International Conference
"Dynamics of Systems on the Nanoscale"

DySoN Conference 2018

Steigenberger Hotel Sanssouci, Potsdam, Germany
October 08 - 12, 2018

DYSON

Book of Abstracts

Table of Contents

Preface

The Fifth International Conference "Dynamics of Systems on the Nanoscale" (DySoN 2018) will be held in Potsdam, Germany 8th -12th October, 2018 in the Steigenberger Hotel Sanssouci located directly in the historical city centre of Potsdam. The Conference will be preceded on 6th and 7th October by the comprehensive training course on multiscale modelling of Meso-Bio-Nano (MBN) systems molecular structure and dynamics with MBN Explorer and MBN Studio – the powerful and universal software being developed by the MBN Research Center in Frankfurt am Main, Germany.

This DySoN conference has been built upon a series of International Symposia "Atomic Cluster Collisions: structure and dynamics from the nuclear to the biological scale" (ISACC 2003, ISACC 2007, ISACC 2008, ISACC 2009, ISACC 2011, ISACC 2013 and ISACC 2015, see isacc-portal.org). During these meetings it has become clear that there is a need for an interdisciplinary conference covering a broader range of topics than just atomic cluster collisions, related to the Dynamics of Systems on a Nanoscale. Therefore, in 2010 the ISACC International Advisory Committee decided to launch a new conference series under the title "Dynamics of Systems on the Nanoscale". The first DySoN conference took place at the National Research Council, Rome, Italy in 2010, the second conference was held in St. Petersburg, Russia in 2012, the third one was held in Edinburgh, UK in 2014, and the fourth one in Bad Ems, Germany in 2016. DySoN 2018 is the fifth conference in this series.

The dynamics on the nanoscale determines a wealth of physical, chemical and biological processes and applications such as the macroscale properties of materials, the catalytical activity of interfaces and the interaction of radiation with biological systems. However, its exploration and description requires unified experimental and theoretical approaches from different fields across the physical, chemical and biological disciplines. A thorough understanding of these systems allows for an exploitation of novel phenomena on the nanoscale leading to an optimization of existing processes or the exploration of novel applications.

Consequently, the DySoN 2018 Conference will promote the growth and exchange of interdisciplinary scientific information on the structure formation and dynamics of animate and inanimate matter on the nanometre scale. There are many examples of complex many-body systems of micro- and nanometre scale size exhibiting unique features, properties and functions. These systems may have very different nature and origin, e.g. atomic and molecular clusters, nanostructures, ensembles of nanoparticles, nanomaterials, biomolecules, biomolecular and mesoscopic systems. A detailed understanding of the structure and dynamics of these systems on the nanometre scale is a difficult and fundamental task, the solution of which is necessary in numerous applications of nano- and biotechnology, materials science and medicine.

Although mesoscopic, nano- and biomolecular systems differ in their nature and origin, a number of fundamental problems are common to all of them: What are the underlying principles of self-organization and self-assembly of matter at the micro- and nano-scale? Are these principles classical or quantum? How does chemical or biological function emerge at the nano- and the meso-scale in systems with different origins? What criteria govern the stability of these systems? How do their properties change as a function of size and composition? How are their properties altered by their environment? What are the interactions of nanomaterials with biological systems? How can interactions of radiation with chemical and biological systems be exploited to create novel materials or enable novel forms of medical treatment? Seeking answers to these questions is at the core of the interdisciplinary DySoN conference.

We have identified urgent key interdisciplinary topics within the nanosciences that are currently discussed within different communities. These include structure formation on the nanoscale, application of nanoparticles in cancer radiation therapies, nanocatalysis and in general the biomedical applications of radiation. The aim of this conference is to bring experts from these different communities together in order foster interdisciplinary discussions and to initiate novel research directions.

Dyson 2018 Program

Monday, 08th October 2018

12^{00} - 16^{00}	Participants registration
14^{30} - 14^{45}	**DySoN 2018 Opening** **Ilko Bald and Ilia A. Solov'yov**
	Afternoon session I: Low-energy electron and ion induced processes (Chair: I. Bald)
14^{45} - 15^{15}	**Amitava Adhikary**, Oakland University, USA *5-Azido-modified pyrimidine nucleosides: electron mediated formation of p-type aminyl radical and its conversion to s-type iminyl radical*
15^{15} - 15^{45}	**Janina Kopyra**, Siedlce University, Siedlce Poland *Electron driven fragmentation of heterocyclic organic compounds.*
15^{45} - 16^{15}	**Stephan Denifl**, University of Innsbruck, Innsbruck, Austria *Low-energy electron interaction from radiosensitizers: associative vs. dissociative attachment*
16^{15} - 16^{45}	**Coffee break**
	Afternoon session II: Self-organization and radiation-induced structure formation on the nanoscale (Chair: I. Solov'yov)
16^{45} - 17^{10}	**Oddur Ingolfsson**, University of Iceland, Reykjavik, Iceland *Dissociative electron attachment as potential means for cross-linking of self-assembled monolayers*
17^{10} - 17^{35}	**Armin Gölzhäuser**, Bielefeld University, Bielefeld, Germany *Carbon nanomembranes: radiation-induced 2D materials for separation technology*
17^{35} - 18^{00}	**David Field**, Aarhus University, Aarhus, Denmark *The optical absorption spectra of spontaneously electrical solids: The case of nitrous oxide*
18^{00} - 18^{15}	**Shyamal Mondal,** Saha Institute of Nuclear Physics, Kolkata, India *Substrate dependent morphology of size-selected soft-landed clusters*
19^{00} - 21^{00}	**Welcome Reception**

Tuesday, 09th October 2018

	Morning session I: Thermal, optical and magnetic properties of nanosystems (Chair: R. Palmer)
9^{30} - 10^{00}	**Andrey V. Solov'yov**, MBN Research Center, Frankfurt am Main, Germany *Dynamics of Meso-Bio-Nano (MBN) systems as seen from computational approach with MBN Explorer*
10^{00} - 10^{30}	**Florent Calvo**, University Joseph Fourier, Grenoble, France *Interplay between external field and temperature on the structure of magnetic colloidal clusters*

10^{30} - 11^{00}	**Victor I. Balykin**, Institute of Spectroscopy, Troitzk, Russia *Planar plasmonic optics and its applications*
11^{00} - 11^{30}	**Coffee break**
	Morning session II: Nanoscale phase and morphological transitions (Chair: S. Khanna)
11^{30} - 12^{00}	**Richard E Palmer,** Swansea University, Swansea, United Kingdom *Massive scale-up of cluster beam deposition (CBD) for the production of functional nanomaterials*
12^{00} - 12^{30}	**Wolfgang Ernst**, Graz University of Technology, Graz, Austria *Core-shell nanoparticles prepared in superfluid Helium droplets: Structure, phase transition, and alloy formation*
12^{30} - 13^{00}	**Poster introductions**
13^{00} - 14^{30}	**Lunch**
	Afternoon session I: Clusters and biomolecular ensembles, complexes, nanostructured materials (Chair: S. Ptasinska)
14^{30} - 15^{00}	**Michal Fárník,** J. Heyrovský Institute of Physical Chemistry Prague, Czech Republic *Dynamics of processes on nano-ices investigated in molecular-beam experiments: interaction with molecules, UV-photons and electrons*
15^{00} - 15^{30}	**Markus Gühr,** University of Potsdam, Potsdam, Germany *New perspectives on molecular dynamics using ultrafast soft x-ray spectroscopy and electron diffraction*
15^{30} - 15^{45}	**Henrike Müller-Werkmeister,** University of Potsdam, Potsdam, Germany *Direct observation of reaction dynamics in spincrossover systems by ultrafast electron diffraction*
15^{45} - 16^{00}	**Masato Nakamura,** Nihon University, Funabashi, Japan *Metallicity and non-metallicity in mercury clusters*
16^{00} - 19^{00}	**Drinks and poster session**

Wednesday, 10th October 2018

	Morning session I: Irradiation driven transformations of complex molecular systems and biodamage (Chair: D. Field)
9^{30} - 9^{55}	**Sadia Bari**, Deutsches Elektronen-Synchrotron (DESY), Hamburg, Germany *Gas-phase biomolecules studied by mass spectrometry at advanced light sources*
9^{55} – 10^{20}	**Franco A. Gianturco**, University of Innsbruck, Innsbruck, Austria *Chemistry in the cold: ionic reactions in traps and processes in the interstellar environments*
10^{20} - 10^{45}	**Sam Eden,** The Open University Milton Keynes, UK *UV-induced dynamics in DNA bases, nucleosides, and clusters*

10^{45} - 11^{00}	**Behnaz Behmand,** Université Paris-Saclay, Gif-sur-Yvette, France *Ionization of guanine nanostructures by absorption of low-energy UV photons*
11^{00} - 11^{30}	**Coffee break**
	<u>Morning session II: Interaction of radiation with biosystems: mechanisms and applications (T. Schlathölter)</u>
11^{30} - 11^{55}	**Andreas Mauracher**, University of Innsbruck, Innsbruck, Austria *Modelling of short DNA single strands*
11^{55} - 12^{20}	**Sylwia Ptasinska**, University of Notre Dame, Notre Dame, USA *Effects of plasma reactive species on biomolecular systems*
12^{20} - 12^{45}	**Eric Suraud,** Université Paul Sabatier, Toulouse, France *Towards the analysis of attosecond dynamics in complex systems*
12^{45} - 13^{00}	**S. V. K. Kumar,** Tata Institute of Fundamental Research, Mumbai, India *Irradiation of protein cytochrome C by low-energy carbon ions and cobalt 60 gamma rays*
13^{00} - 13^{15}	**Conference photo**
13^{15} - 14^{30}	**Lunch**
	<u>Afternoon Session I: Biomedical applications of radiation (A. Korol)</u>
14^{30} - 15^{00}	**Eugene Surdutovich**, Oakland University, Rochester, USA *Multiscale approach to the physics of ion-beam cancer therapy*
15^{00} - 15^{30}	**<u>Steffen Greilich</u>, Lucas Burigo, Mark Bangert, Oliver Jäkel,** German Cancer Research Center, Heidelberg, Germany *Implementation strategies of RBE modelling in current treatment planning for (proton and) carbon ion beams*
15^{30} - 16^{00}	**Jefferson Shinpaugh**, East Carolina University, Greenville, USA *Experimental and computational study of gold nanoparticles as a radiosensitizer for proton and carbon ion irradiation*
17^{00} - 19^{00}	**Conference tour**

Thursday, 11th October 2018

	<u>Morning session I: Electron & spin transport in molecular systems (F. A. Gianturco)</u>
9^{30} - 10^{00}	**Ulrich Kleinekathöfer,** Jacobs University Bremen, Germany *Environmental effects on charge transport through molecular wires: A multi-scale approach*
10^{00} - 10^{30}	**Daniel Kattnig,** University of Exeter, Exeter, United Kingdom *Magnetosensitivity in three-radical systems*
10^{30} - 11^{00}	**Ilia A. Solov'yov**, University of Southern Denmark, Odense, Denmark *Modeling electron transfers in biological systems: applications and examples*
11^{00} - 11^{30}	**Coffee break**

	Morning session II: Reactivity and nanocatalysis (A. Dorn)
11^{30} - 11^{55}	**Emiliano Cortés**, Imperial College, London, United Kingdom *Plasmon induced chemistry*
11^{55} - 12^{15}	**Robin Schürmann**, University of Potsdam, Potsdam, Germany *Hot-electron transfer induced reactions*
12^{15} - 12^{40}	**Shiv Khanna**, Virginia Commonwealth University, Richmond, USA *Nano-catalysts for cross-coupling reactions, CO oxidation, and breaking polar bonds*
12^{40} - 13^{00}	**Nigel Mason**, The Open University, Milton Keynes, UK *Studies of thin films and ice layers; Applications from Astrochemistry to Nanolithography*
13^{00} - 14^{30}	**Lunch**
	Afternoon Session I: Collision processes, fusion, fission, fragmentation (Chair: J. Shinpaugh)
14^{30} - 14^{55}	**Alexander Dorn**, Max-Planck Institute, Heidelberg, Germany *Hydration dependence of ionization and fragmentation reactions in bio-relevant molecules*
14^{55} - 15^{20}	**Rodolphe Antoine**, Université de Lyon1, Lyon, France *New routes to enhance emission properties of gold nanoclusters*
15^{20} - 15^{45}	**Pablo de Vera**, MBN Research Center, Frankfurt am Main, Germany *Molecular dynamics simulations of ion-induced shock wave effects in biological media*
15^{45} - 16^{00}	**Gerhard Hilgers**, Physikalisch-Technische Bundesanstalt, Braunschweig, Germany *Measurement of correlations between two nanometric volumes in the track structure of 241-Am alpha particles*
16^{00} - 16^{30}	**Coffee break**
	Afternoon session II: Propagation of particles through medium (Chair: A. V. Solov'yov)
16^{30} - 16^{55}	**Andrei Korol**, MBN Research Center, Frankfurt am Main, Germany *Investigation of channeling and crystalline undulators with MBN Explorer*
16^{55} – 17^{20}	**Vincenzo Guidi**, Universita di Ferrara, Ferrara, Italy *Steering of GeV and TeV particles via coherent orientational effects in crystals*
17^{20} – 17^{40}	**Vadim Ivanov**, St. Petersburg Polytechnical University, St. Petersburg, Russia *Channeling and radiation of electrons and positrons in bent and periodically bent diamond crystals*
17^{40} - 18^{00}	**Laura Bandiera**, INFN, Ferrara, Italy *Experimental investigation of the electromagnetic radiation emitted by sub-GeV electrons in a bent crystal*
19^{00} - 22^{00}	**Conference Dinner**

Friday, 12th October 2018

	Morning session I: Biological systems and application of nanoparticles (Chair: N. Mason)
9^{30} - 10^{00}	**Jon Golding**, The Open University, Milton Keynes, United Kingdom *Chemo-radiotherapeutic nanoparticles for cancer radiotherapy*
10^{00} - 10^{30}	**Ilko Bald**, University of Potsdam, Potsdam, Germany *Interaction of single molecules with radiation studied by means of DNA origami platforms*
10^{30} - 10^{45}	**Jamoliddin Razzokov,** University of Antwerp, Antwerp, Belgium *Effect of oxidation on the stability of amyloid protofibril*
10^{45} - 11^{00}	**Ida Friis,** University of Southern Denmark, Odense, Denmark *Activation of the DNA-repair mechanism through NBS1 and MRE11 diffusion*
11^{00} - 11^{30}	**Coffee break**
	Morning session II: Structure and dynamics of clusters, nanoparticles and biomolecules (Chair: E. Surdutovich)
11^{30} - 11^{55}	**Thomas Schlathölter,** University of Groningen, Groningen, The Netherlands *Gas-phase interactions of soft X-rays and MeV ions with G-quadruplex DNA*
11^{55} - 12^{20}	**Alexey Verkhovtsev**, German Cancer Research Center (DKFZ), Heidelberg, Germany *Irradiation induced processes with radiosensitizing nanoparticles*
12^{20} - 12^{45}	**Jaroslav Kocisek**, J. Heyrovský Institute of Physical Chemistry, Prague, Czech Republic *Electron attachment in biomolecular models of increasing complexity*
12^{45} - 13^{00}	**Elena Orlenko,** Peter the Great St.Petersburg Polytechnic University, St. Petersburg, Russia *An effect of the space dimension of electron Fermi-gas upon the spin ordering in clusters and nanoparticles*
13^{00} – 13^{30}	**Final Discussion and Conference Closing**
13^{30} - 14^{30}	**Lunch and Departure**

DySoN-2018 Proceedings: Topical Issue in European Physical Journal D: Dynamics of Systems on the Nanoscale

We have the pleasure to announce that a Topical Issue on “Dynamics of Systems on the Nanoscale” will be launched in the European Physical Journal D: Atomic, Molecular, Optical and Plasma Physics (please see the link of the official announcement). All conference participants are encouraged to submit their novel results to this Topical Issue. The deadline for submission is December 30th 2018. Guest Editors are Prof. Ilko Bald, Prof. Ilia Solov’yov, Prof. Nigel Mason and Prof. Andrey Solov’yov.

Conference Venue and Travel Information

The Conference will be hosted by Steigenberger Hotel Sanssouci, Potsdam, Germany.

Potsdam, located southwest of Berlin, is a former seat of the royal Prussian residence and a UNESCO World Heritage Site with an exquisite garden. The symbol of Potsdam is Sanssouci Palace. Frederick the Great had it built according to his own sketches in the middle of the 18th century and it was soon given the nickname of the 'Prussian Versailles'. The palace is only five minutes' walk from the conference site, the Steigenberger Hotel Sanssouci, an ideal starting point for a tour of Potsdam.

On Wednesday, 10th October, a guided tour through the old town of Potsdam will be offered including a short visit of the planetarium located in Potsdam's Dutch quarter.

You can get to Potsdam by public transport from the airports Berlin-Tegel or Berlin-Schoenefeld (both located about 30 km from Potsdam) or from Berlin Main Station.
From Airport Berlin-Tegel: There are many options by public transport. One option is: Take the Bus 109 to "S-Bahnhof Charlottenburg". From there take the S-Bahn S7 to Potsdam Main Station (about 55 min, Ticket "Berlin ABC"). Taxi fare is about 60 €.
From Airport Berlin-Schönefeld: Take the regional train RB22 departing directly from the airport to Potsdam Main Station (about 50 min, Ticket "Berlin BC"). Taxi fare from the airport is about 60 €.
From Berlin Main Station: Take the regional train RE 1 (25 min) or S-Bahn S7 (40 min) to Potsdam Main Station (Ticket "Berlin ABC").
From Potsdam Main Station: Take the Tram 91, Bus 605 or Bus 606 to "Luisenplatz Süd" (6-8 min, Ticket "Potsdam AB" or ticket Berlin region "C" is also valid within Potsdam). The Hotel Steigenberger can be found towards the north close to the entrance to Park Sanssouci.
Detailed train schedules and tickets can be found at www.bahn.de or www.vbb.de.
Potsdam can be reached by car from the A10 and the A115 Highway.

International Advisory Committee

- A.V. Solov'yov (MBN Research Center, Frankfurt am Main Germany), **Chair**
- C. Bréchignac (Laboratoire Aime Cotton, CNRS, Orsay, France)
- M. Broyer (University of Lyon, Lyon, France)
- J.-P. Connerade (Imperial College London, London, UK)
- F. Gianturco (The University of Innsbruck, Innsbruck, Austria)
- J. Jellinek (Argonne National Laboratory, Argonne, Illinois, USA)
- S. Khanna (Virginia Commonwealth University, Richmond, USA)
- N. Mason (The Open University, Milton Keynes, UK)
- E. Surdutovich (Oakland University, Rochester, MI, USA)

Organizing Committee

- Ilko Bald (University of Potsdam, Potsdam, Germany), **Co-Chair**
- Ilia A. Solov'yov (University of Southern Denmark, Odense, Denmark), **Co-Chair**

Contact Information

Prof. Dr. Ilko Bald
DySoN 2018 Co-chair
Institute of Chemistry
University of Potsdam
Karl-Liebknecht-Str. 24-25
14476 Potsdam, Germany
and
BAM Federal Institute for Materials Research and Testing
Richard-Willstätter Str. 11
12489 Berlin
Tel.: +49-0331- 977-5238
Fax: +49-0331-977-6137
Web: www.uni-potsdam.de/en/osci/research.html
E-mail: bald@uni-potsdam.de

Prof. Dr. Ilia A. Solov'yov
DySoN 2018 Co-chair
Department of Physics, Chemistry and Pharmacy
University of Southern Denmark
Campusvej 55
5230 Odense M, Denmark
Tel.: +45-6550-2532
Fax: +45-6615-8780
Web: www.quantbiolab.com
E-mail: ilia@sdu.dk

DySoN Conference Web Page

Updated information on the conference is available at the following internet address:
http://www.dyson-conference.org

Conference e-mail

dyson.conference@gmail.com

Sponsors

The conference will be held under the auspices of the following sponsors:

- MBN Research Center, Frankfurt am Main, Germany
- University of Potsdam, Potsdam, Germany
- University of Southern Denmark, Odense, Denmark
- Lundbeck Foundation, Copenhagen, Denmark
- Deutsche Forschungsgemeinschaft (DFG)

Overview of Abstracts

Talks

Posters

Talks

Low-energy electron and ion induced processes

Mo-I-1

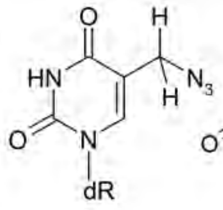
5-AZIDO-MODIFIED PYRIMIDINE NUCLEOSIDES: ELECTRON MEDIATED FORMATION OF π-TYPE AMINYL RADICAL AND ITS CONVERSION TO σ-TYPE IMINYL RADICAL

Zhiwei Wen,[a] Jufang Peng,[a] Paloma Tuttle,[a] Dipra Debnath,[b] Sunny Rishi,[b] Cameron Hanson,[b] Samuel Ward,[b] Yaou Ren,[a] Carol Garcia,[a] Yuan Liu,[a] Yanfeng Liu,[c] Weixi Zhao,[c] Peter M. Glazer,[c] Anil Kumar[b], Michael D. Sevilla,[b] Stanislaw F. Wnuk,[a] and Amitava Adhikary[b]

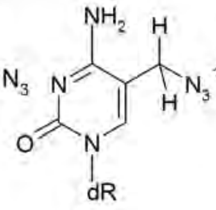
[a]Department of Chemistry and Biochemistry, Florida International University, Miami, Florida 33199, USA
[b]Department of Chemistry, Oakland University, Rochester, Michigan 48309, USA
[c]Department of Therapeutic Radiology, Yale University School of Medicine, New Haven, CT 06520, USA.

