COST Action MP1002, Nano-IBCT
"Nanoscale insights into Ion Beam Cancer Therapy"

Workshop on Nano-IBCT data base development

Vienna, Austria
February 24 - 26, 2012

Scope

Workshop on Nano-IBCT database development is organized as a satellite of the third VAMDC project meeting, and will be held in Vienna (Austria) on February 25th and 26th. The meeting is organized in the framework of the COST Action MP1002 (Nano-scale Insights into Ion Beam Cancer Therapy). The Nano-IBCT database workshop will be devoted to the discussion of a new database to be created within the COST Action Nano-IBCT. The aim of this workshop is to establish contacts between the teams willing to participate in the development of the Nano-IBCT data base, to link this development to the existing project Virtual Atomic and Molecular Data Center (VAMDC, http://www.vamdc.eu), and to establish standards for the newly created Nano-IBCT Data Base.

In particular, the following subjects will be discussed:

- Nano-IBCT data base content
- Database standards and formats
- Software and hardware requirements
- Expandability, maintainability and compatibility of the database
- Experience of VAMDC partners
- Publicity and dissemination issues

About COST Action MP1002 "Nanoscale insights into Ion Beam Cancer Therapy" (Nano-IBCT)
Ion beam therapy offers the possibility of excellent dose localization for treatment of malignant tumours, minimizing radiation damage in normal tissue, while maximizing cell-killing within the tumour. However, the full potential of such therapy can only be realised by better understanding the physical, chemical and biological mechanisms, on a range of time and space scales, that lead to cell death under ion irradiation. The Nano-IBCT COST Action therefore aims to combine, using a multiscale approach, the unique experimental and theoretical expertise available within Europe to acquire greater insight at the nanoscopic and molecular level into radiation damage induced by ion impact.

More information about the COST Action can be found in the on its webpages:
- http://fias.uni-frankfurt.de/nano-ibct/
- http://www.cost.esf.org/domains_actions/mpns/Actions/nano-ibct/

About VAMDC project
VAMDC aims at building an interoperable e-Infrastructure for the exchange of atomic and molecular data. VAMDC is a complex project involving 15 administrative partners representing 24 teams from 6 European Union member states, Serbia, the Russian Federation and Venezuela. It embraces on the one hand scientists from a wide spectrum of disciplines in atomic and molecular (AM) Physics with a strong coupling to the users of their AM data (astrochemistry, atmospheric physics, plasmas) and on the other hand scientists and engineers from the ICT community used to deal with deploying interoperable e-infrastructure.

More information about the VAMDC project can be found in the on its webpages:
- http://www.vamdc.eu/

Sponsors

The workshop will be held under the auspices of the following sponsors:
- COST Action COST Action MP1002, Nano-IBCT
- Frankfurt Institute for Advanced Studies, Frankfurt
- Universität Wien
- The Open University

Important Dates

Distribution of the first announcement	December 22, 2011
Distribution of the second announcement	January 28, 2012
Deadline for registration	January 27, 2012

Scientific Program

The scientific program for this Workshop will consist of sessions, which will include invited and special reports and the round table discussions of all the Workshop participants addressing all the aspects of the envisaged development of the Nano-IBCT data base and the experience of the meeting participants. It is expected that the participants of the Nano-IBCT Data Base Workshop will arrive at least one or two days before the Workshop in order to participate in the VAMDC annual meeting and to get acquainted with the VAMDC project and its participants. The maximum number of the Workshop participants is set to 25 constrained by the capacity of the lecture hall, in which the meeting will take place.

Workshop venue and logistics

The venue of the Nano-IBCT Data Base Workshop will be the Department of East Asian Studies (Japanese Studies) located on the campus of the University of Vienna, see http://campus.univie.ac.at/en/. The meeting room is 2K-EG-29, court 2.4 in court 2. The main entrance to the building is indicated on the following map as "Japanologie" 2.4. It can be reached directly from the (rather small) court 2 near court 1 of the campus, as shown on the map:

For more details, see http://campus.univie.ac.at/en/general-map/#c215355
and http://kenkyuu.eas.univie.ac.at/index.php?id=97

The VAMDC meeting will be held at the 'Hörsaalzentrum' (Lecture Hall C2), court 2.6 of the Campus of the University of Vienna, the Aula at the Campus, court 1.11 and seminar room of the Institute of Japanology, 2K-EG-29, court 2.4. All can be reached directly from the (rather small) court 2.

The on-campus restaurants are on court 1 (1.13 and 1.14). Maps to find the restaurants and their webpages:
http://campus.univie.ac.at/en/restaurants-and-businesses/
http://campus.univie.ac.at/en/restaurants-and-businesses/map-restaurants-and-businesses
Admittedly, the restaurant homepages are mostly in German, but handling everything there in English won't be a problem.

