in 1990. The group rapidly developed a wide ranging research programme studying atmospheric physics (in particular the mechanisms of ozone depletion and global warming), collision physics and plasma physics. He was a co-founder of the UCL Centre of Cosmic Chemistry and Physics commencing a research programme to study molecular formation in the interstellar medium and planetary atmospheres.

Appointed Lecturer in 1998 and Reader in 2000 he joined the Open University in September 2002 as Professor of Physics. Co-founder of the Interdisciplinary Centre for Astrobiology and The Centre of Atomic and Molecular Engineering his research interests have expanded to include research in nanotechnology, radiation chemistry and the origins of life.

He has served on many National and International Committees and co-ordinates several major European projects. He is a keen promoter of physics and public understanding of science having held senior positions in both the Institute of Physics and the British Association of Science. In his spare time (!) he writes on military history, in particular the Napoleonic Wars. Married to Jane they share their house in Heath and Reach with two Turkish Van Cats, Pushkin and Vashka.

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