The chemically stable 5-azidomethyl-2'-deoxyuridine (5-AmdU, **1**) has been utilized for metabolic labeling of DNA as well as fluorescent imaging of live cells. We have synthesized 5-azidomethyl-2'-deoxycytidine (5-AmdC, **2**). The 5-(1-azidovinyl)-2'-deoxyuridine (5-AvdU, **3**), and 5-(1-azidovinyl)-2'-deoxycytidine (5-AvdC, **4**) has been prepared by the regioselective Ag-catalyzed hydroazidation of the 5-ethynyl substrates with $TMSN_3$. The 5-AmdU **1** was converted to its 5'-triphosphate using Yoshikawa protocol followed by coupling with pyrophosphate. Employing DNA replication and repair polymerases, the 5-AmdU-5-TP was enzymatically incorporated into a variety of DNA strands having random sequence, trinucleotide repeats and telomere sequences. Radiation-mediated pre-hydrated electrons which are formed in homogeneous aqueous glassy (7.5 M LiCl) systems in the absence of oxygen at 77 K, led to site-specific formation of neutral aminyl radical **5** from 5-AmdU. ESR spectrum of the π-type aminyl radical shows a prominent doublet of ca. 91 G resulting from the sum of two β-proton hyperfine couplings arising from the two hydrogens from CH_2 group. Radiation-produced electron-mediated site-specific formation of neutral aminyl radical was observed from 5-AvdU **3**, and from 5-AvdC **4** as well. Our ESR spectral studies and DFT calculations showed that the novel π-type neutral aminyl radicals generated from **1-4** undergo facile conversion to σ-type iminyl radicals (e.g., radical 5 converted to **6**). Our work provides the first evidence of π-type aminyl radical and σ-type iminyl radical formation in a modified nucleoside under a reductive environment. These aminyl and iminyl radicals are known to generate DNA damage via oxidative pathways. Furthermore, we present evidence that these azido-nucleosides can be successfully applied as radiosensitizers in cells under hypoxic conditions.

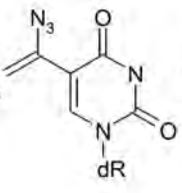
Supported by: NIH NCI R01CA045424; Research Excellence Fund and Center for Biomedical Research at Oakland University



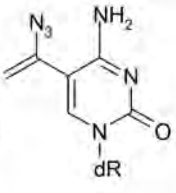
1



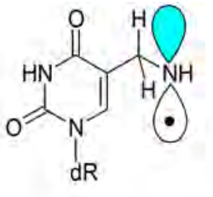
2



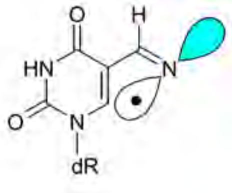
3



4



5



6

ELECTRON DRIVEN FRAGMENTATION OF HETEROCYCLIC ORGANIC COMPOUNDS

Janina Kopyra[1]

[1] Faculty of Sciences, Siedlce University
3 Maja 54, 08-110 Siedlce, Poland
E-mail: kopyra@uph.edu.pl

During the last years investigations of low-energy electron induced damage to biologically relevant molecules have witnessed a remarkable growth. A great effort has been undertaken to explore the intrinsic mechanisms by which such electrons damage biomolecules, e.g., DNA/RNA and their sub-units, amino acids and their agglomerates [1-4].

In the current contribution, the dissociative electron attachment (DEA) to heterocyclic organic compounds consisting of a six-membered ring fused with imidazol ring will be presented and discusses. Such chemical agents are frequently used to mimic the behavior of nucleobases and their metabolic products under reductive conditions. A particular emphasis will be placed on the comparison of the fragmentation patterns of a series of xanthine derivatives. These compounds exhibit an interesting phenomenon in DEA which is based on a site- and bond-selective formation of dehydrogenated parent anions.

REFERENCES
[1] I. Baccarelli, I. Bald, F. A. Gianturco, E. Illenberger, and J. Kopyra, *Phys. Rep.* **508**, 1 (2011).
[2] I. Bald, R. Curic, J. Kopyra, M. Tarana, Dissociative electron attachment to biomolecules. In: Solov'yov, A. (Ed.), Nanoscale Insights Into Ion-Beam Cancer Therapy. Springer, Cham, Switzerland, 159–208 (2017).
[3] L. Sanche, *Eur. Phys. J. D* **35**, 367, 2005 (Review).
[4] J. Kopyra, H. Abdoul-Carime, *J. Chem. Phys.* **132**, 204302 (2010).

LOW-ENERGY ELECTRON INTERACTION FROM RADIOSENSITIZERS: ASSOCIATIVE VS. DISSOCIATIVE ATTACHMENT

S. Denifl[1], R. Meißner[1,2], J. Ameixa[1,2], E. Arthur-Baidoo[1], C. Lochmann[1], L. Feketeova[3], E. Illenberger[1,4], J. Kočišek[5], J. Fedor[5], F. Ferreira da Silva[2], P. Limão-Vieira[2], S. Makurat[6], W. Kozak[6], J. Rak[6]

[1]Institut für Ionenphysik und Angewandte Physik and Center for Molecular Biosciences (CMBI),
Leopold-Franzens Universität Innsbruck, Technikerstraße 25/3, 6020 Innsbruck, Austria
E-mail: Stephan.Denifl@uibk.ac.at
[2]Laboratório de Colisões Atómicas e Moleculares, CEFITEC, Departamento de Física,
Universidade NOVA de Lisboa, Campus de Caparica, 2829-516 Caparica, Portugal
[3]Université de Lyon, Université Claude Bernard Lyon 1, Institut de Physique Nucléaire de Lyon,
CNRS/IN2P3 UMR 5822, 43 Bd du 11 novembre 1918, 69622 Villeurbanne Cedex, France
[4]Institut für Chemie und Biochemie-Physikalische und Theoretische Chemie, Freie Universität
Berlin, Takustrasse 3, 14195 Berlin, Germany
[5]J. Heyrovský Institute of Physical Chemistry v.v.i., The Czech Academy of Sciences, Dolejškova
3, 18223 Prague, Czech Republic
[6]Laboratory of Biological Sensitizers, Physical Chemistry Department, Faculty of Chemistry,
University of Gdańsk, 80-308 Gdańsk, Poland

In the current contribution, we will discuss the formation of negative ions upon electron attachment to the nitroimidazolic radiosensitizers nimorazole and misonidazole as well as the modified nucleobase 5-trifluoromethanesulfonyl-uracil (OTfU). Studies in the gas phase were performed in a crossed electron-molecular beam setup equipped with a high resolution electron monochromator in Innsbruck. In addition, electron attachment to microhydrated nimorazole was studied with the crossed electron-cluster beam setup at the J. Heyrovský Institute of Physical Chemistry in Prague.

Nitroimidazolic molecules are under investigation as potential radiosensitizers for hypoxic tumors, which are characterized by the deprival of oxygen [1]. In Denmark, nimorazole is now considered as a standard compound for the radiotherapy of pharyngeal and supra-glottic carcinoma [1]. Based on *in vitro* studies, misonidazole was suggested to be a more efficient radiosensitizer. However, the dosage of misonidazole in clinical trials was strongly limited due to its neurotoxicity. OTfU is a derivative of uracil with a triflate (OTf) group at the C5-position. This compound was recently synthesized at the University of Gdańsk [2] and was proposed as a possible anticancer agent alternatively to the well-known halouracils.

For all compounds studied, anion efficiency curves for negatively charged (fragment) ions have been measured in the electron energy region below 15 eV. One key observation in the course of the present studies is the high associative electron attachment cross section for the nitroimidazolic compounds in the gas phase, which becomes enhanced in the case of microhydration. In contrast, OTfU predominantly decomposes in the gas phase upon electron attachment into a variety of fragment anions and neutral radicals.

REFERENCES

[1] J. M. Henk, K. Bishop, S. F. Sheperd, *Rad. Onc.* **66**, 65 (2003)
[2] S. Makurat, M. Zdrowowicz, L. Chomicz-Mańka, W. Kozak, I.E. Serdiuk, P. Wityk, A. Kawecka, M. Sosnowska, and J. Rak, *RSC Adv.* **8**, 21378 (2018).

Self-organization and radiation-induced structure formation on the nanoscale

DISSOCIATIVE ELECTRON ATTACHMENT AS POTENTIAL MEANS FOR CROSS-LINKING OF SELF-ASSEMBLED MONOLAYERS

Oddur Ingólfsson[1], Maicol Cipriani[1], Andreas Terfort[3], Sascha Koch[3] and Armin Gölzhäuser[3]

[1]Department of Chemistry and Science Institute, University of Iceland, Dunhagi 3, 107 Reykjavik, Iceland. E-mails: odduring@hi.is and mac31@hi.is
[2]Department of Chemistry, Institute of Inorganic and Analytical Chemistry, Goethe-University, 60438 Frankfurt, Germany. E-mail: aterfort@chemie.uni-frankfurt.de
[3]Physics of Supramolecular Systems and Surfaces, Bielefeld University, 33613 Bielefeld, Germany
E-mails: sascha.koch@uni-bielefeld.de and ag@uni-bielefeld.de

In a recent study by Koch et al. [1] on electron induced cross-linking of self-assembled monolayers (SAMs) from the halogenated biphenyls; 2-X-BPh (X = Cl, Br and I), the cross-linking of SAMs from 2-I-BPh was found to be about 10× more efficient than for the other BPhs.

While these compounds all show similar fragmentation pattern and comparable cross sections for dissociative ionization (DI) through electron impact, the cross section for dissociative electron attachment (DEA) close to 0 eV incident energy is significantly higher for 2-I-BPh, indicating that the higher cross-linking efficiency for this compound is rooted in DEA rather than DI.

DEA is a two-step process [2]; the formation of the transient negative ion (TNI) and its subsequent relaxation through dissociation leading to a negative ion and radical fragment(s):

$$AB + e^- \rightarrow AB^{\#-} \rightarrow A^{(\#)-} + B^{(\#)} \qquad (1)$$

The cross section for the attachment process is inversely proportional to the electron energy close to 0 eV, and thus highest at very low incident energies. And, for single bond rupture (reaction 1), the energy threshold is the bond dissociation energy, BDE(A−B), less the electron affinity of A, $EA(A)$:

$$E_{th}(A^-) = BDE(A-B) - EA(A)$$

This relationship is clearly reflected in the DEA cross sections for the halogenated biphenyls where the thresholds for the formation of X^- and the radical $*C_6H_5\text{-}C_6H_6$ is about 0.54, 0.14 and −0.22 eV for X = Cl, Br and I respectively [3]. Hence, this process is only accessible for 2-I-BPh at 0 eV threshold, where the cross section is the highest, which in turn is reflected in the high cross-linking efficiency of SAMs from this compound.

In this context, we discuss potential means to take advantage of this process to promote the cross-linking efficiency through design of SAMs precursors with enhanced DEA cross sections at very low incident electron energies. Hence, by targeted substitution of suitable SAMs precursors to enhance their electron attachment cross sections and to enable bond ruptures through DEA at very low incident electron energies.

REFERENCES
[1] S. Koch et al. *Beilstein J. Nanotechnol.* 8, 2562 (2017)
[2] I. Bald, J. Langer, P. Tegeder, O. Ingólfsson; *Int. J. Mass Spectrom.* 277, 1–3, 1 (2008)
[3] *NIST Standard Reference Database Num- ber 69 (National Institute of Standards and Technology, National Institute of Standards and Technology, Gaithersburg MD, 20899.*

Acknowledgments: This work was supported by Icelandic Centre for Research (RANNIS) and the University of Iceland Research Fund and conducted within the framework of the COST Action CM1301 (CELINA)

CARBON NANOMEMBRANES: RADIATION-INDUCED 2D MATERIALS FOR SEPARATION TECHNOLOGY

Armin Gölzhäuser

Physics of Supramolecular Systems and Surfaces,
Bielefeld University, 33615 Bielefeld, Germany
E-mail: ag@uni-bielefeld.de

Clean water is a global challenge, and membrane filtration is a key technology to achieve it. There are growing research efforts to explore the use of 2D carbon materials as nanoconduits for molecular transport and separation [1]. Radiation induced chemistry plays a prominent role in these activities as the electron induced modification of molecular surfaces layers is an important step in the fabrication of nanomembranes.

Here, we report on the fabrication and application of carbon nanomembranes (CNMs) with sub-nanometer channels that prove to be excellent water filters, combining a high selectivity with an exceptionally high water permeance. The CNMs are fabricated via the electron induced cross-linking of self-assembled monolayers (SAMs) [2]. CNMs made from terphenylthiol SAMs result in a ~1.2 nm thick membrane perforated by sub-nanometer channels with diameters below ~0.7 nm and areal densities of $\sim 10^{18}$ m^{-2}. When tested as filter membranes, it was found that the CNMs efficiently block the passage of most gases and liquids. However, water passes through with an exceptionally high permeance of $\sim 1.0\times 10^{-4}$ $mol\cdot m^{-2}\cdot s^{-1}\cdot Pa^{-1}$ [3]. This suggests that water fast and cooperatively translocates through a sub-nm channel with a rate of ~66 $molecules\cdot s^{-1}\cdot Pa^{-1}$. As the fabrication of CNMs is scalable, this finding can open new paths towards the use of 2D materials in water purification.

REFERENCES

[1] H.G. Park, Y. Jung: Carbon nanofluidics of rapid water transport for energy applications, *Chem. Soc. Rev.* **2014**, 43 (2), 565-576.

[2] A. Turchanin and A. Gölzhäuser: Carbon Nanomembranes, *Adv. Mater.* **2016,** 28, 6075.

[3] Y. Yang, P. Dementyev, N. Biere, D. Emmrich, P. Stohmann, R. Korzetz, X. Zhang, A. Beyer, S. Koch, D. Anselmetti, A. Gölzhäuser: Rapid Water Permeation Through Carbon Nanomembranes with Sub-Nanometer Channels, *ACS Nano,* **2018**, 12, 4695.

THE OPTICAL ABSORPTION SPECTRA OF SPONTANEOUSLY ELECTRICAL SOLIDS: THE CASE OF NITROUS OXIDE

Rachel James,[a] Anita Dawes,[a] Jérôme Lasne,[b] Andrew Cassidy[c] and David Field[c,d]

[a]School of Physical Sciences, The Open University, Walton Hall, Milton Keynes, MK7 6AA, UK
[b]Laboratoire Interuniversitaire des Systèmes Atmosphériques (LISA), CNRS UMR 7583, Universités Paris-Est Créteil and Paris Diderot, 61 avenue du Général de Gaulle, 94010 Créteil cedex, France
[c]Department of Physics and Astronomy, Aarhus University, Ny Munkegade 120, DL-8000 Aarhus, Denmark
[d]ISA, Centre for Storage Ring Facilities, Department of Physics and Astronomy, Aarhus University, Ny Munkegade 120, DL-8000 Aarhus, Denmark. E-mail dfield@phys.au.dk.

Absorption spectra of films of N_2O, in the range 115-160 nm, will be presented for deposition temperatures between 33K and 64K. Observed shifts in the absorption energy vs deposition temperature are analysed in terms of the temperature-dependent spontaneously electrical ('spontelectric') fields present in the films.[1] Using a simple electrostatic theory, we show (i) that spectra are associated with Wannier-Mott excitons, [2] (ii) that the action of the electric field upon the excitons suffers a blockade at ≤54K for the C-state and ≤52K for the D-state of N_2O, (iii) that the blockade may be attributed to structural defects, which trap the exciton and (iv) that films form with defect-free regions containing 324±3, 168±46 and 95±1 molecules of N_2O at 54K, 52K and 50K respectively. We suggest that films containing these regions represent Ostwald states of the system, precursors to a known phase change at 47K - 48K. Results demonstrate how the spontelectric effect can be used as a tool for exploring the structure of solids, yielding the first experimental indication of the scale size of regular periodicity attendant upon the creation of band structure and an image of the structural changes that take place close to a phase change. These results pose a challenge for chemical modelling which may be addressed using MBN explorer and MBN studio.

REFERENCES

[1] D. Field D, Plekan O, Cassidy AN, Balog R, Jones NC, Dunger J. 2013 *Int. Rev. Phys. Chem.* **32**, 345–392
[2] Chen Y-J, Muñoz Caro G, Aparicio S, Jiménez-Escobar A, Lasne J, Rosu-Finsen A, McCoustra MRS, Cassidy AM, Field D. 2017 *Phys.Rev.Lett.* **119**, 157703-157707

SUBSTRATE DEPENDENT MORPHOLOGY OF SIZE-SELECTED SOFT-LANDED CLUSTERS

Shyamal Mondal[1,2], D. Chowdhury[1,3], S. R. Bhattacharyya[1]

[1]Surface Physics & Material Science Division, Saha Institute of Nuclear Physics,
Sector-1, Block-AF, Bidhan Nagar, Kolkata-700064, India
[2]Department of Physics, Maharaja Manindra Chandra College,
20 Ramkanto Bose Street, 700003, Kolkata, India
[3]ADipartimento di Fisica, University of Genova,
Via Dodecaneso 33 - 16146 Genova, Italy
E-mail: smondal.xray@gmail.com

Amazing size control in supported nanoparticles in pure environment is possible by the controlled deposition of preformed ionized clusters. One of the very important conditions for the control in size after deposition is soft-landing or very low energy deposition (nearly soft-landing). Random movement of clusters as-a-whole or surface-diffusion of clusters is pronounced in such low energy deposition in most of the cluster-substrate combinations [1]. Surface diffusion is the function of cluster-substrate interaction and temperature. Thus it is very interesting fundamentally to investigate the effect of substrates on the final morphology of the supported clusters after room-temperature and elevated-temperature deposition without any substrate treatment. To gain control on the morphological outcome for different cluster-substrate combination is very important for the application perspective too.

Here we report on the morphological property of supported size selected Cu clusters for different cluster-substrate combination. Copper clusters of 3nm diameter produced in a gas aggregation type source [2], based on magnetron sputtering, with very low kinetic energy. As bought substrates of Si, Ge, GaAs, graphite (HOPG), etc., are used for deposition and for morphological characterization SEM and AFM have been employed. In the figure below SEM images are shown.

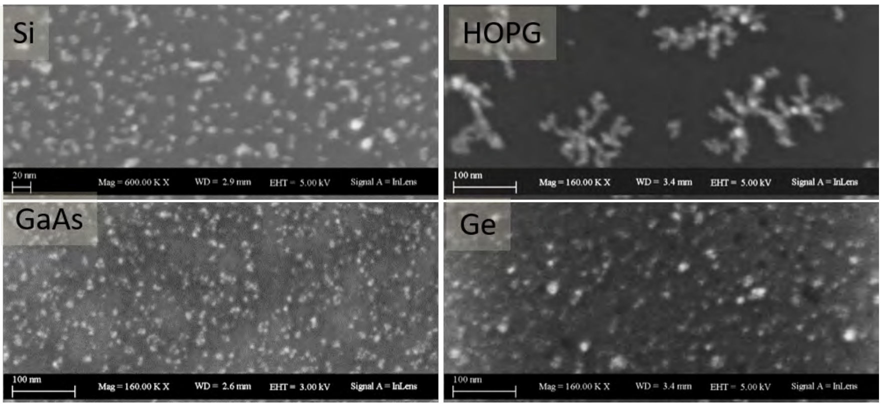


Figure 1: SEM images of cluster assembled films on different substrates.

REFERENCES

[1] P. Jensen, *Rev. Mod. Phys.* **71**, 1695 (1999)
[2] Shyamal Mondal et al, *Rev. Sci. Instrum.* **85**, 065109 (2014)

Thermal, optical and magnetic properties of nanosystems

Tu-I-1

DYNAMICS OF MESO-BIO-NANO (MBN) SYSTEMS AS SEEN FROM COMPUTATIONAL APPROACH WITH MBN EXPLORER

Andrey V. Solov'yov
MBN Research Center, Altenhöferallee 3, 60438 Frankfurt am Main, Germany
E-mail: solovyov@mbnresearch.com

MBN Explorer is a multi-purpose software package developed for advanced multiscale simulations of complex molecular structure and dynamics [1]. It has many unique features and a wide range of applications in Physics, Chemistry, Biology, Material Science, and related industries. A broad variety of algorithms and interatomic potentials are implemented in the program, while its parallelization and computational efficiency allow simulations of the structure and dynamics of very different molecular systems with sizes ranging from atomic to mesoscopic [2]. **Fig. 1** illustrates several fields of application of MBN Explorer. The further information about this can be found on webpages: www.mbnresearch.com/applications, *www.mbnresearch.com/get-mbn-explorer-software* and in the referenced materials [3].

Figure 1. *Different application areas of MBN Explorer.*

Most of the existing codes on Molecular Dynamics (MD) are applicable to a particular class of molecular systems and thus have certain unsurmountable limitations. MBN Explorer overcomes such limitations. The main features of the MBN Explorer such as universality, tuneable force fields, unique algorithmic implementations, multiscale modelling methodologies, modular design and computational efficiency are described in detail on the webpage www.mbnresearch.com/program-features and in the documentation [3], see also www.mbnresearch.com/ bookstore.

MBN Explorer is combined with MBN Studio [1-4] a special multi-task software toolkit with graphical user interface. MBN Studio helps to set up calculations with MBN Explorer, monitoring their progress and examining the calculation results. Such a graphical utility enables the user to visualise selected inputs and outputs. A number of built-in tools allows for the calculation and analysis of specific systems' characteristics. A special modelling plug-in allows the construction of a large variety of molecular systems built of arbitrary atomic and molecular constituents. MBN Studio assists in utilising libraries and databases that provide coordinates and geometries for atomic clusters, nanoparticles, biomolecules, crystals and other MBN systems. The main features of MBN Studio are illustrated in **Fig. 2**.