For more information on the conference venue and other logistic issues, such as transportation from the airport to the Campus of the University of Vienna, accommodation, meals, visas, wireless communication, etc), please visit the Logistics page: http://voparis-twiki.obspm.fr/twiki/bin/view/VAMDC/PmCycleThreeLogistics

Social Program

Event	Date/Time
VAMDC Conference dinner (for those who will arrive on February 23 and pay for the VAMDC Conference dinner)	Thursday, February 23, 2012 19:00 - 22:00
Nano-IBCT Database Workshop dinner will take place at Plachutta Grünspan Biergaststätte, Ottakringer Straße 266, 1160 Wien	Saturday, February 25, 2012 19:00 - 22:00
Vienna city tour could be arranged upon request after the end of the Workshop	Sunday, February 25, 2012 15:00 - 18:00

Tentative scientific program

The Nano-IBCT Database Workshop will be organized according to the following time frame:

Saturday, 25 February 2012

$9^{15} – 9^{30}$	**Nano IBCT Database Workshop Opening** **Friedrich Kupka, Nigel Mason, Andrey V. Solov'yov**
$9^{30} – 11^{00}$	**Session I:** **Chair: I** **A.V. Solov'yov**, Frankfurt Institute for Advanced Studies, Germany *NANO-IBCT COST Action and data needs for multiscale modeling of radiation damage and nanodosimetry* **Friedrich Kupka**, Universität Wien, Austria *VAMDC project* **G. García**, Instituto de Física Fundamental, Madrid, Spain *Data needs for track structure modelling*
$11^{00} – 11^{30}$	**Coffee break**
$11^{30} – 13^{00}$	**Session II:** **Chair: II** **N. Mason**, Open University, Milton Keynes, UK *Electron-biomolecule interactions: experimental state of the art* **B. Marinkovic**, Institute of Physics University of Belgrade, Belgrade, Serbia *Electron scattering and the development of the specified data-base* **Stephen Buckman**, Australian National University, Australia *Positron interactions: state of the art*
$13^{00} – 14^{30}$	**Lunch**

$14^{30} – 16^{00}$	**Session III** **Chair: III** **H. Rabus**, PTB, Braunschweig, Germany *Data collection and dosimetry* **B. Huber**, CEA (Commissariat à l'Energie Atomique et aux Energies Alternatives), France *Data on ion interactions with biomolecular systems* **E. Suraud**, Université Paul Sabatier, Toulouse, France *Data collection on photon interactions with biomolecules and nanoparticles*
$16^{00} – 16^{30}$	**Coffee break**
$16^{30} – 18^{00}$	**Roundtable discussion I** **Moderators: RT-I** **Topics:** *to be announced*
19^{00} - 22^{30}	**Workshop dinner**

Sunday, 26 February 2012

$9^{30} – 11^{30}$	**Morning session IV:** **Chair: IV** **F. Calvo**, CNRS and University of Lyon, France *Anharmonicities in infrared spectra: modeling of action spectroscopies* **A. Mauracher**, University Innsbruck, Austria *DEA with biomolecules: the data base* **G. Mancini**, Caspur, Rome *Data modeling of theoretical e-molecule scattering properties for Molecular Structure Databases* **E. Scifoni**, Helmholtzzentrum für Schwerionenforschung GmbH (GSI), Darmstadt *Ion beam treatment planning and data need*
$11^{30} – 12^{00}$	**Coffee break**
$12^{00} – 13^{00}$	**Roundtable discussion II: Title** **Moderators: TR-1** **Topics:** *to be announced*
$13^{00} –13^{10}$	**Workshop closing**
$13^{10} – 15^{00}$	**Lunch and departure of participants**

International Advisory Committee

- David Field (Aarhus University, Denmark)
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Management Committee of the COST ACTION MP1002, Nano-IBCT

For details, see http://www.cost.esf.org/domains_actions/mpns/Actions/nano-ibct/?management

Local Organizing Committee

- Friedrich Kupka (Universität Wien, Austria)
- Theresa Lueftinger (Universität Wien, Austria)

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Abstracts

POSITRON INTERACTIONS WITH ATOMS AND MOLECULES: FUNDAMENTAL STUDIES AND APPLICATIONS

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Positron collisions with atomic and molecular systems provide an insight into the dynamics of interactions of antimatter with matter. While low energy collisions of positrons are governed by similar Coulomb interactions to those that mediate electron interactions, the nature of the static interaction with the atom is largely repulsive for positrons, and 'exchange', which is critically important in electron interactions, is absent for positrons. On the other hand positrons readily form positronium – the short-lived bound state of an electron-positron pair – which is the major inelastic scattering channel, and which has a threshold at an energy of 6.8 eV below the ionization potential for the atom or molecule concerned. Positronium formation, and as a consequence, ionization, is thus an open channel at very low energies for many atoms and large molecules.

Positrons are also the key projectile in Positron Emission Tomography (PET) scans are becoming increasingly used as a key tool in investigating nanoscale defects and voids in materials, and these applications are driving many of the fundamental investigations – particularly where scattering cross sections and reaction rates are required.

In this talk we shall outline the work of our collaboration on positron interactions with biomolecules, which includes absolute measurements of a range of scattering cross sections, transport theory, and Monte Carlo modeling. We will also discuss the extent of the database that exists for positrons, what is required for the modeling efforts, and what role other contributions from, for example, *ab initio* theory can make.

ANHARMONICITIES IN INFRARED SPECTRA: MODELING OF ACTION SPECTROSCOPIES

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Infrared spectroscopy of gas-phase molecular compounds has undergone decisive progress in the recent years, owing to the advent of new intense and coherent light sources such as free-electron lasers (FELs). These progresses are paralleled with advances in quantum chemistry methodologies, and structural assignment is usually achieved based on static *absorption spectra* at the harmonic level. However, this procedure is disputable, because it neglects anharmonicities and temperature effects, and more importantly all dynamical processes that take place in the experimental determination of *action* spectra. In this contribution, we discuss some possible modeling of infrared multiphoton dissociation spectra, including some explicit account of the various time scales at play from the brief excitation to the much slower fragmentation.

(1) A first multiscale model, applied to the ionic cluster $(NaCl)_{32}$, consists of a fully classical representation of both the potential energy surface and the interaction with the laser field. Statistical molecular dynamics simulations can be carried out over nanoseconds, and the trajectories are subsequently continued on a purely kinetic basis with statistical rate theories. The results obtained for the direct dissociation of the cluster, and for the predissociation of a tagging argon atom, generally indicate that the action spectrum is similar to the anharmonic absorption spectrum, but the bands show some residual red shift that is interpreted as due to the progressive heating of the system as it is exposed to the laser field [1]. Chirping the laser can also have drastic effects [2].

(2) As a complementary model, is is possible to describe the molecule and its interaction with the field on full quantum mechanical grounds. Using an anharmonic quartic force field derived from vibrational perturbation theory, the response to a realistic laser field is modeled by taking into account absorption, stimulated and spontaneous emission of photons, as well as dissociation into the lowest channel. The application of the model to cationic naphthalene also reveals notable differences between the absorption and action spectra, which are of the same magnitude as intrinsic anharmonicities [3].

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REFERENCES

[1] F. Calvo and P. Parneix, *ChemPhysChem* **12**, 212 (2012)
[2] F. Calvo and P. Parneix, submitted for publication.
[3] P. Parneix, M. Basire, and F. Calvo, submitted for publication.

MODELING OF RADIATION INTERACTION WITH BIOLOGICAL MATTER ON THE NANOMETRIC SCALE FOR RADIOBIOLOGY AND RADIOTHERAPY PURPOSES

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Since DNA damage is considered to be the main lesion leading to cell mutation or cell death after irradiation most of the studies nowadays are concentrated on understanding this type of damage to the finest reachable resolution and investigating the cell reaction to different kinds of irradiation. The most common way that is used for these studies is numerical modeling using the so called track structure codes. Using track structure codes it is now possible to reproduce the energy deposit pattern of a certain particle with certain energy in a sub cellular structure and to compare the different irradiation types predicting their relative effects on the cells.

One of the difficulties encountered when leading a numerical modeling study is in the availability of the interaction cross sections for the different particles and with different types of material (mainly here particles crossing DNA bases and other DNA components). Theoretical cross sections are used in the different codes when models are available and they are compared and validated with the available experimental data. When models are absent or not easily accessible one of the methods consists in using the experimental data interpolated and extrapolated directly into the simulation programs (e.g. sub-excitation electrons cross sections in water). This procedure might be very approximate especially for cases where the experimental data is very scarce and hard to find for the studied medium. One example among many others; in the case of sub-excitation electrons in water several studies in the literature are taking data of Michaud et al. (2003) [1] for electrons experiments on ice and "scaling" the results to be suitable for liquid water simulations. In brief, having a common data base where experts within the community can choose the best reliable cross section models to be shared on the database or maybe simply sharing cross section tables calculated and/or also obtained by the available experiments within the community.

Another set of data to be considered is related to experimental results of DNA damage irradiated with different particles. The data would concern different DNA types irradiated at different doses and with different sources. The analysis tool (e.g. Gel electrophoresis or other) is also important to precise. As most of the simulations end points are tending to approximate single and double strand breaks or also lengths of DNA fragments after irradiation, experimental data comes as a validation tool for the theoretical modeling.

REFERENCES

[1] M. Michaud, A. Wen and L. Sanche, *Radiation Research* 159, 3–22 (2003)

DATA NEEDS FOR ELECTRON AND POSITRON TRACK STRUCTURE MODELLING IN CONDENSED MEDIA

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Event by event Monte Carlo simulation methods have become a powerful tool for modelling radiation interactions in soft matter. After a brief review on electron and positron cross section and energy transfer data required by these procedures, a model potential calculation will be presented to investigate how clustering and condensation effects can affect to these data for some atomic and molecular targets, Ar and H_2O, respectively. Single atoms have been represented by an optical potential which includes an absorption term to account for inelastic processes [1]. For positrons, positronium formation has been included in the imaginary part of this complex potential. Ar dimer, trimer and tetramer configurations [2] have been considered by using a screening corrected addition rule (SCAR) procedure which has been confirmed as a successful way to obtain electron scattering cross sections from complex targets [3]. The reliability of this method to calculate electron scattering processes in soft matter will be discussed. Finally some examples of positron and electron tracks in liquid Argon and liquid water will be presented.

REFERENCES

[1] F. Blanco and G. García, Phys. Rev. A **67**, 022701 (2003).
[2] B. Ulrich, A. Vredeborg, A. Malakzadeh, L. Ph. H. Schmidt, T. Havermeier, M. Meckel, K. Colw, M. Smolarski, Z. Chang, T. Jahnke, and R. Dörner, J. Phys. Chem. A **115**, 6936 (2011).
[3] F. Blanco and G. García, J. Phys. B **42**, 145203 (2009).

ION BEAM CANCER THERAPY AND SCIENTIFIC DATA INFRASTRUCTURE FOR SIMULATION METHODS

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Ion beam therapy offers the possibility of excellent dose localization for treatment of malignant tumors, minimizing radiation damage in normal tissue, while maximizing cell-killing within the tumor. However, the full potential of such therapy can only be realized by better understanding the physical, chemical and biological mechanisms, on a range of different time and space scales, that lead to cell death under ion irradiation.