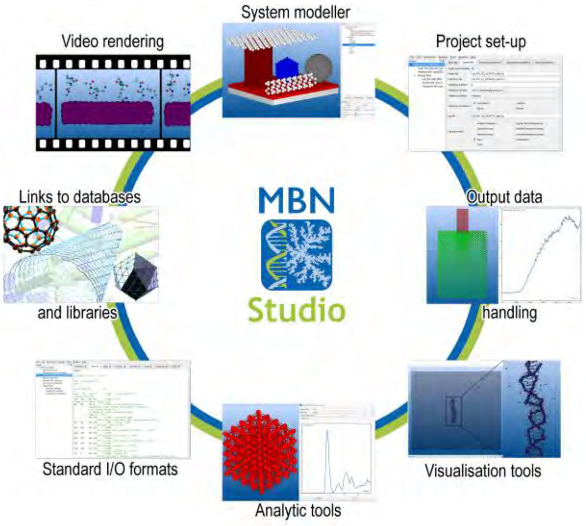


Figure 2. *Main features of MBN Studio.*

Together MBN Explorer & Studio are a powerful and universal instrument of computational research, playing a role of **'virtual microscope and camera'** capable of exploring, simulating, recording and visualising results of multiscale modelling of a large variety of MBN systems.

The talk will give an overview of the main features of the packages and will highlight a number of recent case studies carried out with its use. The selected case studies are in the core of currently running European Research Projects supported within the HORIZON 2020, COST, Marie Skłodowska-Curie, Alexander von Humboldt and other Programmes.

Particular attention will be devoted to the discussion of the multiscale approach towards modelling and the quantitative description of processes occurring in MBN systems on various temporal, spatial and energy scales. Thus, the molecular level assessment of radiation damage in biological targets, being elaborated with the use of MBN Explorer, was designed for the quantitative description of the effects that take place when energetic ions interact with living tissues [5]. A road towards the quantitative understanding physical aspects of ion-beam cancer therapy on the molecular level revealed that this problem has many temporal, spatial, and energy scales, while the main events leading to the cell death happen on a nanometer scale [6]. The multiscale approach allows also to evaluate radio-sensitisation effects caused by metal nanoparticles and other radio-sensitising molecular species [7]. The similar concepts and the computational approach can be also used for important investigations of radiation induced damage in various materials [4].

MBN Explorer and MBN Studio have been utilized for studying the Focused Electron Beam Induced Deposition (FEBID) [8], a very promising direct deposition technique for nanofabrication, for producing free-standing 3D structures of sub-10 nm size. To study the irradiation driven modifications of chemical transformations of complex molecular systems a new molecular dynamics (MD) approach for computer simulations has been suggested [8,9]. The approach is based on the idea that irradiation induced quantum transformations can be treated as random, fast and local processes involving small molecules or molecular fragments. In this way the quantum transformations, such as molecular bond breaks, creation and annihilation of dangling bonds, electronic charge redistributions, changes in molecular topologies, etc, could be incorporated locally into the molecular force fields that describe the classical MD of complex molecular systems under irradiation. The irradiation driven molecular dynamics (IDMD) designed for the molecular level description of the irradiation driven chemistry has been implemented in MBN Explorer [1-3] and successfully applied for the description of the FEBID process [8], as well as in many other irradiation driven and collision processes [2].

There are many other research areas in which MBN Explorer and MBN Studio provide essential molecular and atomistic level insights and computational solutions. A number of such areas and related case studies will be presented at the DySoN 2018 conference, but many more remain intact giving novel topics for investigations that are being conducted by the team of MBN Research Center, www.mbnresearch.com and its partners. You are welcome to join this development!

References

[1] I.A. Solov'yov, A.V. Yakubovich, P.V. Nikolaev, I. Volkovets, and A.V. Solov'yov, J. Comput. Chem., vol. 33, pp. 2412-2439 (2012)

[2] I.A. Solov'yov, A.V. Korol, A.V. Solov'yov, *Multiscale Modeling of Complex Molecular Structure and Dynamics with MBN Explorer*, Springer International Publishing, Cham, Switzerland (2017), 447 p., ISBN: 978-3-319-56085-4, ISBN: 978-3-319-56087-8

[3] I.A. Solov'yov, G.B. Sushko, A.V. Solov'yov, *MBN Explorer Users' Guide: Version 3.0, MesoBioNano Science Publishing*, Germany (2017), ISBN: 978-1-975-63904-4; I.A. Solov'yov, G.B. Sushko, A.V. Verkhovtsev, A.V. Korol, A.V. Solov'yov, *MBN Explorer and MBN Studio Tutorials: Version 3.0*, MesoBioNano Science Publishing, Germany (2017), ISBN: 978-1-976-46092-0

[4] G. Sushko, I.A. Solov'yov, A.V. Solov'yov, www.mbnresearch.com/mbn-studio

[5] E. Surdutovich, A.V. Solov'yov, Eur. Phys. J. D, *Colloquium paper*, **68**, 354-(1-30) (2014); see also *'Nanoscale insights into Ion-Beam Cancer Therapy'*, Editor A.V. Solov'yov, Springer (2016)

[6] E. Surdutovich, A. Yakubovich, A.V. Solov'yov, Sci. Rep. 3, 1289 (2013); A.V. Verkhovtsev, E. Surdutovich, A.V. Solov'yov, Sci. Rep., vol. 6, 27654 (2016)

[7] A.V. Verkhovtsev, A. V. Korol, A.V. Solov'yov, Physical Review Letters, **114,** 063401 (2015);

[8] G.B. Sushko, I.A. Solov'yov, A.V. Solov'yov, Eur. Phys. J. D, vol. 70, 217 (2016)

[9] G.B. Sushko, I.A. Solov'yov, A.V. Verkhovtsev, S.N. Volkov, and A.V. Solov'yov, , Eur. Phys. J. D, vol. 70, 12 (2016)

INTERPLAY BETWEEN EXTERNAL FIELD AND TEMPERATURE ON THE STRUCTURE OF MAGNETIC COLLOIDAL CLUSTERS

Florent Calvo[1], Javier Hernandez-Rojas[2]

[1]LiPhy, CNRS and Université Grenoble Alpes
140 avenue de la Physique, 38402 Saint Martin d'Hères Cedex, France
E-mail: florent.calvo@univ-grenoble-alpes.fr
[2]Departamento de Fisica and IUdEA,
Universidad de La Laguna, 38205 La Laguna, Tenerife, Spain
E-mail: jhrojas@ull.es

Finite sets of nanoscale or mesoscale particles carrying a permanent electric or magnetic dipole moment can self-assemble into a variety of shapes and exhibit collective properties, two features that have attracted much attention in the last decade from both the experimental and computational points of view. At finite temperature, variations in the external field provides some degree of control on the assemblies, and typical motifs of chains, rings, cylinders or branched structures have notably been observed depending on the field magnitude.

In the present contribution, we have developed a simple model to describe clusters of magnetic dipolar spheres with micrometer dimensions, and employed numerical simulations at finite temperature and under external magnetic field to unravel their structure for selected numbers of particles. Our investigation relies on replica-exchange Monte Carlo simulations and an effective potential energy surface that exactly incorporates the fluctuations in external field direction, allowing structural phase diagrams to be delineated in the (temperature,field) plane. The results obtained indicate that both temperature and external field parameters can drastically alter the preferential shape of the colloidal clusters, and through a competition between energetic (ordering) and entropic (disordering) factors do they display compact, elongated, or disordered and fluxional states. The various conformations are connected by multiple first-order-like phase changes, for which a statistical mechanical analysis is presented in terms of the information entropy associated with the inherent structures.

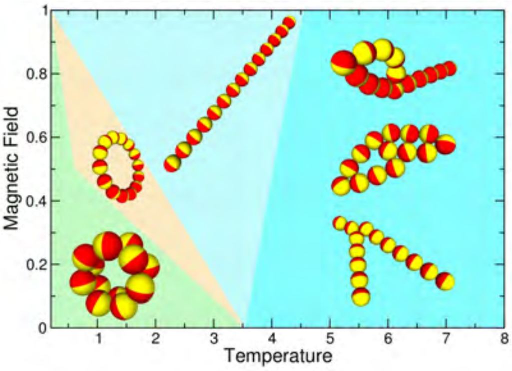


Figure 1: Schematic structural phase diagram in the (temperature,field) plane for the 14-particle colloidal system

REFERENCES
[1] J. Hernandez-Rojas and F. Calvo, *Phys. Rev. E* **97**, 022601 (2018)

PLANAR PLASMONIC OPTICS AND ITS APPLICATIONS

V.I. Balykin

Institute of Spectroscopy, Troitsk, Moscow, Russia

The key advantage of plasmonics is in pushing our control of light down to the nanoscale. It is possible to envision lithographically fabricated plasmonic devices for future quantum information processing or cryptography at the nanoscale in two dimensions. Here we demonstrate the development of the basic elements of planar plasmonic nanooptics: plasmonic optics media, focusing and reflecting plasmonic elements, plasmonic interferometer, plasmonic autocorrelator and planar plasmonic quantum generator.

Nanoscale phase and morphological transitions

MASSIVE SCALE-UP OF CLUSTER BEAM DEPOSITION (CBD) FOR THE PRODUCTION OF FUNCTIONAL NANOMATERIALS

Richard E. Palmer

Nanomaterials Lab
College of Engineering
Swansea University,
Swansea SA1 8EN, UK
Email: R.E.Palmer@swansea.ac.uk

If we imagine a “factory of the future” in which nanoparticle beams are integrated into the production of advanced materials or devices, then a set of critical research challenges emerge for “cluster beam deposition” (CBD). These include control of nanoparticle composition, size, quantity (scale-up), interaction with the support, response to the environment, and performance validation. The prize is a set of applications ranging from water treatment and theranostics to catalysis and memristors. The cluster beam approach is green - it involves no solvents and no effluents; particles can be size-selected; and challenging combinations of metals (nanoalloys) can readily be produced. I will discuss 4 of these research challenges: environment (temperature), scale-up, formulation engineering and performance.

1) **Atomic Structure at High Temperatures** - aberration-corrected Scanning Transmission Electron Microscopy (STEM) is used to investigate, on the atomic scale, the behaviour of deposited clusters in an elevated temperature environment, including structural transformations and (core and surface) melting.

2) **Scale-up** - Industrial catalysis R&D typically requires a gram of catalyst, or 10 mg of clusters at 1% loading on a suitable catalyst support. The “Matrix Assembly Cluster Source” (MACS) is based on ion beam sputtering of a rare gas matrix into which metal atoms are pre-loaded. A scale-up of 5 orders of magnitude in cluster intensity has been achieved to date.

3) **Nanoscale Formulation Engineering** - I will discuss several means by which size-controlled clusters may be presented in a form matching the desired functional application, e.g., catalysis and theranostics. These examples of "formulation engineering on the nanoscale" include direct deposition of metal cluster beams onto powders.

4) **Validation** - Finally I will illustrate the validation challenge to show that cluster-based functional materials are superior to more traditional advanced materials. I will focus on the hydrogenation (both gas and liquid phases) of organic molecules over or applications in the fine chemicals sector and on water splitting.

REFERENCES
For refs see:
https://scholar.google.co.uk/citations?hl=en&user=2pnEX-YAAAAJ&view_op=list_works

Tu-II-2

CORE-SHELL NANOPARTICLES PREPARED IN SUPERFLUID HELIUM DROPLETS: STRUCTURE, PHASE TRANSITIONS, AND ALLOY FORMATION

A. Schiffmann[1],M. Schnedlitz[1], M. Lasserus[1], R. Messner[1], F. Lackner[1], R. Meyer[1], A. W. Hauser[1], D. Knez[2], F. Hofer[2], and W. E. Ernst[1]*

[1]Department of Physics, Graz University of Technology,
Petersgasse 16, 8010 Graz, Austria
E-mail: wolfgang.ernst@tugraz.at
[2]Institute for Electron Microscopy and Nanoanalysis, Graz University of Technology,
Steyrergasse 17, 8010 Graz, Austria

In our labs, superfluid droplets of 10^6 to 10^{10} helium atoms (He_N) are doped with foreign atoms or molecules that can form complexes in this cold environment. In this way, large Cu, Ag, Au, Ni, Pd, and Cr aggregates of different morphology are generated and deposited on solid carbon, BN, or SiN substrates. Employing different pick-up cells for doping the droplets, nanowires of 2 to 5 nm diameter and around 100 nm length, as well as core-shell clusters with one metal surrounding a core of a different species are produced. After surface deposition, the samples are removed and various measurement techniques are applied to characterize the created particles: scanning electron microscopy at atomic resolution, electron tomography [1], temperature dependent SEM and TEM up to 1000 degree C, energy-dispersive x-ray spectroscopy (EDXS), electron energy loss spectroscopy (EELS) and optical absorption. By varying the contents of different metals in core-shell particles, we can tune the plasmon resonance. Furthermore, results of our investigation of the thermal behavior of deposited nanoparticles [2] and the corresponding phase changes on the nanoscale will be reported [3] as well as their chemical reactivity [4].

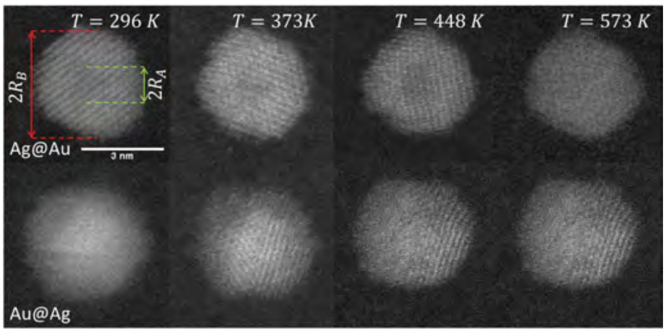


Figure 1: Transmission electron microscopy HAADF scans of a single Ag@Au core@shell cluster as a function of temperature (upper images) and a Au@Ag core@shell cluster scanned at the same temperatures (lower images). With increasing temperature, a softening of the contrast borders between Ag and Au is detected.

REFERENCES

[1] G. Haberfehlner et al., Formation of bimetallic clusters in superfluid helium nanodroplets analyzed by atomic resolution electron tomography, *Nature Communications* **6**, 8779-1-6 (2015).

[2] M. Schnedlitz et al., Thermally induced breakup of metallic nanowires: Experiment and theory, *PhysChemChemPhys* **19**, 9402-9408 (2017).

[3] M. Lasserus et al., Thermally induced alloying processes in a bimetallic system at the nanoscale: AgAu sub-5 nm core-shell particles studied at atomic resolution, *Nanoscale* 10, 2017-2024 (2018), DOI: 10.1039/C7NR07286D .

[4] M. Schnedlitz et al., On the stability of core-shell nanoparticles for catalysis at elevated temperatures: Structural inversion in the Ni-Au system observed at atomic resolution, *ACS Chemistry of Materials* online (2018), DOI: 10.1021/acs.chemmater.7b05075.

Clusters and biomolecular ensembles, complexes, nanostructured materials

Tu-III-1

DYNAMICS OF PROCESSES ON NANO-ICES INVESTIGATED IN MOLECULAR-BEAM EXPERIMENTS: INTERACTION WITH MOLECULES, UV-PHOTONS AND ELECTRONS

M.Fárník, J. Fedor, J. Kočišek, J. Lengyel, A. Pysanenko, K. Grygoryeva, K. Starkbaumová

J. Heyrovský Institute of Physical chemistry, Czech Academy of Sciences,
Dolejškova 3, 18223, Prague 8, Czech Republic
E-mail: michal.farnik@jh-inst.cas.cz

Molecular beams in vacuum, where the molecules can interact with photons, electron or other molecules etc., have long represented the pivotal experimental tool for investigation of molecular reaction dynamics. Clusters add complexity to the studied systems extending them from the gas phase towards bulk. A versatile universal cluster beam apparatus (CLUB) in Prague allows for different experiments with clusters [1]: e.g. deposition of different molecules on large clusters/nanoparticles and observing their reactions triggered by photons and/or electrons of different energies, Figure 1. Such processes can directly mimic in the laboratory the chemistry of aerosols in the atmosphere or astrochemically relevant processes on ices in the space.

We will review several examples of such investigations: (1) pickup and dynamics of molecules on pure argon and water-ice nanoparticles [2]; (2) pickup of atmospheric molecules on small acid nanoparticles [3]. Then the talk will focus on new experiments where different molecules are picked up on the (argon and/or ice) nanoparticles and reactions between them are triggered by UV-photons, fast electrons causing positive ionization or slow electrons leading to the electron attachment and negative ion formation. As an example, the dynamics of reaction between CO and methanol will be discussed, which can be the source of acetic acid CH_3COOH, the second simplest carboxylic acid, detected in the interstellar medium.

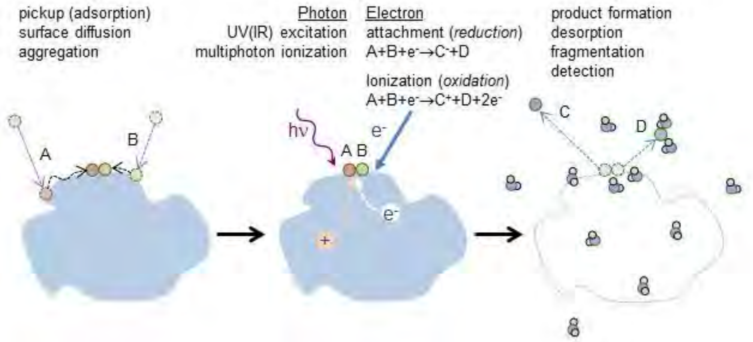


Figure 1: Photon and/or electron triggered chemistry on free nanoparticles.

REFERENCES
[1] M. Fárník and J. Lengyel, *Mass Spec. Rev.* DOI: 10.1002/mas.21554 (2017)
[2] A. Pysanenko et al., *J. Phys. Chem* A **119**, 8991 (2015); P. Rubovič et al., *J. Phys. Chem* A **120**, 4720 (2016); A. Pysanenko et al., *J. Phys. Chem* A **121**, 1069 (2017)
[3] A. Pysanenko et al., *J. Chem. Phys.* **148**, 154301 (2018)

NEW PERSPECTIVES ON MOLECULAR DYNAMICS USING ULTRAFAST SOFT X-RAY SPECTROSCOPY AND ELECTRON DIFFRACTION

Markus Gühr[1,2]

[1]Institut für Physik und Astronomie, Universität Potsdam,
Karl-Liebknecht-Strasse 24/25, 14476, Potsdam, Germany
[2]PULSE, SLAC National Accelerator Laboratory,
Sand Hill Road 2575, 94025, Menlo Park, USA

E-mail: mguehr@uni-potsdam.de

The results were taken by the SLAC UED collaboration and LCLS Nucleobase collaboration (see author lists of publications below).

In this talk, I will present molecular dynamics obtained by diffraction of relativistic electrons exemplified on the rotational and vibrational modes of small model system. The results have been obtained at a new femtosecond ultrafast electron diffraction (UED) source at SLAC. I will point out electron-specific advantages in diffraction of small molecules and discuss future applications on larger molecular systems. So far, we have been able to study rotational wavepackets of nitrogen molecules [1], vibrational wavepackets of iodine molecules [2] as well as dissociation and conical intersection dynamics in CF_3I [3].

In addition, I will present site specific electronic probing of molecular dynamics accomplished by soft x-ray pulses at the oxygen K-edge. We used this scheme to unequivocally observe a molecular intersystem crossing from a $\pi\pi$ state to an $n\pi^*$ state[4]. Combinations of the two techniques for a more complete dynamical description will be discussed.Please, write the title in: Times new roman; bold; capital letters 14 dot. Insert two additional blank lines before the title. Underline the name of the author, who will present the work and give the full contact address as well as e-mail. Please center title, authors and address.

REFERENCES
[1] Yang, J.; Guehr, M.; Vecchione, T.; Robinson, M. S.; Li, R.; Hartmann, N.; Shen, X.; Coffee, R.; Corbett, J.; Fry, A.; Gaffney, K.; Gorkhover, T.; Hast, C.; Jobe, K.; Makasyuk, I.; Reid, A.; Robinson, J.; Vetter, S.; Wang, F.; Weathersby, S.; Yoneda, C.; Centurion, M.; Wang, X. *Nature Communications* **2016**, *7*, 11232.
[2] Yang, J.; Guehr, M.; Shen, X.; Li, R.; Vecchione, T.; Coffee, R.; Corbett, J.; Fry, A.; Hartmann, N.; Hast, C.; Hegazy, K.; Jobe, K.; Makasyuk, I.; Robinson, J.; Robinson, M. S.; Vetter, S.; Weathersby, S.; Yoneda, C.; Wang, X.; Centurion, M. *Physical Review Letters* **2016**, *117*, 173002.
[3] Yang, J.; Zhu, X. L.; Wolf, T. J. A.; Li, Z.; Nunes, J. P. F.; Coffee, R.; Cryan, J. P.; Gühr, M.; Hegazy, K.; Heinz, T. F.; Jobe, K.; Li, R. K.; Shen, X. Z.; Veccione, T.; Weathersby, S.; Wilkin, K. J.; Yoneda, C.; Zheng, Q.; Martinez, T. J.; Centurion, M.; Wang, X. J., *Science* **2018**, *361*, 64-67.
[4] Wolf, T. J. A.; Myhre, R. H.; Cryan, J. P.; Coriani, S.; Squibb, R. J.; Battistoni, A.; Berrah, N.; Bostedt, C.; Bucksbaum, P.; Coslovich, G.; Feifel, R.; Gaffney, K. J.; Grilj, J.; Martinez, T. J.; Miyabe, S.; Moeller, S. P.; Mucke, M.; Natan, A.; Obaid, R.; Osipov, T.; Plekan, O.; Wang, S.; Koch, H.; Gühr, *Nature Communications* **2017**, *8*.