As the underlying dependent physical, chemical and biological processes are to complex to treat them on a purely analytical level, most of our the recent and future understandings will rely on computer simulations, based on mathematical equations, algorithms and last but not least on the available atomic, molecular and transition data. The practicability of the simulated output and the success of a computer simulation is determined by this data, which is treated as input variables in each computer simulation performed. An understanding of a multiscale approach to the physics of ion beam cancer therapy using simulation methods therefore needs to have a joint scientific data infrastructure.

Several computer codes for radiation transport (e.g. Geant4: http://geant4.cern.ch/ , FLUKA: http://www.fluka.org/ , MCNP: http://mcnp-green.lanl.gov/) and track structure analysis (KURBUC, PARTRAC,OREC, SHERBROOKE, ...) are presently used to simulate the underlying physical processes of ion beam therapy. The Meso-Bio-Nano (MBN, http://fias.uni-frankfurt.de/mbn/) Science group at the Frankfurt Institute for Advance Studies has developed a multi-purpose computer code (MBN-Explorer:http://www.mbnexplorer.com/) which is designed to study molecular systems of various degrees of complexity. A broad variety of interatomic potentials implemented in the MBN-Explorer allows to simulate the structure and dynamics of different molecular systems, such as atomic clusters, fullerences, nanotubes, proteins, DNA, composite systems, nanofractals, etc. A recent project focuses on the thermo-mechanical pathways of DNA damage as a consequence of irradiation in ion beam cancer therapy [1,2]. The simulation acts on different space/time scales and needs a variety of reliable input data.

As explained within the previous paragraph, the results of any multi-purpose computer code depend on the input data and therefore a joint scientific data infrastructure is needed. A new database of the Nano-IBCT should base on the relational database of the VAMDC project and could be amplified with the data from simulated outputs (using an database network model), to compare the practicability of different computer codes.

REFERENCES

[1] Alexander V. Yakubovich, Eugene Surdutovich, and Andrey V. Solov'yov, AIP Conf. Proc. 1344, pp. 230-238 (2011)
[2] Alexander V. Yakubovich, Eugene Surdutovich, and Andrey V. Solov'yov, Nuclear Instruments and Methods in Physics Research Section B (2011)

Database for Ion Interactions with Biomolecules in the Gas Phase

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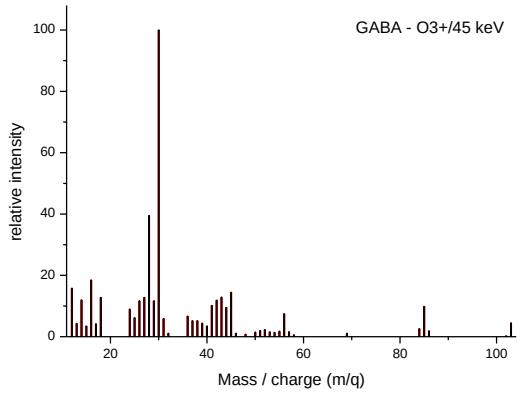
The interaction of ions with biomolecules is studied theoretically as well as in the experiment. For smaller biomolecular systems data, characterizing reaction mechanisms and processes on the molecular level, are often obtained in the gas phase, either for isolated molecules or for biomolecules embedded in a chemical environment (cluster system) or nano-solvated in an aqueous solution. Here detailed information on the processes is obtained by mass spectrometric methods. For larger systems, which cannot be produced easily in the gas phase, ion irradiation of thin films or biomolecules deposited on surfaces have been performed applying very often chemical analysis methods (single and double strand break analysis). Mostly for the reaction probabilities relative values are given only. In a more limited number of studies, absolute cross sections have been reported.

As projectiles light ions as H^{+}, He^{2+}, C^{q+}, N^{q+}, O^{q+} as well as heavy ions (Xe^{q+}) have been used. Typical energies range from the keV region up to several MeV. Shall we restrict ourselves to therapy related ions? Typical target molecules are H_20, nucleobases, nucleotides and –sides, amino acids and peptides isolated and solvated, as well as plasmid DNA or cells.

Data can be documented either in tabular form or in form of standardized mass spectra. In the first case, cross section values can be tabulated as function of collision energy (if available), as for example cross sections for single ionization, cross sections for multiple ionization and total fragmentation cross sections. In the second case, we might document relative cross sections for individual fragmentation channels in form of a standardized mass spectrum showing line intensities for individual fragmentation channels. Similar data sets exist for electron impact (electron energy:70 eV, available under the NIST Electron Ionization (EI) Mass Spectral Library [1]. For all these data a procedure has to be established to guarantee the quality and precision of the data.



The given example shows the fragmentation mass spectrum obtained in collisions of O^{3+} ions with the amino acid GABA ($NH_2(CH_2)_3COOH$), measured at a collision energy of 45 keV. In addition, a Table identifying the corresponding fragment molecular ions should be given.

As ordering parameter we might consider: i) type of process (ionization, fragmentation) ii) type of target molecule, iii) type of environment, iv) type of projectile (element, charge state, kinetic energy), or we may exchange i) and ii).