DIRECT OBSERVATION OF REACTION DYNAMICS IN A SPIN-CROSSOVER SYSTEM BY FEMTOSECOND ELECTRON DIFFRACTION

Henrike M. Müller-Werkmeister[1,2*], Yifeng Jiang[1,3], Lai Chung Liu[3], R. J. Dwayne Miller[1,3]

[1] Max Planck Institute for the Structure and Dynamics of Matter,
Luruper Chaussee 149, 22607 Hamburg, Germany
[2] Institute of Chemistry, Physical Chemistry, University of Potsdam,
Karl-Liebknecht-Str. 24-25, 14476 Potsdam, Germany
[3] Departments of Chemistry and Physics, University of Toronto,
80 St. George Street, Toronto M5S 3H6, Canada
*Email: henrike.muellerwerkmeister@uni-potsdam.de

Femtosecond electron diffraction (FED) is a sensitive tool to directly study molecular dynamics in structural detail. Here, we present recent results focused on the direct observation of reaction dynamics on the ultrafast timescale. All experiments have been performed in a 95 keV DC-RF hybrid FED setup [1] to allow for the best temporal and spatial resolution.

The investigated phenomenon is photoinduced spin crossover (SCO). We have studied the structural dynamics in the coordination compound $[FeII(PM\text{-}AzA)_2](NCS)_2$ (or AZA) in single crystalline form using FED to investigate the transient structural changes associated with this spin transition [2]. The unique capability of FED allows us to directly probe atomic motions and to track ultrafast structural changes within the crystal lattice of AZA. By monitoring the time-dependent changes of the Bragg reflections, we observed the formation of a photoinduced structure similar to the thermally induced high spin state. The data and refinement calculations indicate the global structural reorganization within 2.3 ps, as the metal–ligand bond distribution narrows during intramolecular vibrational energy redistribution (IVR), driving the molecular rearrangement. Three independent dynamical groups are identified to model the structural dynamics upon photoinduced SCO.

REFERENCES

[1] M. Gao, C. Lu, H. Jean-Ruel, L. Liu, A. Marx, K. Onda, S. Koshihara, Y. Nakano, X. Shao, T. Hiramatsu, G. Saito, H. Yamochi, R. R. Cooney, G. Moriena, G. Sciaini, and R. J. D. Miller, Nature **496**, 343 (2013).

[3] Y. Jiang, L. Liu, H. M. Müller-Werkmeister, C. Lu, D. Zhang, R. L. Field, A. Sarracini, G. Moriena, E. Collet, and R. J. D. Miller, Angew. Chemie **129**, 7236 (2017).

METALLICITY AND NON-METALLICTY IN MERCURY CLUSTERS

Masato Nakamura[1], René-Jean Tarento[2]

[1]College of Science and Technology, Nihon University
Narashinodai, Funabashi, 274-8501, Japan
E-mail:mooming@phys.ge.cst.nihon-u.ac.jp
[2]Laboratoire de Physique des Solides, *CNRS UMR 8502*
Université Paris-Sud, Université *de Paris-Saclay*
F91405, Orsay, France
E-mail: tarento@lps.u-psud.fr

A mercury atom has electronically shell closing structure like rare gas atoms. Thus, the bonding in a small mercury cluster is due to van der Waals interactions. As the cluster size increases, metallic bonds are formed in the cluster. This metal non-metal transition has been extensively studied through the measurements on ionization potential, band gaps, or plasmon oscillation [1].

Here we shed light on the mechanism of the transition through the dynamic process of clusters. An experimental study on the fragmentation of multiply charged mercury clusters was performed by a group at Osaka University [2]. It was reported that nearly symmetric fragmentation was main decay process in the fragmentation of doubly charged clusters while strongly asymmetric fragmentation for triply charged clusters. We calculate the energy barrier for various decay channels with the liquid drop model [3]. Experimental finding can be clearly explained in terms of the energy barrier. The energy barrier takes the minimum value for nearly symmetric (strongly asymmetric) fragmentation for doubly (triply) charged clusters [4]. The appearance sizes, the minimum size at which a multiply charged cluster becomes stable, were measured. It is shown that that the energy barrier for fission and the monomer evaporation energy take nearly the same value at the size. As a result of these analyses, small mercury clusters behave as van der Waals clusters in the dynamics of fragmentation.

On the other hand, large mercury clusters show metallic property. The electronic shell effects are often observed in metallic clusters. When the cluster size increases as much as 10^3, the shell structure bunches and the supershell structure [5] is formed. The suppershell effect has been observed in the mass abundance spectrum of large mercury clusters [6].

REFERENCES

[1] H. Haberland et al., J. Chem. Soc. Faraday Transaction 86, 2473 (1990)
[2] Sato et al., *J. Mass. Spectrom. Jpn.* 51, 393 (2003)
[3] O. Echt et al., *Phys. Rev. A* 38, 3236 (1988)
[4] M. Nakamura and R.-J. Tarento, *J. Chem. Phys.,* **148**, 084312 (2018)
[5] H. Nishioka, K. Hansen, and B. R. Mottelsen, Phys. Rev. B **42**, 9377 (1990).
[6] H. Itoh et al. *Phys. Rev. B* 48, 4741 (1993)

Irradiation driven transformations of complex molecular systems and biodamage

GAS-PHASE BIOMOLECULES STUDIED BY MASS SPECTROMETRY AT ADVANCED LIGHT SOURCES

Sadia Bari[1]

[1]Deutsches Elektronen-Synchrotron DESY
Notkestr. 85, 22607, Hamburg, Germany
E-mail: sadia.bari@desy.de

Investigating the interaction of light with biologically relevant molecules has gained interest for a wide variety of research fields including photochemical reactions such as light harvesting as well as radiation damage in proteins and DNA related to cutting-edge cancer treatment techniques. However, in the condensed phase, disentangling direct and indirect radiation effects is often difficult. Electrospray ionization introduces biomolecular ions from solution into the gas phase, allowing for studies of molecular systems in a well-defined state.

The coupling of electrospray ionization sources with synchrotrons [1,2] and free-electron lasers [3] opens the way to the investigation of the electronic structure of biomolecular systems and of a fine description of their relaxation mechanisms in the VUV and soft X-ray energy range. The wide-ranging photon energy available at the synchrotrons enables systematic studies of ionization and dissociation as a function of the photon energy. Inner-shell excitations provide a localized site of energy deposition. The extremely high photon flux and fs pulse duration offered by free-electron lasers allow studying the molecular properties in intense fields. Furthermore, using the assets of free-electron lasers in a pump-probe scheme enables the study of the dynamics of charge migration and charge transfer within gas-phase biomolecules.

Results will be presented of mass-spectrometric experiments at advanced light sources with different gas-phase biomolecules, e.g. proteins [4] and oligonucleotides.

REFERENCES

[1] S. Bari et al., *J. Chem. Phys* **134**, 024314 (2011)
[2] A. Milosavljević et al., *J. Phys. Chem. Lett.* **3**, 1191 (2012)
[3] T. Schlathölter et al., *Angew. Chem. Int. Ed. Engl.* **128**, 10899 (2016)
[4] S. Bari et al., *Chem. Eur. J.* **24**, 7631 (2018)

CHEMISTRY IN THE COLD: IONIC REACTIONS IN TRAPS AND PROCESSES IN THE INTERSTELLAR ENVIRONMENTS

Franco A. Gianturco

Institute of Ion Physics, University of Innsbruck, Innsbruck, Austria

Ion traps are the core technology utilized to confine charged particles over a long period of time, allowing further application of different cooling techniques [1,2] and the manipulation of single molecules on the quantum level. The well-established technique of buffer-gas cooling is one of the chief methods that has led to the production of translationally as well as internally cold molecular ions to the few kelvin range.

Experiments attempting to reach these temperatures by buffer gas cooling have found that although the molecular motion and rotation are quickly cooled to the cryogenic temperature, in some cases the molecular vibration relaxes at impractically long timescales.

For this kind of problems theory can provide important information to overcome some of the experimental limitations and to explain the behavior of specific systems. Modeling the molecular de-excitation under physical conditions of ion traps by accurate quantum calculations has helped to identify a specific class of systems that exhibit efficient ro-vibrational cooling [3,4]. At present, cold molecular ions are at the center international research because its applications go beyond the study of chemical reactions; they are also important in fundamental precision measurements [5] and quantum information processing [6].

In this talk I shall endeavour to show that highly sophisticated experimental results in cold ion traps under the above conditions can be explained and modelled very accurately by combining high-level structural calculations of the interaction forces and quantum dynamical methods to describe the collisional energy exchanges [7-9].

REFERENCES

[1] Roland Wester. Phys. Chem. Chem. Phys., 16:396{405, 2014.

[2] S. Trippel, M. Stei, J. A. Cox, and R. Wester. Phys. Rev. Lett., 110:163201, 2013

[3] M. Tacconi, F. A. Gianturco, E. Yurtsever, and D. Caruso. Phys. Rev. A, 84:013412, 2011.

[4] Roland Wester. J. Phys. B, 42:154001, 2009

[5] J. Biesheuvel, J.-P. Karr, L. Hilico, K. S. E. Eikema, W. Ubachs, and J. C. J. Koelemeij. Nature Communications, 7:10385, 2016.

[6] A. Andre, D. DeMille, J. M. Doyle, M. D. Lukin, S. E. Maxwell, P. Rabl, Schoelkopf R. J., and Zoller P. Nat Phys, 2:636, 2006.

[7] P. F. Staanum, P. S. Skyt, A. K. Hansen, and M. Drewsen. Nat Phys, 6:271, 2010.

[8] D. Hauser, S. Lee, F. Carelli, S. Spieler, O. Lakhmanskaya, E. S. Endres, S. S. Kumar, F. Gianturco, and R. Wester. Nature Physics, 11:467,470, 2015.

[9] M. Hernandez-Vera, F. A. Gianturco, R. Wester, H. da Silva Jr, O. Dulieu, S. Schiller, J.Chem.Phys.(in press).

UV-INDUCED DYNAMICS IN DNA BASES, NUCLEOSIDES, AND CLUSTERS

J. Bocková[1], A. Rebelo[1,2], D. Mészáros[3], T. da Fonseca Cunha[1,2], P. Limão-Vieira[2], P. Papp[3], V. Vizcaino[4], J. C. Poully[4], S. Eden[1]

[1] School of Physical Sciences, The Open University, Walton Hall, Milton Keynes, MK7 6AA, UK
[2] Laboratório de Colisões Atómicas e Moleculares, CEFITEC, Departamento de Física, FCT - Universidade NOVA de Lisboa, P-2829-516 Caparica, Portugal
[3] Department of Experimental Physics, Faculty of Mathematics Physics & Informatics, Comenius University, Bratislava 84248, Slovakia
[4] CIMAP/GANIL, Boulevard Henri Becquerel, BP 5133, 14070 Caen Cedex 5, France
E-mail: s.p.eden@open.ac.uk

Radiation induced processes in biomolecules have been investigated intensively recently, notably to better understand the fundamental processes that can initiate lesions in key macromolecules [1]. This talk focuses on how comparing fragment ion production by electron impact ionization (EII) and UV multi-photon ionization (MPI) of biological building blocks such as nucleobases can provide evidence for structural changes (tautomeric transitions, isomeric transitions, and / or dissociation) in neutral electronic excited states. While studies of isolated molecules generally provide the clearest mechanistic interpretations, equivalent measurements on clusters enable closer analogies to be drawn with biological environments where different unimolecular or intermolecular reactive pathways can be significant. Studying the radiation response of sequentially more complex biomolecules in the gas phase provides a complementary route towards biologically-relevant systems. As a case study of scaling complexity, I will discuss ring opening in neutral electronically excited uracil in the gas phase [2], in various clusters [3], and in its RNA nucleoside uridine (brought into the gas phase using the *laser thermal desorption* method [4] developed at Queen's University Belfast). Finally, I will report on the development of experiments at the OU to analyze low-energy electron interactions with Stark-selected neutral isomers and clusters.

REFERENCES
[1] K. Kleinermanns, D. Nachtigallová, M. S. De Vries, Int. Rev. Phys. Chem. **32**, 308 (2013)
[2] B. Barc, M. Ryszka, J. Spurrell, M. Dampc, P. Limão-Vieira, R. Parajuli, N. J. Mason, S. Eden, J. Chem. Phys. **139**, 244311 (2013)
[3] M. Ryszka, R. Pandey, C. Rizk, J. Tabet, B. Barc, M. Dampc, N. J. Mason, S. Eden, Int. J. Mass Spectrom. **396**, 48 (2016)
[4] O. Ghafur, S. Crane, M. Ryszka, J. Bockova, A. Rebelo, L. Saalbach, S. De Camillis, J. Greenwood, S. Eden, D. Townsend, J. Chem. Phys. **149**, 034301 (2018)

We-I-4

IONIZATION OF GUANINE NANOSTRUCTURES BY ABSORPTION OF LOW ENERGY UV PHOTONS

Behnaz Behmand, Akos Banyasz, Lara Martinez-Fernandez, Gérard Baldacchino, Dimitra Markovitsi

LIDYL, CEA, CNRS, Université Paris-Saclay, F-91191 Gif-sur-Yvette, France
E-mail: behnaz.behmand@cea.fr

Guanine rich DNA strands have the ability to form four-stranded structures (G-quadruplexes) whose building blocks are guanine tetrads. In addition to their key role in biological functions, G-quadruplexes are studied as targets for anti-cancer therapy as well as for their potential applications in nanotechnology. During the past decade, our group carries out a systematic study of the photophysical and photochemical processes occurring following photon absorption by these nanostructures [1].

Here, we focus on tetramolecular G-quadruplexes formed by association of four DNA single strands TGGGGT. Using nanosecond transient absorption with low intensity excitation at 266 nm, we study the primary species, ejected electrons and guanine radicals, resulting from photo-ionization.

We found that the quantum yield for one photon ionization is $\phi = (4.5 \pm 0.6) \times 10^{-3}$. This value is similar to that determined previously for G-quadruplexes formed by the human telomeric sequence [2]. Under the same experimental conditions, the monomeric constituents TMP and dGMP do not undergo one photon ionization of ($\phi < 0.5 \times 10^{-4}$). This means that the specific organization of guanines in four-stranded structures rules their propensity to undergo oxidation by photons whose energy is at least 2.7 eV lower than the ionization potential of the bases.

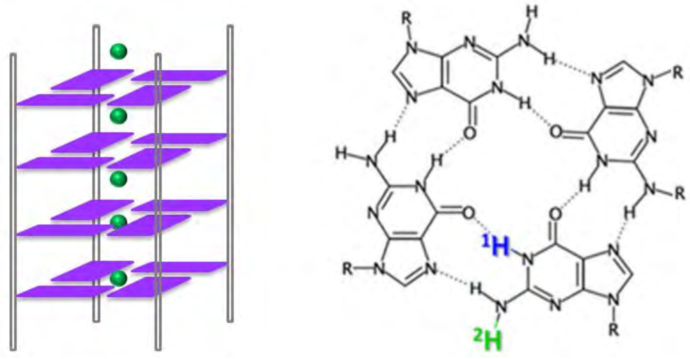


Figure 1: Schematic representation of the studies G-quadruplexes and the guanine tetrads.

The transient absorption spectra recorded after the decay of hydrated electrons, are identified as guanine radicals. At 3 μs, their concentration is equal to that of ejected electrons. We distinguish three types of radicals: (i) radical cations decaying on the μs time scale, (ii) deprotonated radicals $(G\text{-}H_2)^\bullet$ in which a proton at position 2 is missing, which decay within a few ms, and (ii) deprotonated radicals $(G\text{-}H_1)^\bullet$ in which a proton at position H_1 is missing. The latter are the longest lived species.

The nature of the metal ion present in the central cavity does not affect the propensity of electron detachment from these nanostructures. In contrast, it does play a role in the reaction dynamics of the generated radicals, as observed for the dynamics of electronic excited states [3]. In particular, in the presence of K^+, $(G\text{-}H_2)$ radicals survive longer than in the presence of Na^+.

REFERENCES
[1] P. Changenet-Barret, Y. Hua, D. Markovitsi, *Top. Curr. Chem.* **356**, 183 (2015)
[2] A. Banyasz, L. Martinez-Fernandez, C. Balty, M. Perron, T. Douki, R. Improta, D. Markovitsi, *J. Am. Chem. Soc.* **139**, 10561 (2017)
[3] Y. Hua, P. Changenet-Barret, R. Improta, I. Vayá, T. Gustavsson, A. B. Kotlyar, D. Zikich, P. Šket, J. Plavec, D. Markovitsi, *J. Phys. Chem. C.* **116**, 14682 (2012)

Interaction of radiation with biosystems: mechanisms and applications

MODELLING OF SHORT DNA SINGLE STRANDS

Andreas Mauracher, Stefan E. Huber

Institute of Ion Physics and Applied Physics, University of Innsbruck
Technikerstraße 25/3, 6020 Innsbruck, Austria
E-mail: andreas.mauracher@uibk.ac.at

Radiation therapy is among the most commonly applied modalities against tumours next to chemotherapy and surgery [1]. To increase the effect of the radiation, certain therapeutic agents, i.e. radiosensitizers, are applied in combined chemoradiotherapy [2]. A review on damage of DNA labelled with electrophilic nucleobases induced by ionizing radiation summarizes the most important factors deciding about radiation damage as (i) electron affinity of the modified nucleoside, (ii) local surroundings of the label and (iii) strength of the chemical bonding between substituent and nucleobase [3]. Furthermore, radiosensitivity is also assumed to be related to hydration as well as secondary organic radicals in the cell environment [4].

For a detailed understanding of the fundamental processes governing radiosensitivity, results from both experimental studies and theoretical investigations need to be combined. From a computational point of view, the choice of an appropriate theoretical model is often a tedious task not least because of the general difficulty of finding a reasonable balance of accuracy and computational expenses. In particular, in the framework of radiation effects on DNA, this is further complicated by the intrinsic complexity of the biological systems of interest. This contribution aims at giving an overview of selected difficulties in this context but also of resultant opportunities for possible methodological improvements as well as a better understanding of radiation induced DNA damage in general.

REFERENCES

[1] M. Joiner, A. van der Kogel, Eds. Basic Clinical Radiobiology, Hodder Arnold: London, 2009. ISBN 978-0-340-92966-7

[2] G. D. Wilson, S. M. Bentzen, P. M. Harari, Semin. Radiat. Oncol. 16 (2006) 2. DOI: 10.1016/j.semradonc.2005.08.001

[3] J. Rak, L. chomicz, J. Wiczk, K. Westphal, M. Zdrowowicz, P. Wityk, M. Zyndul, S. Makurat, L. Golon, Mechanisms of Damage to DNA Labeled with Electrophilic Nucleobases Induced by Ionizing or UV Radiation. J. Chem Phys. B 119 (2015) 8227.

[4] M. Zdrowowicz, L. Chomicz, J. Miloch, J. Wiczk, J. Rak, G. Kciuk, K. Bobrowski, Reactivity Pattern of Bromonucleosides Induced by 2-Hydroxypropyl Radicals: Photochemical, Radiation Chemical, and Computational Studies, J. Phys. Chem. B 119 (2015) 6545-6554. DOI: 10.1021/acs.jpcb.5b01904

EFFECTS OF PLASMA REACTIVE SPECIES ON BIOMOLECULAR SYSTEMS

Ek R. Adhikari[1,2], Xu Han[1,2], James Kapaldo[1,2], Vladimir Samara[1], Kemo B.S. Jammeh[1,3], Sylwia Ptasinska[1,2]

[1]Radiation Laboratory, University of Notre Dame,
Notre Dame, Indiana 46556, USA
[2]Department of Physics, University of Notre Dame,
Notre Dame, Indiana 46556, USA
[3]Berea College,
Berea, Kentucky 40404, USA
Notre Dame, Indiana 46556, USA
E-mail: sptasins@nd.edu

An atmospheric pressure plasma is a unique non-equilibrium system that has electron temperatures of a few to 10 eV that is relatively high in comparison to ion and gas temperatures, which are typically close to room temperature. Because the fractional ionization (less than a few percent) of this type of plasma, a distinctive set of conditions can be obtained, in which plasma treatment benefits from chemical interactions, rather than the energetics of plasma components. These chemical interactions are induced due to plasma species; i.e., photons, electrons, ions, radicals, excited neutrals, and electric and magnetic fields and due to their synergistic effects.

To date, research, particularly focused on biological effects, including DNA damage, impairment of cell substructures and cell death caused by plasma species, has been performed using atmospheric pressure plasmas [1]. Specifically, recent findings showed that cancer cells are more susceptible to damage by the reactive species than normal cells subjected to plasma exposure. This outcome of cell responses to plasma treatment has inspired the potential application of plasma as an effective and safe tool for novel cancer therapy. Despite the rapid growth of this field, the development of plasma-based cancer therapy is still far from the stage of clinical trials around the world. The key hurdle is the lack of fundamental and comprehensive knowledge of processes in which plasma interacts with biomolecular systems.

Therefore, understanding of the physical, chemical, and biological mechanisms that underlie plasma-biomolecule interactions, which ultimately will lead to plasma cancer therapy, is essential. To obtain this goal, one of the research directions is to qualify and quantify plasma reactive species which allow for obtaining detailed mechanisms of their effects.

Our recent investigations focused on effects of plasma reactive species on DNA [2-4] and cell [5-6] using an atmospheric pressure plasma source under different experimental conditions. In addition, we used a variety of spectroscopic techniques to detect plasma reactive species in the atmospheric pressure plasma as well in plasma treated targets [7]. At the meeting, the most thrilling results and conclusions will be reported as well as remaining challenges and open questions will be addressed.