[1] NIST link: http://www.sisweb.com/software/ms/nist.htm#ei

VAMDC PROJECT

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The Virtual Atomic and Molecular Data Centre (VAMDC, see M.L. Dubernet et al. [1]) is an EU-FP7 e-infrastructure project (under the ``Combination of Collaborative Projects and Coordination and Support Actions" funding scheme, call topic: INFRA-2008-1.2.2 Scientific Data Infrastructure, Grant Agreement number: 239108) devoted to building a common electronic infrastructure for the exchange and distribution of atomic and molecular data. It involves two dozen teams from six EU member states (Austria, France, Germany, Italy, Sweden, United Kingdom) as well as Russia, Serbia, and Venezuela. Scientists from many different disciplines in atomic and molecular physics collaborate within VAMDC. They include creators and users of the data sets as well as scientists and engineers from the information and communication technology community. In this talk an overview of the status of VAMDC and its capabilities in its current form as presented at the 3rd VAMDC Annual Meeting (Cycle Three Project Meeting) will be given.

REFERENCES

[1] Marie-Lise Dubernet et al., J. Quant. Spectrosc. Rad. Transf. **111**, 2151 (2010)

ELECTRON INDUCED DISSOCIATION AS STUDIED BY ATOM-(BIO)MOLECULE COLLISIONS

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Owing to the absence of free electrons in the physiological environment, electron transfer mechanisms may be considered as a better matching of electron attack to the target molecules. Though, potassium-(bio)molecule collisions can be used as a model to investigate such key targets. Electron transfer-induced processes in neutral low energy atom-molecule collisions are presently a relatively unexplored field, particularly in respect to biological relevant molecules. As the outermost electron in potassium is weakly bound, the experiments may provide an analogy for electron transfer from electronically excited secondary neutrals in biological material.

The present set of experiments performed in the Lisbon laboratory, have allowed the observation of peculiar differences in nucleobase anion fragmentation pathways in respect to free electron interactions. The fragmentation patterns of nucleobase anions, notably thymine/uracil [1] and some radiosensitizers [2], produced in collisions with accelerated potassium atoms, have revealed several fragment anions that were not reported in free electron attachment studies. However the most striking difference was the enhanced yield of anions stemming from bond breaks in the ring, most notably CNO^-. Though, these have been referred as being relevant from a radiobiological standpoint as well as from a fundamental point of view.

Within the scope of a data base, Nano-IBCT could include two sets of data that would be used either for radiobiological simulation purposes or just for fundamental reasons. Though, wherever possible, cross sections for biomolecular decomposition by charge transfer experiments should be included, as well as an extensive list of all fragment ions produced.

REFERENCES

[1] D. Almeida, R. Antunes, G. Martins, S. Eden, F. Ferreira da Silva, Y. Nunes, G. García and P. Limão-Vieira, *Phys. Chem. Chem. Phys.* **13**, 15657 (2011)

[2] F. Ferreira da Silva, D. Almeida, R. Antunes, G. Martins, Y. Nunes, S. Eden, G. García and P. Limão-Vieira, *Phys. Chem. Chem. Phys.* **13**, 21621 (2011)

PROGRESS ON BELGRADE E-RACP DATA BASE AND INFORMATION SYSTEM

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Development of the information system that would cover fundamental aspects of the research conducted in the area of atomic collision physics has been of our interest since last decade when we put forward process model and data model with the examples of implementation [1]. That information system encompasses both bibliographic entries and specific data base with the cross sections derived in the research of atomic collisional physics (RACP).

Belgrade e-RACP data base is seen as a part of the large scale effort to maintain the distributed Virtual Atomic Molecular Data Centre (VAMDC) [2]. Selection of the papers could be done by larger number of parameters such as key words, authors, categories, experimental or theoretical methods of study, PASC, DOI, etc. Publications that consider data in electron/atomic and molecular collision physics are presented in this data base in the structured way and every spreadsheet has an abstracts with the tagged data that enable fast survey. Data input is supervised by the specialist evaluating the published work and extracting and categorizing the relevant data and parameters of the experiment or theoretical treatment.

Figure 1: The mask of entry point to the RACP information system maintained at the Institute of Physics, University of Belgrade.

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REFERENCES

[1] V. M. Cvjetković, B. P. Marinković, and D. Šević, “Information System i Atomic Collision Physics”, in *Advances and Innovations in Systems, Computing Sciences and Software Engineering*, Ed. Khaled Elleithy, pp. 485-490, Springer, Dordrecht, The Netherlands (2007).
[2] B. P. Marinković, V. Bočvarski, N. Nikolić, Dj. Lazović, D. Šević, G. García, and N. J. Mason, *Proc.* EIPAM09/PEIC, Joint EU – Australia Meeting 2009 and The Fifth Annual Meeting of ESF Programme on ‘*Electron Induced Processing at the Molecular Level*’ (EIPAM09), 12 – 16 Oct. 2009, Trieste, Italy.

Electron-biomolecule interactions: experimental state of the art

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Since the publication of the seminal paper by Sanche and co-workers[1] in 2000 demonstrating the possible link between basic electron molecular interactions and the propagation of damage in DNA, research on the interaction of electrons with larger biomolecular systems has grown at a rapid rate leading to more than 500 publications. Several national and international research collaborations have developed, including the COST RADAM and NANO-IBCT programmes, bringing together researchers to;

1. Develop an understanding of the fundamental interactions between different types of radiation (ions, electrons) and basic biomolecular systems.
2. Study and quantification of electron induced damage to DNA and to biomolecular assemblies (DNA-protein, lipid-protein complexes and membranes) and
3. explore the role of electron induced processes in Radiation Damage models.