REFERENCES

[1] K. P. Arjunan, V. K. Sharma, S. Ptasinska, *International Journal of Molecular Sciences* **16**, 2971-3016 (2015)

[2] X. Han, W. A. Cantrell, E. E. Escobar, S. Ptasinska, *European Physical Journal D* **68**, 46 (2014)
[3] E. R. Adhikari, S. Ptasinska, *European Physical Journal D* **70**, 180 (2016)
[4] E. R. Adhikari, V. Samara, S. Ptasinska, *Journal of Physics D: Applied Physics* **51**, 185202 (2018)
[5] X. Han, M. Klas, Y. Liu, S. M. Stack, S. Ptasinska, *Applied Physics Letters* **102**, 233703 (2013)
[6] K. P. Arjunan, A. Obrusník, B.T. Jones, L. Zajíčková, S. Ptasinska, *Plasma Processes and Polymers* **13**, 1087-1103, (2016)
[7] E. R. Adhikari, V. Samara, S. Ptasinska, *Biological Chemistry* (2018) doi: 10.1515/hsz-2018-0203

TOWARDS THE ANALYSIS OF ATTOSECOND DYNAMICS IN COMPLEX SYSTEMS

P. M. Dinh[1], P. G. Reinhard[2], E. Suraud[1;3]

[1]Laboratoire de Physique Théorique, UMR 5152, Université Paul Sabatier, 118 route de Narbonne, F-31062 Toulouse Cedex, France
2Institut für Theoretische Physik, Universität Erlangen Staudtstr. 7, D-91058 Erlangen, Germany
3School of Chemistry and Chemical Engineering, Queen's University Belfast, Belfast BT7 1NN, United Kingdom

The progress in laser technology over the last decades has opened up new avenues for the exploration of properties of clusters and molecules. A laser pulse is characterized by its frequency but also by the laser intensity as well as the laser time profile. While for years the variations of these parameters were heavily constrained by technology, the last two decades and even more so the last years have seen tremendous increases in the range of attainable parameters. This is true for intensity, which since the 1990's can reach huge values which can lead to very large energy deposits and possibly violent disintegration of the irradiated species. But this is also true for the tuning of the time profile which can now be tailored up to time scales of the order of magnitude of electronic motion and even below. This allows the follow up of the detail of electronic dynamics at its own "natural" time. The latest breakthroughs were attained in terms of laser frequency with the ongoing possibility of reaching very large frequencies up the X domain. This opens up new possibilities of imaging which are progressively being explored.

We shall focus in this presentation on the recent explorations of electron dynamics down to the attosecond time scale. We shall first present some experimental cases, whose characteristics can be well reproduced by time dependent microscopic theories. We shall then seek for a detailed explanation of observed trends and introduce a schematic model which surprisingly enough provides a remarkable account of experimental trends. It shows in particular that the response of the system is heavily biased by properties of the laser used for exciting and testing the system, especially its IR component. Using the ideas developed in the schematic model we shall reanalyze former computed data and show how much one can attain system's properties.

REFERENCES

[1] Mechanisms of cluster ionization in strong laser pulses, U. Saalmann, C. Siedschlag,, J. M. Rost, J. Phys. B 39 (2006) R39.
[2] Non linear electron dynamics in metal clusters, F. Calvayrac, P. G. Reinhard, E. Suraud, C. Ullrich, Phys. Reports 337(2000)493-578
[3] Laser-driven nonlinear cluster dynamics, Th. Fennel, K.-H. Meiwes-Broer, J. Tiggesbumker, P.-G. Reinhard, P. M. Dinh, E. Suraud, Rev. Mod. Phys. 82 (2010) 1793
[4] Probing Time-Dependent Molecular Dipoles on the Attosecond Time Scale, C. Neidel et al Phys. Rev. Lett 111 (2013) 033001.
[5] Towards the analysis of attosecond dynamics in complex systems, C.-Z. Gao, P. M. Dinh, P.-G. Reinhard, E. Suraud , Phys. Chem. Chem. Phys. 19 (2017) 19784

We-II-4

IRRADIATION OF PROTEIN CYTOCHROME *C* BY LOW ENERGY CARBON IONS AND COBALT 60 GAMMA RAYS

Juliah J. Chelliah[1], Thupten Tsering[1], Pragya Bhatt[2], C. P. Safvan[3] and S. V. K. Kumar[4]

[1,4]Tata Institute of Fundamental Research,
Homi Bhabha Road, Colaba, Mumbai 400005, India
[4]E-mail: svkk@tifr.res.in
[2,3]Inter University Accelerator Centre,
Aruna Asaf Ali Marg, New Delhi 110 067, India,
[3]E-mail: safvan@iuac.res.in

Research to understand the efficacy of different types of radiation at the molecular level has mostly been concentrated on DNA. Other molecules like proteins, carbohydrates, lipids also play an important role in cell survival and division. Effect of radiation on these molecules and its role in cancer therapy has not drawn much attention of the scientific community. However, it is now realized that proteomes can play an important role in cancer diagnosis and treatment and a recent review by Winter *et al* [1] has drawn attention to the response of different types of radiation to proteome. In a first of a kind experimental study on native proteins, we have chosen a small 12.3 kDa heme containing protein, Cytochrome *c*, which is present in cells, as a model to understand the effect of radiation induced damage to proteins [2].

Purified1.21mM solution of Cytochrome *c* was spotted on a clean tantalum foil and irradiated by 328 eV C^+ ions and 1ml of the protein solution was irradiated by ^{60}Co γ-Rays in an irradiation chamber. Both the irradiations were carried out at the Low Energy Ion Beam Facility and ^{60}Co γ-Ray irradiation facilities respectively, at the Inter University Accelerator Centre. The irradiated samples were analyzed by a Bruker Ultraflex MALDI – ToF mass spectrometer at Tata Institute of Fundamental Research.

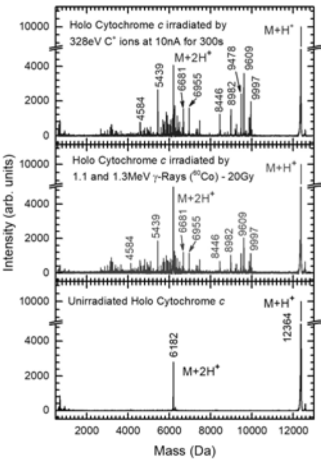


Figure 1: Mass Spectrum of Cytochorme *c* irradiated by low energy carbon ions and γ - Rays.

It is observed from figure 1 that both low energy C^+ ions and ^{60}Co γ-Rays fragment the protein giving rise to largely same set of fragment ions, however, fragment ion yield is more when irradiated by C^+ ions. The fragment ions arising due to single scission of the peptide backbone have been assigned. It is to be noticed that most of the major fragment ions detected are without the heme group indicating that the heme bonding to the backbone is weak and gets detached during the fragmentation process. However, the mass spectrum does not indicate the removal of heme alone from the protein giving rise to either an apo protein ion or a heme ion. The fragmentation seems to preferentially yield higher mass ions as compared to small fragment ions. As there is no water present during the irradiation by C^+ ions and the fragmentation pattern is similar for both types of radiation, protein breakage is unlikely to be caused by $OH^•$ radicals but more likely by direct energy transfer.

REFERENCES

[1] M. Winter, et al, *Mol. & Cell. Proteomics* **16**, 855 (2017)
[2] J. J. Chelliah, et al, (*manuscript under preparation*)

Biomedical applications of radiation

MULTISCALE APPROACH TO THE PHYSICS OF ION-BEAM CANCER THERAPY

Eugene Surdutovich[1], Andrey V. Solov’yov[2]

[1]Physics Department, Oakland University,
Rochester, MI 48309, USA
E-mail: surdutov@oakland.edu
[2]MBN Research Center,
60438 Frankfurt am Main, Germany
E-mail: solovyov@mbnresearch.com

A multiscale approach to the physics of radiation damage with ions (MSA) has been developed in order to relate the biological damage as a result of irradiation with ions to physical, chemical, and biological effects [1,2]. In contrast to other methods, the MSA attempts to give a predictive assessment of survival probabilities on dose and linear energy transfer (LET) based on the analysis of phenomena that happen on different temporal, spatial, and energy scales. The multiscale approach leads to the development of the recipe for the calculation of cell survival probabilities.

The major physical prediction of MSA is the effect of ion-induced shock waves [3]. They are produced due to high gradients of energy deposited in the vicinity of high-LET ion paths. High pressures initiate collective radial flows capable of propagating reactive species formed near the ions’ paths to larger distances. This changes the initial conditions for the chemical phase [4].

The MSA developed a scenario of radiation damage with ions and cell-survival probabilities are calculated on its basis. The key understanding is that lesions that bring about cell inactivation are not caused by dose per se. Rather, lesions result from impact of secondary electrons or other reactive species formed as a consequence of energy deposition. The criterion of lesion lethality based on its complexity is suggested based on experimental survival curves [2]. The predictability of cell survival by the MSA has been successfully tested on a variety of cell lines with different values of LET and oxygenation conditions [5]. The oxygen enhancement ratio is obtained as a byproduct of those calculations.

The MSA was applied to the development of an algorithm of obtaining a uniform profile for cell survival along the spread-out Bragg peak (SOBP) [6]. That work is a step towards the development of a novel treatment planning system. In the most recent work, the effect of high ion fluences was considered in order to take into account the interaction between different ion tracks [7]. The suggested analytical method can be applied to the assessment of radiation damage of plasmid-DNA at high doses and that done by ultrafast laser-driven ion beams.

REFERENCES

[1] A.V. Solov'yov *et al.*, *Phys. Rev.* E **79**, 011909 (2009)
[2] E. Surdutovich and A.V. Solov’yov, *Eur. Phys. J.* D **68**, 353 (2014)
[3] E. Surdutovich and A.V. Solov’yov, *Phys. Rev.* E **82**, 051915 (2010),
[4] P. de Vera, *et al.*, *Eur. Phys. J.* D, **72**, in press (2018)
[5] A.V. Verkhovtsev, E. Surdutovich, and A.V. Solov’yov, *Sci. Rep.* **6**, 27654 (2016)
[6] E. Surdutovich and A.V. Solov’yov, *Eur. Phys. J.* D **71**, 210 (2017)
[7] E. Surdutovich and A.V. Solov’yov, *Eur. Phys. J.* D, **72**, in press (2018)

IMPLEMENTATION STRATEGIES OF RBE MODELLING IN CURRENT TREATMENT PLANNING FOR PROTON AND HEAVIER ION BEAMS

Steffen Greilich[1,2], Alexey Verkhovtsev[1], Lucas Burigo[1], Mark Bangert[1], Oliver Jäkel[1,2,3]

[1]German Cancer Research Center (DKFZ), Heidelberg, Germany
[2]National Center for Radiation Research in Oncology (NCRO), Heidelberg Institute for Radiation Oncology (HIRO), Heidelberg, Germany
[3]Heidelberg Ion-Beam Therapy Center (HIT), Heidelberg, Germany
E-Mail: s.greilich@dkfz-heidelberg.de

The use of swift protons and other light atomic nuclei for the treatment of cancerous lesions started in the 1950s when radiotherapy with X- or gamma-rays (or electrons) had already matured into an established approach practiced for half a century. Thus, despite the obvious differences regarding beam interactions and biological effects, the concepts of prescribing, delivering and reporting radiation dose for ion-beam cancer therapy (IBCT) were largely adopted from existing experience with photon irradiation. Most notably, the entire clinical knowledge on values needed for tumor control and normal tissue toxicity relied on photon dose. One of the remarkable biological effects of ion beams, however, is their ability to deliver significantly higher cell kill than keV and MeV photon or even fast proton beams at the same physical dose. To be able to relate the ion and the photon doses that yield the same effect, the concept of relative biological efficiency was introduced.

To assure the delivery of sufficient dose to a lesion for tumor control and at the same of minimal dose to healthy tissue to avoid toxicity, any external radiotherapy treatment is carefully tailored to the treatment site, the patient anatomy and the properties of the tissue the beam interacts with. While delineation of target volumes and organs at risk is still mostly done manually, the optimization of the dose distribution and the related machine parameters is heavily automatized as part of clinical ‘treatment planning systems’ (TPSs). TPSs that are used for proton and heavier ion therapy have thereby to provide an estimate of RBE.

This presentation will introduce the main concepts of ion radiotherapy planning, give an overview on radiobiological models currently used in clinics and their implementation in TPSs. It will illustrate that new ion species and more complex irradiation techniques may require more powerful models and that such models have to be concurrent with the specifics of TPSs actually used in the clinics.

We-III-3

EXPERIMENTAL AND COMPUTATIONAL STUDY OF GOLD NANOPARTICLES AS A RADIOSENSITIZER FOR PROTON AND CARBON ION IRRADIATION

J.L. Shinpaugh[1], E.C. Maertz[1], W.L. Hawkins[1], N. Carlson[1], C. Boyd[1], J. Teller[1],
C. Putnam-Evans[2], R.A. McLawhorn[3], L.H. Toburen[1], and M. Dingfelder[1]

[1]Department of Physics, East Carolina University
Greenville, North Carolina, 27858 USA
E-mail: shinpaughj@ecu.edu
[2]Department of Biology, East Carolina University
Greenville, North Carolina, 27858 USA
[3]21st Century Oncology
Greenville, North Carolina, 27834 USA

Enhancement of tumor cell killing using nanoparticles is widely being studied for increasing the efficacy of radiation therapy in the treatment of cancer. At East Carolina University, we have initiated an experimental and computational study of gold nanoparticles as a radiosensitizer for particle radiation. Results are presented for cell survival and radiation damage for *in-vitro* irradiation by protons of malignant prostate and breast epithelial cells treated with gold nanoparticles in an energy range approaching the Bragg peak. These results are intended to serve as benchmark data as interest expands for using a wide range of materials as radiosensitizers in hadron therapy; comparison to our previous results for proton irradiation of nonmalignant and cancer cells treated with cerium oxide nanoparticles will be presented.

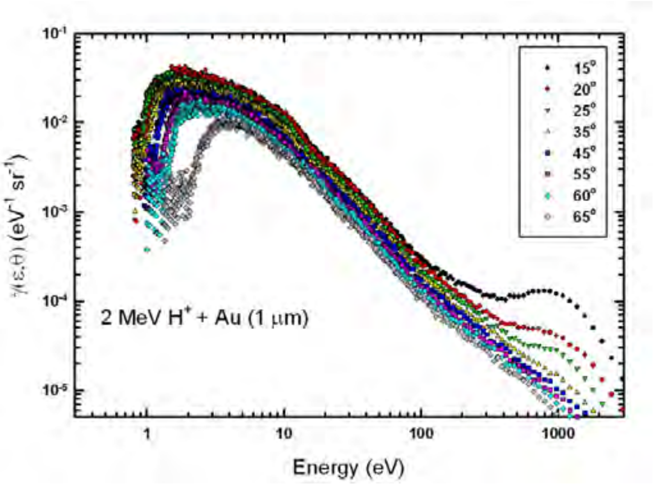


Figure 1: Absolute doubly differential electron emission yields for 2-MeV protons incident on a 1-μm gold foil. Spectra are shown for various emission angles relative to the incident beam.

In addition, we are expanding current Monte Carlo track structure simulation models to include secondary electron production from gold. To test the models, we have measured absolute doubly differential electron emission yields from gold surfaces, hydrated gold surfaces, and amorphous solid water induced by fast proton and carbon ion impact; representative spectra are shown in figure 1 for electron emission following the transmission of 2 MeV protons through a 1-μm gold foil. The experimental results are compared to electron transport simulations using the PARTRAC track structure code.

Electron and spin transport in molecular systems

ENVIRONMENTAL EFFECTS ON CHARGE TRANSPORT THROUGH MOLECULAR WIRES: A MULTI-SCALE APPROACH

Ulrich Kleinekathöfer

Department of Physics and Earth Sciences
Jacobs University Bremen
Campusring 1, 28759 Bremen, Germany
E-mail: u.kleinekathoefer@jacobs-university.de

Charge as well as excitation energy transfer processes are important and ubiquitous in biological systems but at the same time complicated to model at the molecular level. In a multi-scale approach (classical) molecular dynamics simulations and electronic structure calculations need to be combined. The results of such a treatment can subsequently be employed in quantum approaches to determine the respective charge and energy transfer scenarios as well as optical responses. As examples, the charge transport through a DNA molecule is detailed with a special emphasis on the time-dependent effects caused by the liquid environment.

Concerning the quantum transport through molecular wires, several theoretical approaches rely on assuming a molecule-lead coupling composed of Lorentzian functions and a decomposition of the Fermi function in connection with quantum master equations, hierarchical schemes or non-equilibrium Green's functions. The underlying assumptions make this strategy very unattractive due to the limitations in the form of the molecule-lead coupling and its inefficiency at low temperatures. To overcome these restrictions, a Chebyshev expansion is applied to derive a set of coupled ordinary differential equations within the non-equilibrium Green's functions formalism. The new scheme has been tested for molecular junctions under the influence of strong time-dependent perturbations leading, for example, to coherent destruction of tunneling.

REFERENCES

T. Kubar, M. Elstner, B. Popescu and U. Kleinekathöfer, Polaron Effects on Charge Transport through Molecular Wires: A Multi-scale Approach, J. Chem. Theory Comput. 13, 286–296 (2017).

M. Wolter, M. Elstner, U. Kleinekathöfer und T. Kubar, Microsecond Simulation of Electron Transfer in DNA: Bottom-up Parametrization of an Efficient Electron Transfer Model Based on Atomistic Details, J. Phys. Chem. B 121, 529–549 (2017).

M. I. Mallus, M. Aghtar, S. Chandrasekaran, G. Lüdemann, M. Elstner and U. Kleinekathöfer, Relation between Dephasing Time and Energy Gap Fluctuations in Biomolecular Systems, J. Phys. Chem. Lett. 7, 1102–1108 (2016).

B. Popescu, H. Rahman and U. Kleinekathöfer, Using the Chebyshev Expansion in Quantum Transport Calculations, J. Chem. Phys. 142, 154103 (2015).

MAGNETOSENSITIVITY IN THREE-RADICAL SYSTEMS

Robert H. Keens[1], Salil Bedkihal[1], P. J. Hore[2] and Daniel R. Kattnig[1]

[1]University of Exeter, Living Systems Institute and Department of Physics,
Stocker Road, Exeter, EX2 4TP, UK
[2]Physical and Theoretical Chemistry Laboratory, University of Oxford,
South Parks Road, Oxford, OX1 3QZ, UK
E-mail: d.r.kattnig@exeter.ac.uk

The Radical Pair Mechanism (RPM) is a canonical model for the magnetosensitivity of chemical reaction processes [1]. Its governing principle is the coherent interconversion of the singlet and triplet spin states of the radical pair, the key ingredient to which is the hyperfine interaction. This, in combination with spin-selective reaction channels, gives rise to magnetic field effects (MFEs) in the reaction yields. This model underpins the radical pair-based magnetic compass attributed to many migratory birds in the form of the blue-light sensitive flavo-protein cryptochrome [1]. The RPM is also discussed in the context of putatively adverse health effects resulting from the exposure to weak static and oscillatory magnetic fields [2].

This truly quantum mechanism is now at the forefront of the emerging field of quantum biology and, here, I will focus on new aspects of reaction magnetosensitivity that are peculiar to systems comprising three instead of two radicals.

Firstly, I will show that the hyperfine interaction is not a categorical requirement to realize magnetosensitivity to weak magnetic fields. Instead, in systems comprising more than two radicals, dipolar interactions provide an alternative, so far undiscovered, pathway for MFEs [3]. By considering the role of symmetries and energy level crossings, I will present a model that demonstrates a directional sensitivity to fields weaker than the geomagnetic field, and remarkable spikes in the reaction yield, as a function of the magnetic field intensity, that can be tuned by the exchange interaction. These results further our current understanding of weak-field reaction magnetosensitivity and could be particularly relevant to MFEs on lipid autoxidation.

Secondly, I will report on a surprising effect that can boost the magnetosensitivity of radical pairs in the putative magnetosensory protein cryptochrome [4,5]. We have found that MFEs can be vastly amplified if one of the radicals of the primary pair undergoes a spin-selective electron transfer reaction with a spin-bearing scavenger (chemical Zeno effect).[6] This new scheme offers clear and important benefits such as a greatly enhanced sensitivity to the orientation of a 50 μT magnetic field (by up to two orders of magnitude in the relative anisotropy) and magnetosensitivity for radicals that are more than 2 nm apart [4]. This means that radical pairs too distant to undergo spin-selective recombination reactions could also be viable magnetic compass sensors and that the detrimental effects of inter-radical exchange and dipolar interactions can be minimized. Even more surprisingly, the effect immunizes the sensor to fast decoherence processes in one of the radicals [5]. Consequently, magnetic field effects on radical pairs involving swiftly spin-relaxing species, such as superoxide, are no longer to be precluded.

REFERENCES

[1] P. J. Hore and H. Mouritsen, Annu. Rev. Biophys. 45, 299 (2016).
[2] J. Juutilainen, M. Herrala, J. Luukkonen, J. Naarala, and P. J. Hore, Proc Biol Sci 285 (2018).
[3] R. H. Keens, S. Bedkihal, and D. R. Kattnig, Phys. Rev. Lett. accepted (2018).
[4] D. R. Kattnig and P. J. Hore, Sci. Rep. 7, 11640 (2017).
[5] D. R. Kattnig, J. Phys. Chem. B 121, 10215 (2017).
[6] A. S. Letuta and V. L. Berdinskii, Dokl. Phys. Chem. 463, 179 (2015).

MODELING ELECTRON TRANSFERS IN BIOLOGICAL SYSTEMS: APPLICATIONS AND EXAMPLES

Ilia A. Solov‘yov

University of Southern Denmark, Department of Physics, Chemistry and Pharmacy
Campusvej 55, 5230 Odense M, Denmark
E-mail: ilia@sdu.dk

The photoreceptor protein cryptochrome is thought to host, upon light absorption, a radical pair that is sensitive to very weak magnetic fields, endowing migratory birds with a magnetic compass sense, see Fig. 1.

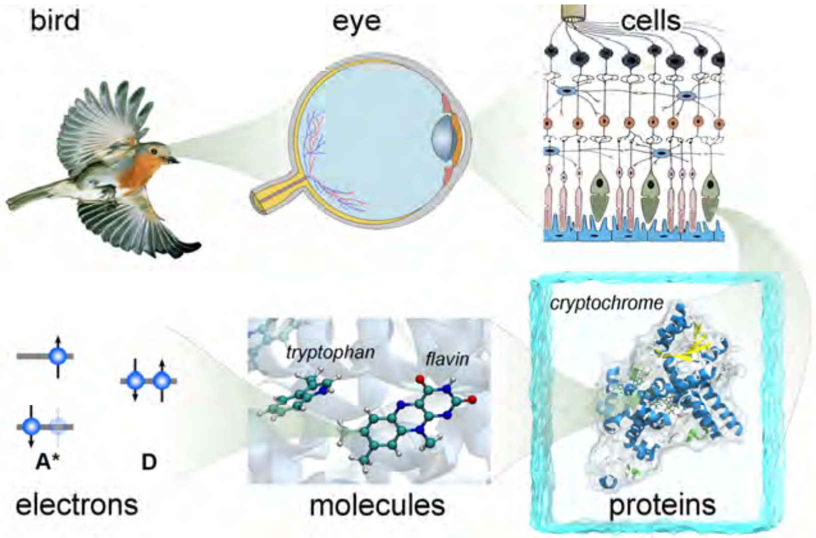


Fig. 1. Avian magnetoreception is a multiscale problem.

The molecular mechanism that leads to formation of a stabilized, magnetic field sensitive radical pair has despite various theoretical and experimental efforts not been unambiguously identified yet. We challenge this unambiguity through a unique quantum mechanical molecular dynamics approach [1] where we perform electron transfer dynamics simulations considering the motion of the protein upon the electron transfer. This approach allows us to follow the time evolution of the electron transfer in an unbiased fashion and to reveal the molecular driving force that ensures fast electron transfer in cryptochrome guaranteeing formation of a persistent radical pair suitable for magnetoreception. We argue that this unravelled molecular mechanism is a general principle inherent to all proteins of the cryptochrome/photolyase family and that cryptochromes are, therefore, tailored to potentially function as efficient chemical magnetoreceptors.

We further extent our analysis for Xenopus laevis cryptochrome DASH, where recent experimental studies [2] have shown that even if some of the amino acids in the active site are mutated, radical pair formation is still observed. We employ dynamical quantum mechanical calculations [3] to study this phenomenon in molecular detail by first constructing a homology model of Xenopus laevis cryptochrome DASH, and then mutate key amino acids involved in the electron transfer. We report several new alternative electron transfer pathways resolved at the molecular level, consistent with experiment, and compare the amino acid sequences of different cryptochrome species to show that one of the alternative electron transfer pathways could be general for all cryptochrome DASH proteins.

REFERENCES

[1] G. Lüdemann, I.A. Solov'yov, T. Kubař, M. Elstner, J. Am. Chem. Soc. **137** (2015), 1147.
[2] T. Biskup, B. Paulus, A. Okafuji, K. Hitomi, E.D. Getzoff, S. Weber, E. Schleicher, J. Biol. Chem. **288** (2013), 9249-9260.
[3] E. Sjulstok, G. Lüdemann, I.A. Solov'yov, T. Kubař, M. Elstner, Biophysical Journal **114** (2018), 2563.

Reactivity and nanocatalysis

Th-II-1

PLASMON INDUCED CHEMISTRY

Emiliano Cortés[1,2]

[1]Blackett Laboratory, Physics Department, Imperial College London,
South Kensington Campus, SW7 2AZ, London, UK
E-mail: e.cortes@imperial.ac.uk
[2]Faculty of Physics, Nanoinstitute Munich, LMU
Schellingstrasse 4, 80799, Munich, Germany

Progress in controlling and tuning light-matter interactions has expanded our ability to collect, store, and convert energy at the nanoscale. Plasmonic materials have played a crucial role in enhancing such interactions due to localized surface plasmon resonances (LSPRs) that can be excited after light impinges on a metal nanoparticle (NP). The incident electric field of a given frequency drives the conduction electrons of the NP in collective oscillations, known as LSPRs. The interaction with light is so intense that the typical extinction cross section of a metal NP illuminated at its LSPR is more than ten times larger than its geometrical size.

Enhanced absorption of photons in metal nanostructures - in comparison to bulk metal surfaces - and the subsequent excitation and non-radiative decay of LSPRs offer exciting opportunities for light-into-chemical energy conversion. A deeper understanding of plasmonic−photonic interactions allows for the predesign of specific functionalities on either sub-particle surfaces or nanosized elements of complex metallic nanoclusters. Our results can be exploited for the design, fabrication, and applications of functional platforms in the nanoscale regime [1-4].

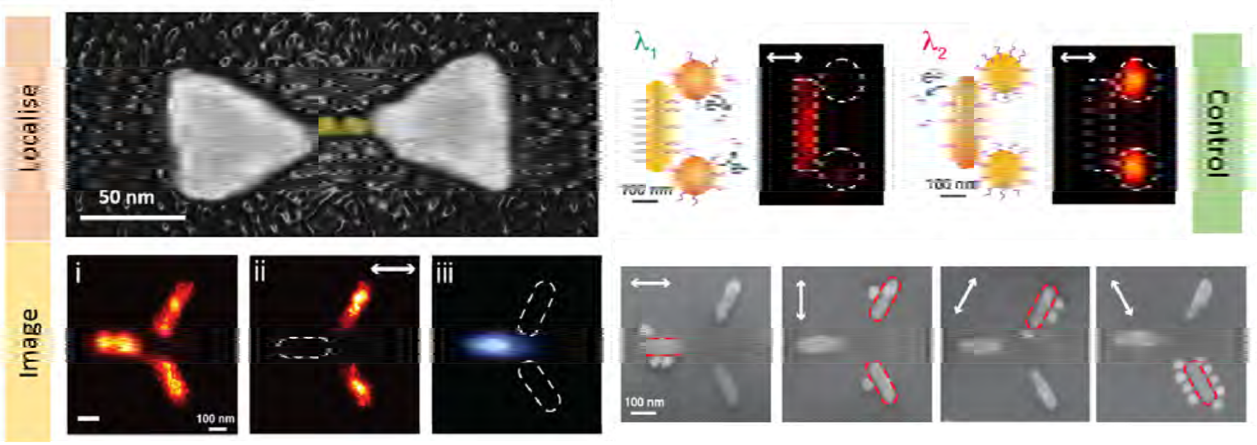


Figure 1: Examples of nano-localised chemical modifications induced by plasmon excitation in metal nanostructures [1-4].

REFERENCES
[1] E. Cortes, et al. Nature Comm. 14880 (2017)
[2] E. Cortes, Adv. Opt. Mat **5**, 1700191 (2017)
[3] S. Simoncelli, et al. ACS Nano **12**, 3, 2184–92 (2018)
[4] S. Simoncelli, et al. Nano Letters **18**, 6, 3400–06 (2018)

HOT-ELECTRON TRANSFER INDUCED REACTIONS

R. Schürmann[1], S. Vogel[1,2], K. Ebel[1,2], C. Nicolas[3], A. R. Milosavljević[3] and I. Bald [1,2]

[1] Institute of Chemistry, University of Potsdam,
Karl-Liebknecht-Str. 24-25, 14476 Potsdam-Golm, Germany
[2] Federal Institute of Material Research and Testing,
Richard-Willstätter-Str. 11,12489 Berlin, Germany
[3] Synchrotron SOLEIL,
L'Orme des Merisiers, Saint Aubin, BP 48, 91192 Gif-sur-Yvette Cedex, France
E-mail: rschuerm@uni-potsdam.de

Chemical reactions on light illuminated gold (Au) and silver (Ag) nanoparticles (NPs) provide versatile applications ranging from solar energy storage [1] to novel cancer therapies [2],[3]. Such reactions are often induced by so called "hot-electrons", which are generated in the decay of localized surface plasmon resonances (LSPRs) of the NPs. Typically surface enhanced Raman scattering (SERS) is used to study hot-electron induced reactions in real-time and identify the reaction products. Among the most widely studied plasmon catalyzed reactions is the reduction of 4-Nitrothiophenol (4-NTP) to p,p'-dimercaptoazobenzene (DMAB) [4].

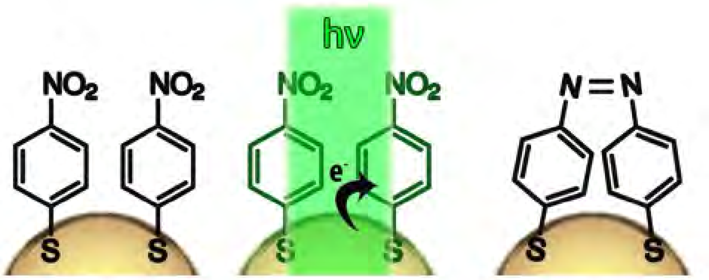


Figure 1: Sceme of the plasmon mediated reaction from 4-NTP to DMAB

In general, the extraordinary high signal enhancement on noble metal SERS substrates originate from nanoscopic gaps between NPs, so called "hot-spots". In consequence, also the hot electrons are inhomogenously distributed over the substrate leading to time-dependent reaction rates, which can be described by fractal kinetics [5]. The observed reaction rates show a strong dependency on the wavelength of the incident light. However, the wavelength dependency of the hot electron induced reactions cannot be fully explained by the plasmonic enhancement of the NPs. In order to obtain complementary information on the system, synchrotron X-ray photoelectron spectroscopy (XPS) measurements of isolated 4-NTP capped AuNP-clusters have been performed to monitor the valence band states. In this way, a dependency of the reaction rates on the available electronic states of the NPs has been demonstrated. Furthermore, the work function of the system has been determined and the binding of 4-NTP on AuNPs has been elucidated. Besides 4-NTP also the hot electron induced reactions of the potential DNA-radiosensitizer 8-Bromoadenine (8-BrA) [6] has been studied under different environmental conditions. A detailed understanding of the interaction of electrophilic radiosensitizers with plasmonic NPs might help to improve the cancer photothermal therapy.

REFERENCES

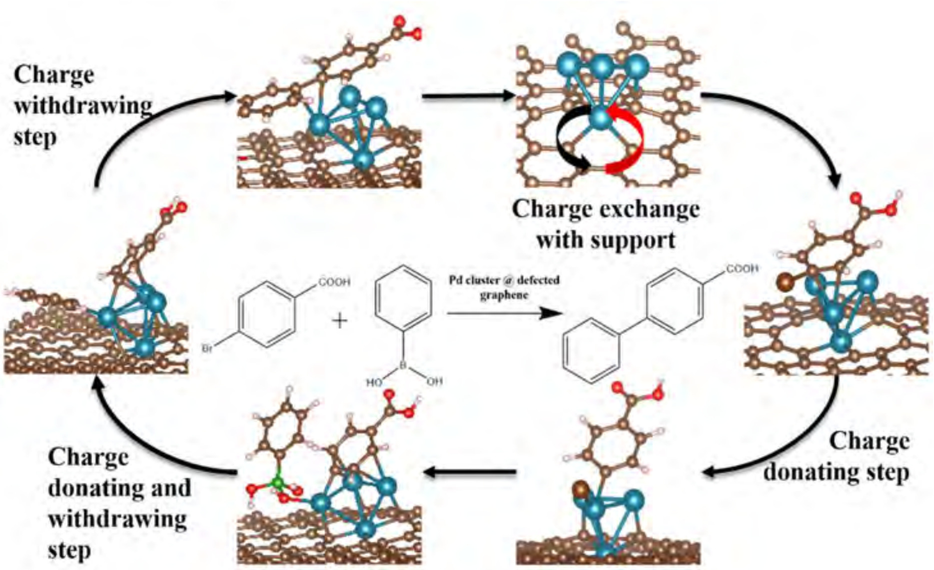
[1] S. Yu, A. J. Wilson, G. Kumari, X. Zhang, P. K. Jain; *ACS Energy Lett*. 2017 2(9), 2058
[2] N. S. Abadeer, C. J. Murphy, *J. Phys. Chem. C* 2016, *120*, 4691–4716.
[3] R. Schürmann, I. Bald, *J. Phys. Chem. C* 2016, *120*, 3001–3009.
[4] X. Ren, E. Cao, W. Lin, Y. Song, W. Liang, J. Wang, *RSC Adv* 2017, *7*, 31189–31203.
[5] R. Schürmann, I. Bald, *Nanoscale* 2017, *9*, 1951–1955.
[6] R. Schürmann, T. Tsering, K. Tanzer, S. Denifl, S. V. K. Kumar, I. Bald, *Angew. Chem. Int. Ed.* 2017, *56*, 10952–10955.

Th-II-3

NANO-CATALYSTS FOR CROSS-COUPLING REACTIONS, CO OXIDATION, AND BREAKING POLAR BONDS

S. N. Khanna and A. C. Reber
Department of Physics, Virginia Commonwealth University, Richmond, VA 23284-2000.
Y. Yang and B. Frank Gupton
Department of Chemical and Life Science Engineering, VCU, Richmond, VA 23284.
snkhanna@vcu.edu

The talk will highlight two distinct aspects of nano-catalysts, (1) Graphene as a solid state ligand for Palladium catalyzed cross-coupling reactions used for drugs, and (2) Using ligands to induce reactivity in metallic clusters by selective positioning.



The carbon-carbon cross coupling reactions using palladium catalysts are one of the most important chemical transformations in the preparation of complex organic molecules. The Suzuki coupling reaction is particularly important in pharmaceutical applications due to its mild reaction conditions and broad application across a wide range of functionalized substituents. These reactions are generally carried out under homogeneous conditions that cannot be used in continuous flow processes, and leads to product contamination, and loss of expensive catalyst. Binding the palladium catalyst to a conventional support fails to overcome these limitations because the active sites are adversely affected and the catalytic activity is still homogenous because it is performed by palladium that has leached into solution. We demonstrate that a catalyst consisting of palladium clusters supported on reduced graphene not only minimizes leaching but also offers superior catalytic activity with extremely high turnover frequencies and remarkable recyclability. Theoretical investigations reveal that while the vacancy/void sites strongly bind the clusters thereby reducing leaching, the support also serves as a reservoir of charge for the donor and acceptor of electrons allowing the supported clusters to reduce the barriers for both the oxidation and reduction steps operating in a heterogeneous mode. I will also discuss our recent efforts to further improve the catalytic activity via mixed clusters.

I will then talk about our efforts in inducing reactivity in metallic clusters using ligands. Quantum confinement in small metal clusters leads to a bunching of states into electronic shells enabling the classification of stable clusters as superatoms. We demonstrate that these superatoms exhibit dual reactivity patterns in that clusters with closed electronic shells are inert towards reactivity with oxygen; however, clusters with closed electronic shells can still react with polar reactants such as methanol. We demonstrate this unique reactivity pattern by considering the reactivity of methanol with aluminum clusters ligated with iodine ($Al_nI_m^-$). Through a combined experimental and theoretical effort we show that the reactivity is dominated by Lewis acid and Lewis base active sites that can be reactive irrespective of the shell closure. We demonstrate how selective positioning of the ligands and structure of the metal core one can induce such pairs the cluster leading to a new paradigm where ligands can be employed to induce reactivity or stability towards polar molecules.

STUDIES OF THIN FILMS AND ICE LAYERS; APPLICATIONS FROM ASTROCHEMISTRY TO NANOLITHOGRAPHY

Nigel J Mason[1,2]

[1]School of Physical Sciences, The University of Kent
Canterbury, CT2 7NH United Kingdom
E-mail: N.J.Mason-OBE@kent.ac.uk

[2]School of Physical Sciences, The Open University
Walton Hall, Milton Keynes, MK7 6AA, United Kingdom
E-mail: nigel.mason@open.ac.uk

The study of the morphology and reaction dynamics within thin films and ice layers has implications in many disparate fields of science and technology from the study of molecular formation on dust grains in the Interstellar medium to the fabrication of nanostructures by both top down etching or bottom up deposition. Until recently the 'granularity' or nanoscale structure of such thin films and ices was largely ignored but in recent experiments we have shown that knowledge of such morphology is crucial in understanding chemical transformations and molecular synthesis. For example the enhanced growth rate of ozone in molecular oxygen films at temperature below 2OK is due to the oxygen molecules forming dimers allowing internal dimer conversion to ozone which is lost at higher temperatures when the dimer is not able to form [1]. Similarly the observations of excitons in the UV transmission of ammonia ice explains the granularity of ammonia ice and ammonia/water ice limiting transport of radiation induced radicals at certain temperatures [2].

In this presentation I will discuss the role of UV and IR spectroscopy in probing the morphology of thin films and ice layers and how they may be used to explore reaction dynamics leading to molecular synthesis. I will explain the relevance of such studies to Astrochemical modelling and importance in nanolithography. I will also discuss a unique set of experiments to explore the morphology of ice films grown on micron sized 'dust' particles isolated within an ultrasonic trap [3] and their relevance to observational astronomy.

REFERENCES

[1] On the electron-induced isotope fractionation in low temperature $^{32}O_2/^{36}O_2$ ices—ozone as a case study B. Sivaraman , A. M. Mebel, N. J. Mason , D. Babikov and R. I. Kaiser *Phys. Chem. Chem. Phys.* **13**, 421-427 (2011)

[2] A morphological study of ammonia ice under astrochemical conditions using VUV Spectroscopy. A Dawes, R J Mukerji, M P Davis, P Holtom, S M Webb, S V Hoffmann, D A Shaw and N J Mason *J Chem Phys* ***126*****:** Art. No. 244711 (2007)

[3] The Spectroscopy And Chemical Dynamics of Microparticles Explored Using An Ultrasonic Trap N J Mason, A Dawes, E A Drage, S M Webb, R McPheat and G Hayes *Faraday Discussions*: **137** 367-376 (2008)

Collision processes, fusion, fission, fragmentation

Th-III-1

HYDRATION DEPENDENCE OF IONIZATION AND FRAGMENTATION REACTIONS IN BIO-RELEVANT MOLECULES

Xueguang Ren, Enliang Wang and Alexander Dorn

Max Planck Institute for Nuclear Physics, 69117 Heidelberg, Germany
E-mail: A.Dorn@mpi-k.de

Primary ionizing radiation penetrating biological tissue produces large numbers of low-energy secondary electrons which effectively induce damages in biological material. In order to understand the underlying reactions electron collisions with molecules are regularly studied in the gas phase, e.g. in kinematically complete (e, 2e) experiments where the scattered and ionized electrons are detected [1] or in experiments using mass spectrometers [2]. We combine both techniques in a so-called reaction microscope where for electron impact ionization (with energy E_0) of gas-phase molecules the momentum vectors of two outgoing electrons (energies E_1 and E_2) are detected in coincidence with the residual ion(s). This enables to correlate the ionized electron orbital (according to the measured binding energy) and the subsequent fragmentation pathway [3].

Here we discuss how hydration of organic molecules modifies their fragmentation and gives rise to new reaction pathways. As a model system we use tetrahydrofuran (C_4H_8O, THF) a five membered heterocyclic ring that is often regarded as the simplest surrogate for the sugar deoxyribose in the DNA backbone. Oxygen in THF is capable of one hydrogen-bonding link to water (Fig. 1a) and forms reasonable simple THF-water dimers for which electronic structure calculations are feasible. In these systems we were able to experimentally identify intermolecular Coulombic decay (ICD) [4]. This is an energy transfer process where energy stored in an inner-valence vacancy in water is transferred to THF ionizing it. As illustrated in Fig. 1 the starting point is the creation of an inner-valence (iv) vacancy by direct electron-impact ionization of the water molecule (a). Then the energy released by de-excitation of an outer-valence (ov) electron at the same molecule is transferred to the neighboring THF molecule, which consequently emits a low-energy electron (b). Finally, both molecules are charged and a Coulomb explosion occurs with back-to-back emission of the fragment ions. In this indirect ionization of THF we observe that the fragmentation probability of the THF ion is significantly higher compared to direct electron impact ionization of THF. This ICD process can be relevant for radiation damage since starting with a single secondary electron it produces within a small volume two energetic ions and three reactive slow electrons which can produce further damage in the close

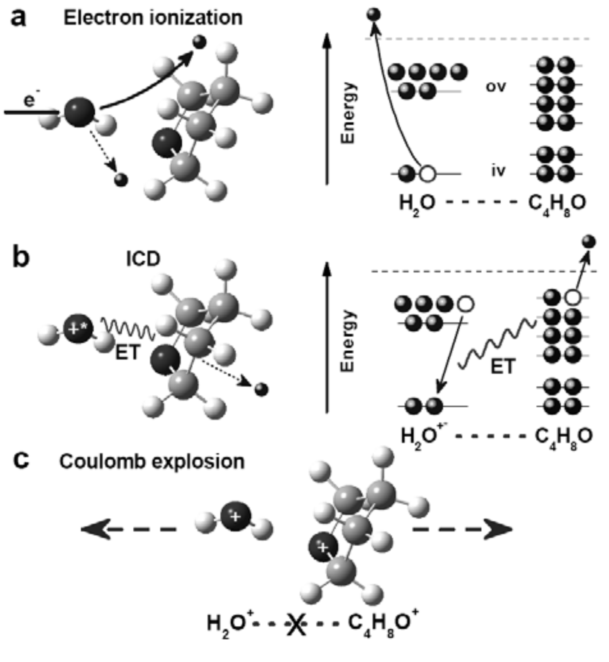


Figure 1: Schematic representation of intermolecular Coulombic decay (ICD) in a hydrogen-bonded THF-water dimer (for details see text).

vicinity. Our calculations of the state energies also show that ICD can follow carbon *2s* ionization in THF dimers and, therefore, it can occur in biological tissue in general [4]. Thus, ICD is expected to be a widespread phenomenon in loosely bound matter that can lead to the direct damage of hydrated biomolecules such as DNA, as well as for the efficient production of reactive ions and secondary electrons.