The amount of data generated over the last decade is impressive but to date such data has been dispersed across a wide range of journals and there exists no single database that assembles, reviews and recommends standards for the radiation community. It is therefore timely to review the current status of the field and consider how the community may both collate such data and thence identify new data needs. We will then be able to address such questions as;

- How is such data being used to improve radiation damage models ? and
- Is it possible to use data from fundamental science to develop better radiation therapy techniques and if so
- What are other questions that must be answered before clinical practice may be changed ?

In this talk I will briefly discuss these issues and suggest how a IBCT Nano database may assist in the development of next generation research.

REFERENCES

[1] L Sanche, *Mass Spectrometry Reviews* **21** (2002) 349 and M A Huels *et al*, *J Am Chem Soc.* **125** (2003) 4467

DEA TO BIOMOLECULES – THE DATA BASE

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Dissociative electron attachment (DEA) to biomolecules in the gas phase reveals a wealth of information. In the course of the VAMDC EU project we present a possible way to build up a data base containing the most important features which can be obtain from experimental DEA studies. In addition we could provide in some cases results from quantum-chemical calculations concerning the structure of molecules and fragments as well as energetics for certain reactions observed in the experiment. DEA experiments are carried out at the Institute of Ion Physics and Applied Physics mainly with two different setups, a double-focusing two sector field instrument (VG ZAB2) [1] and an electron monochromator followed by a quadrupole mass filter or a home build time-of-flight mass spectrometer, respectively [2].

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Despite the language in which the data base should be written, it should contain the following information: a) a list of all negatively charged ions which are detected in our experiments, b) the resonant positions of the electron efficiency curves for all fragments, and c) the records of the ion efficiency curves themselves. It will be important to achieve a proper data retrieval which will allow the user to search for different pieces of information, e.g. all biomolecules which form a certain negative ion or all ions which are formed at a certain range of energy.

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REFERENCES

[1] T. Hamann, A. Edtbauer, F. Ferreira da Silva, S. Denifl, P. Scheier, P. Swiderek, Dissociative electron attachment to gas-phase formamide. *Phys. Chem. Chem. Phys.* 26/**13** (2011) 12305-12313
[2] V. Vizcaino, P. Bartl, D. Gschliesser, S. E. Huber, M. Probst, T. D. Märk, P. Scheier, S. Denifl, Dissociative Electron Attachment to beta-Alanine. *ChemPhysChem* 7/**12** (2011) 1272-1279

ATOMIC AND MOLECULAR DATA FOR DOSIMETRY

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Dosimetry in general aims to quantify the energy deposited by ionizing radiation in matter. Atomic and molecular data are required for computer programs that simulate radiation transport and energy deposition in matter and also for the conversion from measured quantities to the dose quantity of interest (e.g. ionization to air kerma; air kerma to absorbed dose to water). For high-energy photons, neutrons, electrons, protons and alpha particles, extensive data libraries have been compiled (e.g. [1]) and often been cast into easy-access online calculation tools (e.g. [2]).

Advanced approaches such as nanodosimetry aim to complement the absorbed dose by a quantitative descriptor of radiation quality based on particle track structure, i.e. the microscopic pattern of energy deposition. For simulation of track structure as well as for data analysis and uncertainty evaluation of measured parameters of track structure additional atomic and molecular data are needed, such as: (a) cross sections for the interaction of ions at energies below the Bethe regime and their low-energetic secondary electrons with water, DNA constituents and detector operating gases; (b) production rates, reaction rates, life times and diffusion coefficients of radical species; (c) fragmentation probabilities of different DNA constituents after ionization or excitation.

Such experimental or theoretical data should always be reported as absolute values including an appropriate estimate of uncertainty, ideally determined following the ISO guidelines [3]. Interdependencies between data sets from different sources (e.g. for relative measurements converted to absolute values by reference to data of other molecules) should be explicit in the data base. Data sets should be evaluated for consistency using established procedures [4] and the results should be reported as integral part of the information provided. In an online data base, a hierarchical structure would be ideal which provides, at the top level, a calculation tool for an interpolation based on theoretical models whose consistency with the experimental data is established quantitatively. Below this top level, a synopsis of evaluated data would be provided with underlying links to the individual original data sets and their reference.

REFERENCES

[1] D.E. Cullen et al., Lawrence Livermore National Laboratory, UCRL-50400, Vol. 30, October 1991.
[2] M. J. Berger et al., *ESTAR, PSTAR, and ASTAR*, [Online] URL: http://physics.nist.gov/Star.
[3] Joint committee on guidelines in metrology, Report JCGM 100:2008, [Online] URL: http://www.bipm.org/utils/common/documents/jcgm/JCGM_100_2008_E.pdf.
[4] H. G. Paretzke, M. J. Berger, In: J. Booz, H. G. Ebert (eds) Proceedings of the 6th Symposium on Microdosimetry, EUR 6064, Harwood, London, pp 749-758.

Data modeling of theoretical e-molecule scattering properties for Molecular Structure Databases

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High Performance Computing (HPC) applications are currently struggling with an increasing demand of performance in Data Handling infrastructures. To this end, Caspur is at the forefront of the problem by proposing innovative solutions to the outstanding requirements of modern HPC applications. Applications, fueled by the performance of modern many-core systems based on GPU technologies will lack, without a supporting high performance data management, the real possibility to accumulate large data set and, consequently to estimate observables intimately affected by the overall simulating sampling. This aspect is becoming a real bottleneck in many HPC processing workflows in life-science and in particular, in computational science.