In a second experiment we studied how the direct electron impact ionization and fragmentation dynamics of a THF monomer is modified if neighbors are present. Studies were done for pure THF clusters and hydrated clusters which both were produced in a supersonic gas jet. Interestingly, we see a destabilizing effect of the environment as it is illustrated in Fig. 2 where the binding energy (*BE*) spectra of the ionized orbitals are shown for (in coincidence with) different residual ion species as indicated. Considering first monomers, the molecule stays intact and the parent ion is observed for ionization of the HOMO orbital (*BE* = 10 eV, bottom curve with full squares). The ring-breaking reaction leading to $C_2H_4O^+$ requires more energy and the ionization of an inner orbital (HOMO-4,5) with *BE* around 13 eV (open squares, third spectrum from top). Interestingly for dimers the required energy for this ring breaking reaction is strongly reduced: For the hydrated dimer $H_2O^{\cdots}$THF only 10.5 eV (open circles, second spectrum from top) is required and for the THF_2 dimer 10 eV are sufficient (open diamonds, top spectrum). In both cases no stable parent ions are observed. From that and the binding energies we conclude that in the clusters even HOMO ionization leads to ring breaking and not to the stable parent ion as in the monomer. Using quantum chemical calculations we find that the reaction barriers for the ring-breaking reactions are lowered if hydrogen-bonded neighbors are present.

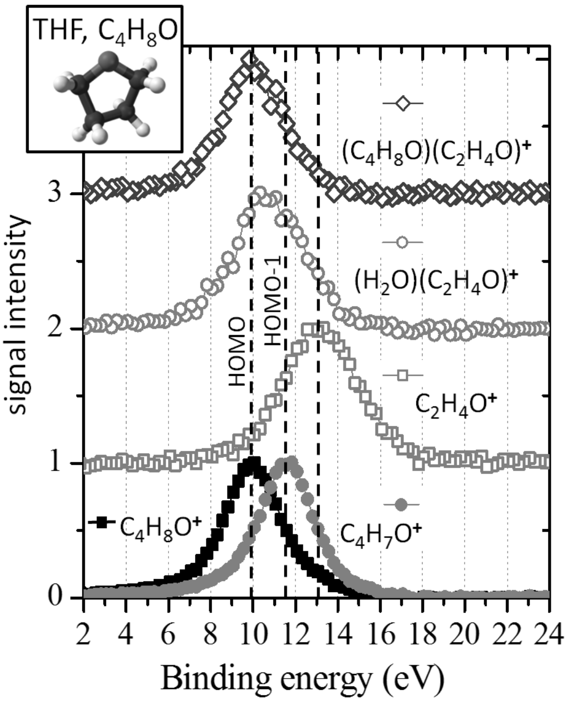


Figure 2: Binding energy spectra ($BE = E_0 - E_1 - E_2$) for production of different fragment ions. For ionization of THF monomers (two bottom curves and third curve from top) hydrated THF (second curve from top) and THF dimers (top curve) and fragmentation into the ion species given in the diagram.

REFERENCES

[1] D. B. Jones *et al*, *J. Chem. Phys.* **145**, 164306 (2016)
[2] M. Dampc *et al*, *J. Phys. B* **44**, 055206 (2011)
[3] X. Ren *et al*, *J. Chem. Phys.*, **141**, 134314 (2014)
[4] X. Ren *et al*, *Nature Physics*, DOI: 10.1038/s41567-018-0214-9

NEW ROUTES TO ENHANCE EMISSION PROPERTIES OF GOLD NANOCLUSTERS

Rodolphe Antoine

University Lyon[1], France

Functional ligand-protected noble metal cluster nanomaterials with enhanced two-photon absorption and two-photon excited emission may lead to new technologies in the fields of bio-imaging applications. In this talk, I will review experimental and theoretical methodologies allowing detailed investigation and analysis of two-photon absorption/emission properties of ligand-protected silver and gold metal clusters, coined “ligand-core” NLO-phores. Then I will thoroughly analyze physical phenomena and trends leading to large two-photon absorption/emission responses of a few series of model nanoclusters focusing on the effects of the relaxation pathways in the linear and nonlinear optical regime, as well as innovative strategies aiming at enhancing their two-photon emission responses.

REFERENCES

[1] Bertorelle F, Moulin C, Soleilhac A, Comby-Zerbino C, Dugourd P, Russier-Antoine I, Brevet PF, Antoine R (2018) Bulky Counterions: Enhancing the Two-Photon Excited Fluorescence of Gold Nanoclusters. ChemPhysChem 19 (2):165-168. doi:doi:10.1002/cphc.201701186

[2] Russier-Antoine I, Bertorelle F, Calin N, Sanader Z, Krstic M, Comby-Zerbino C, Dugourd P, Brevet P-F, Bonacic-Koutecky V, Antoine R (2017) Ligand-core NLO-phores: a combined experimental and theoretical approach to the two-photon absorption and two-photon excited emission properties of small-ligated silver nanoclusters. Nanoscale 9 (3):1221-1228. doi:10.1039/C6NR07989J

[3] Sanader Z, Krstic M, Russier-Antoine I, Bertorelle F, Dugourd P, Brevet P-F, Antoine R, Bonacic-Koutecky V (2016) Two-photon absorption of ligand-protected Ag15 nanoclusters. Towards a new class of nonlinear optics nanomaterials. Physical Chemistry Chemical Physics 18:12404-12408. doi:10.1039/C6CP00207B

[4] Russier-Antoine I, Bertorelle F, Hamouda R, Rayane D, Dugourd P, Sanader Z, Bonacic-Koutecky V, Brevet P-F, Antoine R (2016) Tuning Ag29 nanocluster light emission from red to blue with one and two-photon excitation. Nanoscale 8 (5):2892-2898. doi:10.1039/C5NR08122J

[5] Russier-Antoine I, Bertorelle F, Vojkovic M, Rayane D, Salmon E, Jonin C, Dugourd P, Antoine R, Brevet P-F (2014) Non-linear optical properties of gold quantum clusters. The smaller the better. Nanoscale 6:13572-13578

MOLECULAR DYNAMICS SIMULATIONS OF ION-INDUCED SHOCK WAVE EFFECTS IN BIOLOGICAL MEDIA

Pablo de Vera[1], Eugene Surdutovich[2], Nigel J. Mason[3], Fred J. Currell[4], Andrey V. Solov’yov[1]

[1]MBN Research Center, Altenhöferallee 3, 60438, Frankfurt am Main, Germany
E-mail: pablodevego@gmail.com
[2]Department of Physics, Oakland University, 48309, Rochester, Michigan, USA
[3]School of Physical Sciences, The Open University, MK7 6AA, Milton Keynes, UK
[4]The Dalton Cumbrian Facility, University of Manchester, CA24 3HA, Moor Row, Cumbria, UK

Among the many applications of energetic ion beams, ion beam cancer therapy (IBCT) is gaining much attention in the last years. IBCT is a modern radiotherapy technique for cancer treatment, which exploits the characteristics of energy deposition in condensed matter by ions, namely, small angular deflection and a depth-dose curve presenting a sharp maximum at the end of the ions’ trajectories (the so-called Bragg peak). Both characteristics result in a highly collimated beam which selectively deposits most of its energy in the cancerous region, sparing surrounding healthy tissues [1]. Furthermore, ion beams present an increased relative biological effectiveness, meaning that, for the same amount of dose, they can kill many more cells as compared to photons. This effect arises due to physico-chemical processes following irradiation and mainly occurring at the atomic and molecular level [2]. Thus, IBCT is also a very interesting problem from the fundamental point of view, since basic processes happening on the nanoscale have to be understood in order to better control and exploit therapy.

Within the multiscale scenario of IBCT [1, 2], ions lose most of their energy by ionizing the medium (mainly liquid water) and producing large numbers of low energy electrons (LEE) and free radicals. LEE thermalize within a few nanometers around the ion’s path, building up intense radial doses. This concentrated pattern of energy deposition, together with high densities of produced radicals, can induce clustered DNA damage leading to cell death. Such damage is primarily inflicted by LEE or radicals. If the linear energy transfer (LET) is sufficiently high, the transport of these agents is significantly affected by shock waves cylindrically propagating from ions’ paths, caused by the large gradients of deposited energy [3]. The shock waves affect the radiation chemistry scenario by propagating free radicals out of the ion tracks [4] and, at extremely high LET in the Bragg peak of heavy ions, they can rupture DNA bonds by thermo-mechanical effects [5, 6].

In this contribution, we will show how the molecular dynamics technique can be used to simulate the response of the liquid medium to the energy deposited by swift ions, in order to get insights into the physico-chemical mechanisms leading to biomolecular damage by shock waves.

REFERENCES
[1] A.V. Solov’yov (ed.), *Nanoscale Insights into Ion- Beam Cancer Therapy* (Springer International Publishing, Cham, Switzerland, 2017)
[2] A. Verkhovtsev, E. Surdutovich, A.V. Solov’yov, *Sci. Rep.* **6**, 27654 (2016)
[3] E. Surdutovich, A.V. Solov'yov, *Phys. Rev. E* **82**, 051915 (2010)
[4] P. de Vera, E. Surdutovich, N. J. Mason, F. J. Currell, A. V. Solov'yov, *Eur. Phys. J. D* (In press, 2018). DOI: 10.1140/epjd/e2018-90167-x. arXiv:1703.09150 [physics.bio-ph]
[5] E. Surdutovich, A.V. Yakubovich, A.V. Solov'yov, *Sci. Rep.* **3**, 1289 (2013)
[6] P. de Vera, N. J. Mason, F. J. Currell, A. V. Solov'yov, *Eur. Phys. J. D* **70**, 183 (2016)

MEASUREMENT OF CORRELATIONS BETWEEN TWO NANOMETRIC VOLUMES IN THE TRACK STRUCTURE OF ^{241}AM ALPHA PARTICLES

G. Hilgers, H. Rabus

Physikalisch-Technische Bundesanstalt,
Bundesallee 100, D-38116 Braunschweig, Germany
E-mail: gerhard.hilgers@ptb.de
E-mail: hans.rabus@ptb.de

Although there are radiobiological data indicating the relevance of correlations in damages to DNA [1], it is assumed that the local ionisation density in a single nanometre-sized site is the most important quantity. For denser ionising particles, however, the spatial correlation of ionisation clusters becomes also important. A double or even multiple clustered damage, which causes two DSBs in two spatially separated sensitive volumes each of several nanometres in size, can result in the loss of a whole DNA loop. This loop can be of substantial length depending on the geometrical position of the two target volumes and the degree of damage produced in the respective targets by a passing primary particle.

Correlations of ionisations created by the same primary particle in two spatially separated nanometre-sized target volumes were investigated using the ion-counting nanodosimeter operated at PTB. The measured quantity is a two-dimensional probability distribution $P_{\nu,\mu}(Q,V_1,V_2)$ that exactly ν ions are created in the target volume V_1 and μ ions are created in the target volume V_2 for a primary particle of radiation quality Q. Measurements of correlated ionisations were carried out with ^{241}Am alpha particles in different target gases, which represent different mechanisms leading to DNA damage.

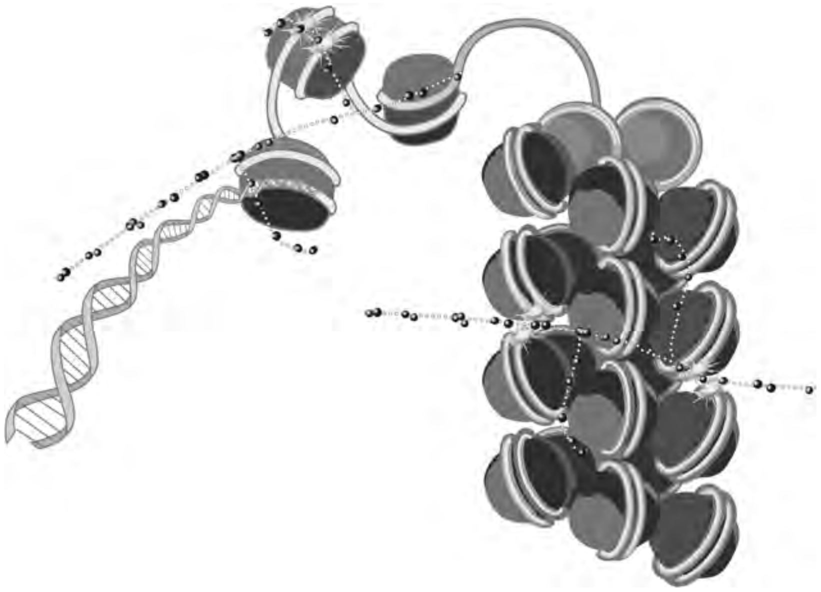


Figure 1: Loss of DNA loops due to the correlated creation of DSBs by the same primary ion in two spatially separated target volumes.

REFERENCES

[1] J.A. Simmons, D.E. Watt, *Radiation Protection Dosimetry – A Radical Reappraisal*. Medical Physics Publishing (1999).

Propagation of particles through medium

INVESTIGATION OF CHANNELING AND CRYSTALLINE UNDULATORS WITH MBN EXPLORER

A.V. Korol[1,2], G.B. Sushko[2], A.V. Solov'yov[2]

[1]St. Petersburg State Maritime University, Leninsky ave. 101, 198262, St. Petersburg, Russia
[2]MBN Research Center, Altenhöferallee 3, 60438 Frankfurt am Main
E-mail: korol@mbnexplorer.de, solovyov@mbnresearch.de

The main phenomenon addressed is the radiation formed in a Crystalline Undulator (CU) [1]. In this device, the radiation is generated by a bunch of ultra-relativistic particles channeling through a periodically bent crystal. Such a system becomes a source of intensive radiation of the undulator type, and, under certain conditions, also a source of the laser light within the energy range from tens-hundreds keV up to MeV [1] which is unachievable in conventional FEL devices.

Propagation of ultra-relativistic electrons and positrons in crystalline structures was simulated by means of the channeling module [2] of the MBN Explorer software package [3]. The universal design of the package allows one to integrate relativistic equations of motion with simultaneous generation of the crystalline environment in the course of the particle propagation as well as to compute spectral and spectral-angular distributions of the emitted radiation.

At the Conference, an overview will be given of the CU research field with particular emphasis of the progress which can be achieved by means of numerical simulations of high level of predictivity. Also, new results will be presented and discussed. These results include, in particular:

(1) Emission spectra from 5–20 GeV positrons and electrons channeling in a diamond(110)-based CU. The periodic bending considered implies the bending amplitude a and period λ_u to be much larger than the interplanar spacing d and the period of channeling oscillations λ_{ch}, respectively.

(2) Quantitative analysis of the channeling process and of the radiation emitted by 855 MeV electrons and positrons in straight, bent and periodically bent Ge(110).

(3) Comparison of the channeling efficiencies of graphite(002), diamond(110), Ge(110) and W(110) for the light projectile of the energy within the range 855 MeV–20 GeV.

The current theoretical results and the numerical data are highly relevant in view of the ongoing channeling experiments carried out with 195–855 MeV electron beams at the Mainz Microtron (Germany) facility and with 20–35 GeV projectiles at the SLAC facility (USA).

The work was supported in part by the Alexander von Humboldt Foundation Linkage Grant and by the HORIZON 2020 RISE-PEARL project.

REFERENCES

[1] A.V. Korol, A.V. Solov'yov, W. Greiner. *Channeling and Radiation in Periodically Bent Crystals*. Springer Berlin Heidelberg, 2014 (2nd edition).
[2] G. Sushko, V.Bezchastnov, A. Korol, W. Greiner, A. Solov'yov: *J. Comp. Phys.* **252** (2013) 404
[3] I.A. Solov'yov, A.V. Yakubovich, P.V. Nikolaev, I. Volkovets, A.V. Solov'yov: *J. Comp. Chem.* **33** (2012) 2412–2439

STEERING OF GeV AND TeV PARTICLES VIA COHERENT ORIENTATIONAL EFFECTS IN CRYSTALS

Vincenzo Guidi[1],
On behalf of the AXIAL experiment

[1]Department of Physics and Earth Sciences, University of Ferrara,
and INFN Sezione di Ferrara, Italy
E-mail: guidi@fe.infn.it

The possibility to manipulate the trajectories of charged particle beams through coherent interaction of the particles with a bent crystal has fascinated the community of high-energy and accelerator physicists. In fact, the phenomena of channeling and of the recently discovered volume reflection appear to be promising techniques in this sense. The strong electric field experienced by a beam particle in proximity of an ordered structure of the atoms in a crystal exerts a strong confinement force onto the particle and may bound its trajectory to proceed parallel to a crystalline plane or an atomic string, which become preferential pathways in the crystal. As the crystal is being bent, the pathways are bent in turn and the particles are diverted towards a different direction with respect to incoming direction, i.e., beam steering is accomplished.

Owing to a strong R&D carried out at some labs worldwide on the technology for crystal manufacture and bending, steering of particle beams has become a mature technique for particle accelerators. Selection of the crystal geometry is strongly bound up to the energy of a particle beam that one wants to manipulate. As an example, at some GeV energy, the usage of quasi-mosaicity allows one to fabricate tens-of-um-thin bent plates, the secondary curvature of which can be used for particle steering. At the energy of hundreds GeV or some TeV a crystalline strip some-mm-thick along the beam bent by anticlastic deformation is probably the preferable solution.

Particle steering can be done by using either the under-bound confined motion of particles within neighboring atomic planes, i.e., planar channeling or the over-barrier motion of particles moving at grazing angle with respect to atomic planes or strings, such as for volume reflection, multi-volume reflection and axial channeling assisted by stochastic motion. Each regime offers advantages and disadvantages, which may be adapted to each individual situation.

Even though channeled negative particles are de-channeled at faster rate than positive particles due to repeated collisions with nuclei, steering of negatively charged particles can be envisaged. Steering of negatively charged particles can also be performed provided that the crystal is thinner than the de-channeling length of particles at the energy under consideration. In this case, the usage of an unbound regime of particles partly circumvents the problem of collisions with nuclei, leading to performance similar to that for positive particles.

In this talk, we review the state-of-the art on the science and technology about particle steering via coherent orientational effects in bent crystals and present the results achieved at international labs on this subject.

CHANNELING AND RADIATION OF ELECTRONS AND POSITRONS IN PERIODICALLY BENT DIAMOND CRYSTALS

K.B. Agapev[1], A.V. Pavlov[1,2], V.K. Ivanov[1], A.V. Korol[2,3], A.V. Solov'yov[3]

[1]Department of Experimental Physics, Peter the Great St. Petersburg Polytechnic University,
Polytekhnicheskaya 29, 195251, St. Petersburg, Russia
E-mail: ivanov@physics.spbstu.ru
[2]St. Petersburg State Maritime University, Leninsky ave. 101, 198262, St. Petersburg, Russia
[3]MBN Research Center, Altenhöferallee 3, 60438 Frankfurt am Main, Germany
E-mail: korol@mbnexplorer.com, solovyov@mbnresearch.com

Channeling and radiation phenomena are studied for ultra-relativistic electrons and positrons passing through straight, bent and periodically bent diamond crystals. Comprehensive quantitative analysis of the channeling and radiation emission processes is presented based on numerical simulations carried out by means of the MBN Explorer package [1,2]. The motion of a channeling particle in a uniformly bent crystal contains two components: the channeling motion and the translation along the arc. The latter motion gives rise to the synchrotron-type radiation. Periodic bending results in additional peaks in the emission spectra so that such crystals can be considered as Crystalline Undulators (CU) operating in the ($10^{-1}\ldots10^{0}$) MeV photon-energy range [3].

Both electron and positron channeling along the (110) crystallographic planes was studied for the energies ε=270, 375, 600 and 855 MeV and for different values of (i) bending radius R (uniformly bent crystals), and (ii) bending amplitude a (Periodically Bent Crystals, PBCs). Similar simulations of 855 MeV electron and positron channeling have been performed for Si crystal [4]. In the current simulations the diamond crystal thickness L was set to 20 μm. The periodic bending was assumed to have of a harmonic shape $S(z) = a\cos(2\pi z/\lambda_u)$ where the coordinate z is measured along the incident beam direction. The bending period λ_u was set to 5 μm, the range of the bending amplitude includes the values a = 1.2, 2.5, 4.0 Å. The quoted values of ε, L, λ_u and a correspond to the electron beam energies and to parameters of the 4-period CU used in recent experiments at the MAMI facility [5]. At the first stage of the simulation, for each case we calculated 6000 trajectories analyzing which we defined the main parameters which characterize the channeling process. As expected, the average channeling length of electrons is an order of magnitude smaller than that for positrons and it decreases with the increase of the bending amplitude. For positrons, the channeling length for is comparable with L for all values of a thus indicating that significant part of positrons passes through the whole crystal staying in the channeling mode.

The simulated trajectories were used further as the input data for numerical analysis of the intensity of emitted radiation. Four graphs in Figure 1 illustrate the evolution of the spectral distributions with the bending amplitude. The data presented refer to 855 MeV electrons and positrons and to to the emission aperture 0.24 mrad.

In the straight crystal (graph a), the spectra are dominated by powerful peaks due to the channeling radiation (ChR). For positrons, the main narrow peak, located at ca 3 MeV, corresponds to the emission into fundamental harmonic of ChR. In the electron case, strong anharmonicity of the channeling oscillations results in noticeable widening of the peak and in decreasing of its intensity (note the factor 5 used to plot the electron spectra).

Graphs b-d show the emission spectra in PBCs with different bending amplitudes *a*. Main novel feature is associated with the CU radiation, the fundamental peak of which is located at $\omega_1 \approx 1$ MeV for both electrons and positrons. As expected, the peak intensity for positrons is much larger than for electrons. As a function of *a*, the peak intensity acquires the maximum value at $a = 2.5$ Å.