In recent years Caspur devoted attention and resources to the building of an innovative tool through which it will be possible both to manage and share very large datasets of molecular data following the whole HPC work-flow of numerical experiments from the beginning (*pre*) to the end (*post*) of the data processing. A similar proposal has to rely on a layered infrastructure and ultimately, has to be based on the best solutions for the geographical access/distribution of data and related services, like those offered by modern service oriented cloud systems. This activity was born within COST:CODECS action, and contributed to the establishment of a on-the-field experience which Caspur is willing to share with the Nano-IBCT community and the VAMD project. Caspur is already involved in the Nano-IBCT activities concerning the interaction of secondary, low energy electrons with biomolecules. Such involvement focused on the use of high-throughput computational tools, recently optimised for the use of GPU platforms, by which the calculation of electron-molecule elastic cross sections and the characterisation of the crucial Transient Negative Ions can be carried out on large molecules with a significant efficiency. The population of the molecular database with structure-dependent data relevant to electron-molecule scattering is the natural continuation of the project.

At the Nano-IBCT database meeting a progress report on the status of the workflow will be presented and the core database architecture explained in full detail. A dataset of about 2000 molecular systems will serve as a test case to show the capabilities of the core driver able to manage, leverage and retrieve large amount of quantum chemical information. Then, a preliminary data model to include e-molecule scattering properties from theoretical calculations into the structural database will be presented together with a comprehensive planning of future activities able to accumulate critical data and optimize the whole workflow on the basis of the Nano-IBCT requirements.

ION BEAM TREATMENT PLANNING AND DATA NEED

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Ion beam therapy is keeping developing in Europe and Japan, thanks to outstanding tumor control results, even if the debate on cost/benefits is still considered an open question. The latter debate, further challenges the exploitation of the capabilities of this therapy through improved treatment planning.

The TRiP98 program, first treatment planning system (TPS) for particles, was developed and used for treating all the 440 patients during the successful GSI pilot project for ion therapy [1], and it is now keeping on developing as a research prototype used in all the centers presently dealing with ion beams for therapy [2]. Among the major directions of present investigation there is the treatment of hypoxic tumors [3, 4] and the possibility to perform a multi-ion treatment [5]. The core of the program is in the optimization of the particle fluences which are delivered to tumor volume elements, matching a prescribed biologically effective dose on the tumor and explicitly imposing the sparing of surrounding organ at risks (OAR).

An overview of the TRiP98 features will be reported, together with an analysis of its present structure, the type of data which are loaded, and on which data there is presently a major need, with a focus on those ones which, directly or indirectly, may be related to nanoscale models and experiments.

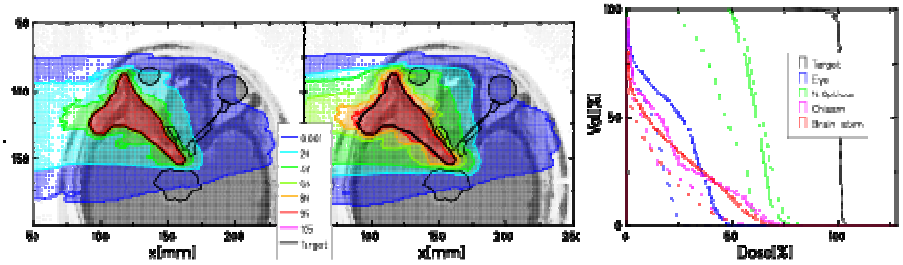

Figure 1: TRiP98 optimized dose distributions considering different radiosensitivity data

REFERENCES

[1] M. Krämer et al., *Phys Med Biol.* **45**, 3319 (2000).
[2] M. Krämer and M. Durante, *Eur. Phys. J. D* 2010 **60**, 195 (2010).
[3] E. Scifoni, M. Krämer and M.Durante, *GSI Sci. Rep.* **2010**, 489 (2011).
[4] E. Scifoni, M. Krämer, W. Tinganelli, W.Kraft-Weyrather and M. Durante, *in prep for Phys Med Biol.*
[5]] M. Krämer, E. Scifoni and M.Durante *GSI Sci. Rep.* **2011** (2012) *submitted.*

COST ACTION NANO-IBCT AND DATA NEEDS FOR MULTISCALE MODELING OF RADIATION DAMAGE AND NANODOSIMETRY

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The talk will introduce the COST Action MP1002 'Nanoscale insights into Ion-Beam Cancer Therapy' (Nano-IBCT) and its main goals.

Ion beam therapy offers the possibility of excellent dose localization for treatment of malignant tumours, minimizing radiation damage in normal tissue, while maximizing cell-killing within the tumour. However, the full potential of such therapy can only be realised by better understanding the physical, chemical and biological mechanisms, on a range of time and space scales, that lead to cell death under ion irradiation [1]. The COST Action MP1002: NANOSCALE INSIGHTS INTO ION BEAM CANCER THERAPY (NANO-IBCT), therefore aims to combine, using a multiscale approach, the unique experimental and theoretical expertise available within Europe to acquire greater insight at the nanoscopic and molecular level into radiation damage induced by ion impact. For more information see http://www.cost.esf.org/domains_actions/mpns/Actions/nano-ibct/) and http://fias.uni-frankfurt.de/nano-ibct/**.**

The basic approaches for multiscale modeling of radiation damage and nanodosimetry effects will be introduced and the needs for the collection of appropriate experimental and theoretical data and their storage in the Nano-IBCT data base will be outlined.

REFERENCES

[1]] A. V. Solov'yov, E. Surdutovich, E. Scifoni, I. Mishustin, and W. Greiner. *Phys. Rev. E* **79**, 011909 (2009).

THE DATABASE FOR X-RAY PHOTON PROCESSES

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The basic damage mechanisms to DNA and other biomacromolecules within the cell have recently been brought into question by new studies of X-ray irradiation of such molecules. Previously radiation damage has been commonly attributed solely to ionisation via direct impact of high-energy quanta or by reactive radicals. However, recently the role of secondary electrons inducing such damage has been explored and it has been shown that the probability of causing strand breaks within the DNA is one to two orders of magnitude larger for electrons than for photons of the same energy. Furthermore, such electron interactions are highly localized being targeted at specific sites within the DNA. Thus radiation damage may be described at an individual molecule level.

These radiation induced physical and chemical processes may be exploited both to understand the risk of exposure to different types of radiation and to explore the pathways with cellular compounds localized in close proximity of DNA (especially the presence of amino acids, lipids and water). However such research requires the collection and curation of databases of fundamental atomic and molecular data, related to experiment and theory, that will help to gain a comprehensive understanding of the key interactions between investigated systems.

Our work to measure binding energies related to many more biologically significant molecules (e.g., intercalants, radiosensitizers) using X-ray Photoelectron Spectroscopy (XPS) is one of what remains a limited number of explorations being pursued internationally and many more experiments are still needed. In this roundtable discussion I will review progress of these experiments and how it is being used to gain a deeper understanding of DNA damage induced by the abundant secondary low energy electrons. The cross correlation between the site damage indicted by XPS and the formation of DNA strand breaks detected via agarose or polyacrylamide gel electrophoresis (AGE or PAGE), high performance liquid chromatography (HPLC) and/or mass spectrometry will also be discussed.

DATA COLLECTION ON PHOTON INTERACTIONS WITH BIOMOLECULES AND NANOPARTICLES

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We discuss various scenarios of interaction between clusters and molecules and lasers of various characteristics both from the experimental and theoretical point of view. The developments of new tools of investigation of properties of emitted electrons, especially energy and angular resolved ones, opens the door to rather detailed descriptions of irradiation scenarios. These data are furthermore rather accessible from the theoretical point of view with currently developed/available theories. This should help disentangle the various dynamical underlying scenarios at work in the course of such irradiation processes.

REFERENCES

Th. Fennel, K.-H. Meiwes-Broer, J. Tiggesbaumker, P.-G. Reinhard, P. M. Dinh, and E. Suraud, Laser-driven nonlinear cluster dynamics : from single- and multiphoton excitations to the strong-field domain, Rev. Mod. Phys. 82 (2010) 1793

DISTRIBUTED SOFTWARE DEVELOPMENT: TOOLS AND PRACTICES

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Distributed development projects (the projects done across many worksites or locations) are becoming the norm for today's software industry. During the last ten years multiple tools and techniques helping to facilitate distributed projects emerged and became popular.

For example, a traditional documentation in form of a solid file covering a certain subject has multiple drawbacks when used as a tool for communication between remote development teams due to the problems with changes tracking and notification. These problems can be solved using a Wiki tool for document control, with additional benefits like a very low cost of change, full document history and a full-text search.

In order to communicate software change requests, bug reports and feature propositions, task trackers are widely used. They provide a centralized storage of categorized change requests which helps to track a project history and to create a project schedule. A typical software project with 10 developers involved accumulates about a thousand small change requests per year.

Other tools are available and widely used; software development groups should carefully build a project infrastructure before starting an actual work.

MULTISCALE APPROACH: A THEORETICAL TOOL FOR UNDERSTANDING RADIATION DAMAGE

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Understanding of fundamental physical processes accompanying propagation of fast heavy ions in biological medium is important, because this knowledge can be utilized in the ion-beam cancer therapy, which is one of the most advanced modern techniques to cure certain type of cancer. The central element of the multiscale approach [1] is the theoretical evaluation and quantification of the DNA damage within cell environment. To achieve this goal one needs a significant amount of data on various atomic and molecular processes involved into the cascade of events starting with the ion entering and propagation in the biological medium and resulting in the DNA damage [2].

In recent years it has been shown that a detailed understanding of these processes is indeed possible due to new advances in the theoretical and experimental tools developed in molecular physics. An impressive example, among others, has been a discovery of a resonant mechanism to be at the origin of the damage carried out by low energy electrons [3], via the occurrence of dissociative electron attachment. This understanding on a quantum mechanical level paved the way to new research on possible low energy damage effects [4]. Thus, the atomic and molecular physics community has become more involved in this field of research and has initiated an increasingly fruitful collaboration with the radiation research community all over the world, especially in Europe.

Novel developments require that the atomic and molecular physics community provides data, such as cross sections, as well as models for understanding of the processes of damage of molecules under various treatment methods and conditions. The newly created database should contain not only the experimental data but also provide the user with theoretical models for applications of the results of experimental measurements.

REFERENCES

[1] A.V. Solov'yov, E. Surdutovich, E. Scifoni, I. Mishustin and W. Greiner *Phys Rev E* **79**, 011909 (2009)
[2] A.V. Yakubovich, E.Surdutovich, A.V. Solov'yov *AIP Conf. Proc*. **1344**, 230 (2011)
[3] B. Boudaiffa, P. Cloutier, D. Hunting and L. Sanche *Science* **287** 1658 (2000)
[4] B. Michael and P. O'Neill, *Science* **287** 1603 (2000)

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