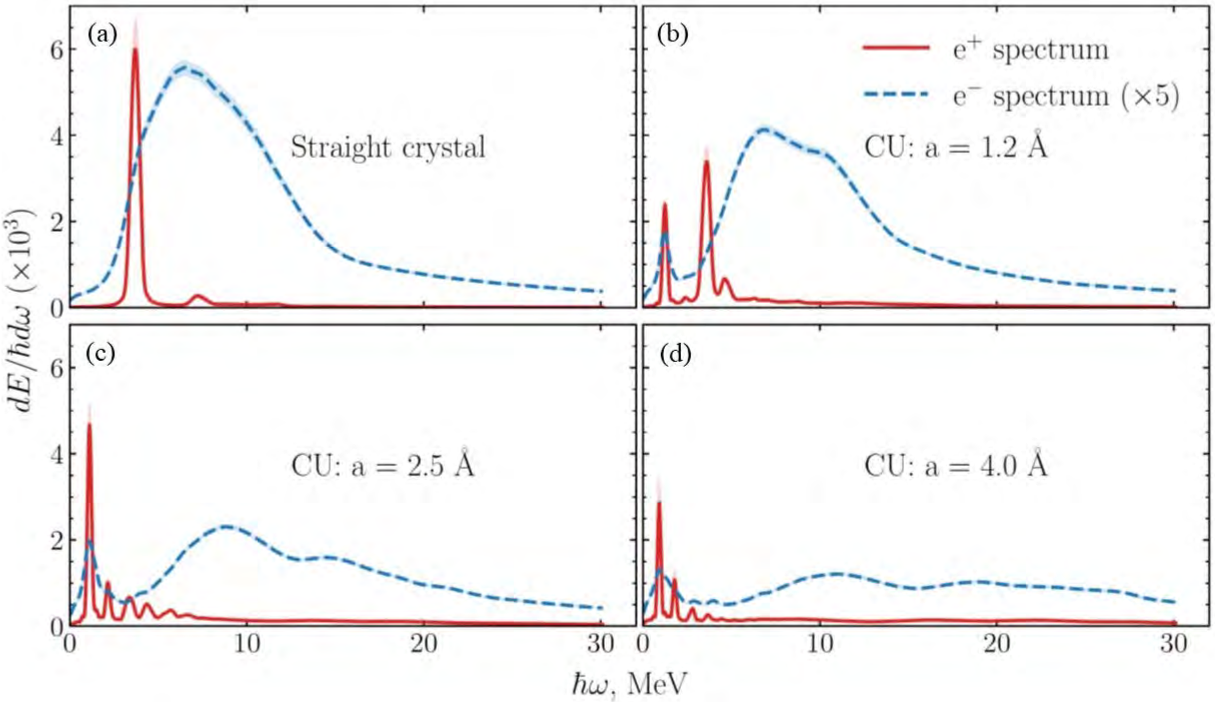


Figure 1: Spectral distribution of radiation by 855 MeV electrons and positrons for the straight (graph a) and periodically bent diamond (110) crystal for different bending amplitudes *a* (graphs b-d). The electron spectra are multiplied by factor 5. The spectra correspond to the aperture 0.24 mrad. Grey shading indicates statistical errors due to the finite number of simulated trajectories.

Several other features are to be noted in the emission spectrum of positrons. First, the ChR peak, which is very pronounced in the straight crystal and for a=1.25 Å, virtually disappears for a=2.5 and 4.0 Å. This this is due to the increasing centrifugal force in a PBC which results in dramatic decrease in the allowed values of the channeling oscillations amplitude. Second, with increase of the bending amplitude, the emission into higher harmonics, $\omega_n = n\omega_1$ (n=2,3,...), of the CU radiation becomes more pronounced (see graphs c, d).

More results obtained will be presented and discussed at the conference.

The work was supported in part by the Alexander von Humboldt Foundation Linkage Grant and by the HORIZON 2020 RISE-PEARL project. We acknowledge the Peter the Great Saint-Petersburg Polytechnic University Supercomputing Center (www.spbstu.ru) for providing the opportunities for carrying out large-scale computer simulations.

REFERENCES

[1] I.A. Solov'yov, A.V. Yakubovich, P.V. Nikolaev, I. Volkovets, A.V. Solov'yov, J. Comput. Chem. **33** (2012) 2412-2439

[2] http://mbnresearch.com/get-mbn-explorer-software

[3] A.V. Korol, A.V. Solov'yov, W. Greiner, *Channeling and Radiation in Periodically Bent Crystals*. (Second ed., Springer-Verlag, Berlin Heidelberg, 2014)

[4] A.V. Korol, V.G. Bezchastnov, G.B. Sushko, A.V. Solov'yov, *Nucl. Instrum. Meth.* B **387** (2016) 41

[5] H. Backe, W. Lauth, *Nucl. Instrum. Meth*. B **355** (2015) 24

EXPERIMENTAL INVESTIGATION OF THE ELECTROMAGNETIC RADIATION EMITTED BY SUB-GEV ELECTRONS IN A BENT CRYSTAL

L. Bandiera[1], A. Sytov[1], A. Mazzolari[1], M. Romagnoni[1], V. Guidi[1], D. De Salvador[2], P. Klag[3], W. Lauth[3], V. Tikhomirov[4]

[1]INFN, Sezione di Ferrara
Via Saragat 1, 44122 Ferrara, Italy
E-Mail corresponding author: bandiera@fe.infn.it
[2]INFN, Laboratori Nazionali di Legnaro
Viale dell'Università 2, 35020 Legnaro (PD), Italy
[3]Institut für Kernphysik, Johannes Gutenberg-Universität Mainz,
Johann-Joachim-Becher-Weg 45, 55128 Mainz, Germany
[4]Institute for Nuclear Problems of Belarusian State University
Ulitsa Bobruyskaya 11, Minsk, Belarus

In this work we report the investigation of electromagnetic radiation emitted by 855 MeV electrons deflection and radiation by ultrathin silicon and germanium crystals, bent along (111) planes, carried on at the MAinzer Mikrotron. The crystal length of 15 μm was chosen to be comparable with the dechanneling length of electrons. In order to make the measurements for different values of bending radius of the same crystal we used a piezo-actuated dynamical holder, allowing one a remote change of the crystal curvature [1].

For silicon the measured channeling efficiency exceeded 35 %, being a new record for negatively charged particles [2]. On the other hand, for germanium the efficiency turned out slightly below 10% due to the stronger contribution of multiple scattering. However, this is the first evidence of negative beam steering by planar channeling in a Ge crystal at sub-GeV energies.

The radiation spectra were measured in dependence on the crystal curvature and its orientation for both silicon and germanium bent crystals. All the results were critically compared with Monte Carlo simulations [3,4].

These results are relevant for crystal-based beam steering as well as for the generation of e.m. radiation in either bent or periodically bent crystals.

REFERENCES

[1] D. De Salvador et al., JINST 13 (2018) C04006.
[2] A. Sytov, L. Bandiera et al., Eur. Phys. J. C 77 (2017) 901.
[3] L. Bandiera et al., Nucl. Instr. Meth. Phys. Res. B 355 (2015) 44.
[4] A. Sytov, V. Tiknomirov, Nucl. Instr. Meth. Phys. Res. B 355 (2015) 383.

Biological systems and application of nanoparticles

CHEMO-RADIOTHERAPEUTIC NANOPARTICLES FOR CANCER RADIOTHERAPY

Jon Golding

The Open University, Milton Keynes, United Kingdom

Monte Carlo simulations predict a minimal effect of element choice on megavoltage radiosensitisation. We have examined the radiosensitising potential of several metal oxide nanoparticles and find that there are differences in the amount of hydroxyl radicals produced upon irradiation. Moreover, nanoparticles exhibit differences in toxicity towards HSC-3 skin cancer cells. The combination of chemo-toxicity and radiation-induced radical production highlight interesting element choices for the development of nanoparticle radiosensitisers.

INTERACTION OF SINGLE MOLECULES WITH RADIATION STUDIED BY MEANS OF DNA ORIGAMI PLATFORMS

Ilko Bald[1,2], Jenny Rackwitz[1], Robin Schürmann[1,2], Kenny Ebel[1,2]

[1]Institute of Chemistry, University of Potsdam,
Karl-Liebknecht-Str. 24-25, 14476, Potsdam, Germany
[2]Department of Analytical Chemistry and Reference Materials, BAM Federal Institute for Materials Research and Testing,
Richard-Willstätter-Str. 11, 12489, Berlin, Germany
E-mail: bald@uni-potsdam.de

DNA origami nanostructures allow for the precise placement of functional entities such as metal nanoparticles, fluorescent dyes and specific DNA sequences. We have recently demonstrated that gold nanoparticles can be arranged on DNA origami structures to create intense hot spots for surface-enhanced Raman scattering (SERS).[1] The advantages of using DNA origami nanostructures as SERS substrates are the high control over the interparticle gap size and the possibility to place a single analyte molecule precisely into the hot spot in between the particles. In this way it is possible to detect single molecules by Raman spectroscopy by depositing the DNA origami nanostructures on surfaces and by correlating Raman images with atomic force microscopy (AFM) images.[2] DNA origami can also be used to create more complex plasmonic nanostructures consisting of more than two particles of defined size and distance.[3,4] In this way single protein molecules can be detected by SERS.[4] The longterm goal is to follow chemical reactions on a single-molecule level by SERS in order to identify the most relevant intermediates in chemical reactions.

DNA origami platforms can also be used to quantify DNA strand breaks in oligonucleotides induced by low-energy electrons and VUV photons, which is pivotal for a fundamental understanding of DNA radiation damage and the processes underlying cancer radiation therapy. [5] DNA strand breaks in specific target sequences on a single-molecule level can be detected by AFM. In the present contribution DNA strand breaks in oligonucleotides modified with electrophilic radiosensitizers, such as 5-Bromouracil, induced by low-energy electrons und VUV photons will be discussed.[5-7]

REFERENCES

[1] J. Prinz, B. Schreiber, L. Olejko, J. Oertel, J. Rackwitz, A. Keller, I. Bald *J. Phys. Chem. Lett.* **4**, 4140 (2013).
[2] J. Prinz, C. Heck, L. Ellerik, V. Merk, I. Bald *Nanoscale* **8**, 5612 (2016).
[3] C. Heck, J. Prinz, A. Dathe, V. Merk, O. Stranik, W. Fritzsche, J. Kneipp, I. Bald *ACS Photonics* **4**, 1123 (2017).
[4] C. Heck, Y. Kanehira, J, Kneipp, I. Bald, *Angew. Chem. Int. Ed.* **57**, 7444 (2018).
[5] R. Schürmann, S. Vogel, K. Ebel, *Chem. Eur. J.* **24**, 10271 (2018).
[6] J. Rackwitz, J. Kopyra, I. Dabkowska, K. Ebel, M. Lj. Rankovic, A. R. Milosavljevic, I. Bald, *Angew. Chem. Int. Ed.* **55**, 10248 (2016).
[7] R. Schürmann, T. Tsering, K. Tanzer, S. Denifl, S. V. K. Kumar, I. Bald, *Angew. Chem. Int. Ed.* **56**, 10952 (2017).

Fr-I-3

EFFECT OF OXIDATION ON THE STABILITY OF AMYLOID PROTOFIBRIL

Jamoliddin Razzokov, Maksudbek Yusupov, Annemie Bogaerts

PLASMANT research group, Department of Chemistry, University of Antwerp,
Universiteitsplein 1, 2610, Antwerp, Belgium
E-mail: jamoliddin.razzokov@uantwerpen.be

Alzheimer's disease (AD) is associated with the aggregation and accumulation of amyloid peptides in neural tissue [1]. These amyloid aggregates interact with the cell membrane, increasing its permeability, such as calcium influx, eventually leading to the activation of apoptotic signaling pathways in neuronal cells [2, 3]. Hence, amyloid aggregates or self-assembled forms of amyloid peptides (Aβ) are believed to be linked with neuronal cell death in AD. It was shown in literature that cold atmospheric plasma (CAP) considerably reduces amyloid aggregates in aqueous solution [4]. Since CAP produces a cocktail of reactive oxygen and nitrogen species (RONS), the degradation of amyloid aggregates probably occurs due to their oxidation by these RONS. Despite the tremendous investigations on the inhibition of amyloid aggregates, the effect of oxidation on the Aβ stability has not been studied in detail.

Therefore, in this study we perform molecular dynamics simulations to get insight into the conformational changes of Aβ pentamer in the presence of oxidized residues. We also estimate the effect of oxidation on the dissociation free energy of terminal peptide in Aβ pentamer, using the umbrella sampling method [5]. The specific modification (or oxidation) of Aβ residues is defined based on the reactivity of amino acids caused by CAP [6]. We create three oxidation states of Aβ pentamer, i.e., 4% (OX1), 12% (OX2) and 16% (OX3).

Our simulation results indicate that oxidized Aβ pentamer becomes more flexible upon increasing oxidation degree, thereby affecting its conformation. We also find that the role of salt bridge Asp23-Lys28 in native, OX1 and OX2 is significant to maintain the integrity of the hydrophobic core of the Aβ pentamer. On the other hand, in the case of OX3 substantial hydrophobic core opening is observed due to the disruption of the salt bridge. In order to obtain detailed information on conformational changes, we perform secondary structure analysis as given in Table 1. As is clear, in all oxidized structures the β-sheet content is reduced, which is responsible for the structural stability.

Table 1: Secondary structure analysis computed by means of STRIDE. All values are given in %.

System/ Conformation	β-sheet	β-bridge	Turn	coil	α;- 5;- 3-helix
Native	64.4	0.9	12.7	22.0	0
OX1 (4%)	62.8	1.2	12.5	23.5	0
OX3 (12%)	61.6	0.8	10.4	27.2	0
OX4 (16%)	52.5	1.4	15.5	30.6	0

The results of the umbrella sampling simulations reveal that the dissociation free energy of terminal peptide decreases upon increasing oxidation degree. This is a hallmark for the inhibition of and stability of the protofibril structure. Our results are in line with experimental observations on the degradation of amyloid aggregates induced by CAP treatment [4].

REFERENCES

[1] I.W. Hamley, *Chemical reviews*, **10**, 112 (2012).
[2] B.A. Yankner, L.K. Duffy, D.A. Kirschner, *Science*, **250**, 4978 (1990).
[3] A. Demuro, I. Parker, G.E. Stutzmann, *Journal of Biological Chemistry*, **17,** 285 (2010).
[4] D. Bayliss, J.L. Walsh, G. Shama, F. Iza, M.G. Kong, *New Journal of Physics*, **11**, 11 (2009).
[5] J. Kästner, Wiley Interdisciplinary Reviews: Computational Molecular Science, **6**, 1 (2011).
[6] E. Takai, T. Kitamura, J. Kuwabara, S. Ikawa, S. Yoshizawa, K. Shiraki, H. Kawasaki, R. Arakawa, K. Kitano, *Journal of Physics D: Applied Physics*, **28**, 47 (2014).

ACTIVATION OF THE DNA-REPAIR MECHANISM THROUGH NBS1 AND MRE11 DIFFUSION

Ida Friis[1], Ilia A. Solov'yov[1]

[1]Department of Physics, Chemistry and Pharmacy, University of Southern Denmark,
Campusvej 55, 5230, Odense, Denmark
E-mail: friis@sdu.dk
E-mail: ilia@sdu.dk

The non-homologous end joining of a DNA double strand break is initiated by the MRE11-NBS1-RAD50 complex whose subunits are the first three proteins to arrive to the breakage site thereby making the recruitment time of MRE11, NBS1 and RAD50 essential for cell survival. In the present investigation, the nature of MRE11 and NBS1 transportation from the cytoplasm to the nucleus, hosting the damaged DNA strand, is hypothesized to be a passive diffusive process.

The feasibility of such a mechanism is addressed through theoretical and computational approaches which permit establishing the characteristic recruitment time of MRE11 and NBS1 by the nucleus. A computational model of a cell is constructed from a set of biological parameters will be presented and the kinetic Monte Carlo algorithm is used to simulate the diffusing MRE11 and NBS1 particles as a random walk process. To accurately describe the experimented data, it is discovered that MRE11 and NBS1 should start diffusion from significantly different starting positions.

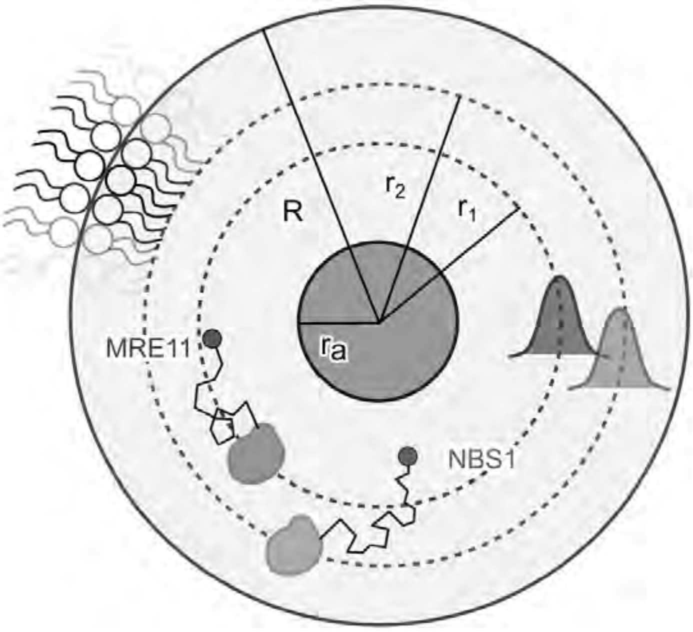


Figure 1: Model of a cell used to model the diffusion of DNA repair signaling proteins MRE11 and NBS1. The two proteins are here shown on their way from the starting point of a ribosome into the nucleus, which contains the broken DNA.

Structure and dynamics of clusters, nanoparticles and biomolecules

GAS-PHASE INTERACTIONS OF SOFT X-RAYS AND MEV IONS WITH G-QUADRUPLEX DNA

Wen Li[1], Xin Wang[1], Wessel Douma[1], Klaas Bijlsma[1], Ronnie Hoekstra[1], Marwa Abdelmouleh[2],
Michal Ryszka[2], Mathieu Lalande[2], Jimmy Rangama[2], Violaine Vizcaino[2], Jean-Christophe Poully[2],
and Thomas Schlathölter[1]

[1]Zernike Institute for Advanced Materials, University of Groningen, Nijenborgh 4, 9747AG
Groningen, The Netherlands
[2] CIMAP, UMR 6252 (CEA/CNRS/ENSICAEN/Université de Caen Normandie), Caen, France
E-mail: t.a.schlatholter@rug.nl

For almost two decades, interactions of photons and ions with gas phase biomolecules have been investigated to improve our understanding of the molecular mechanisms of radiation therapy [1]. Initially, most experimental and theoretical studies focused on relatively small DNA building blocks. In 2011, for the first time a combination of electrospray ionization and radiofrequency ion trapping was interfaced with synchrotron and ion beamlines [2,3]. A pioneering study focused on soft X-ray ionization and keV ion induced ionization of the doubly protonated oligonucleotide $[dGCAT+2H]^{2+}$. It was found that key findings obtained with DNA building blocks (for instance high stability of nucleobases and fragile nature of deoxyribose) are also found in oligonucleotides, even though fragmentation patterns are entirely different [4].

In living organisms, however, DNA occurs in de-protonated form. Our current studies therefore focus on ionization and fragmentation of oligonucleotide anions. Such studies are experimentally more challenging, because fragmentation competes with electron detachment. Furthermore, not only negatively charged product ions are formed, but also cations and neutrals.

In particular, we study interactions of soft X-rays (at the carbon, nitrogen and oxygen K-edges) and MeV carbon ions (at Bragg peak energies) with oligonucleotides of different structure (single and double stranded, G-quadruplex). For all systems under study, electron detachment is the dominant channel. For soft X-ray absorption, positive fragments are only observed for the case of relatively small oligonucleotides such as the telomeric sequence dTTAGGG. Single telomere-containing sequences tend to break in the GGG region of the sequence. In G-quadruplexes of the same telomere sequence, fragmentation is almost entirely quenched.

MeV carbon ions on the other hand, even lead to formation of small positive fragments when colliding with duplex DNA. This is in line with the notion that ions can induce complex DNA damage, such as clustered lesions.

REFERENCES

[1] G. García and M. C. Fuss (Eds.), *Radiation damage in biomolecular systems*, (Springer, Netherlands, 2012).
[2] A. R. Milosavljević et al., Phys. Chem. Chem. Phys. 13, 15432 (2011)
[3] S. Bari et al., J. Chem. Phys. 134, 024314 (2011)
[4] O. Gonzalez-Magaña et al. , J. Phys. Chem. A 87, 032702 (2013)

IRRADIATION INDUCED PROCESSES WITH RADIOSENSITIZING NANOPARTICLES

Alexey Verkhovtsev[1,2], Kaspar Haume[2], Pablo de Vera[2], Eugene Surdutovich[3], Nigel J. Mason[4], Andrey V. Solov'yov[2]

[1]German Cancer Research Center (DKFZ), 69120 Heidelberg, Germany
[2]MBN Research Center, 60438 Frankfurt am Main, Germany
[3]Department of Physics, Oakland University, Rochester, 48309 Michigan, USA
[4]School of Physical Sciences, The Open University, MK7 6AA Milton Keynes, UK
E-mail: a.verkhovtsev@dkfz-heidelberg.de

Metal nanoparticles (NPs) made, e.g., of gold, platinum or gadolinium have been proposed as novel agents for more efficient treatment of tumors with ionizing radiation. It is believed that NPs made of these metals have capacity to enhance the biological damage induced by energetic photon and ion-beam irradiation, i.e. to act as radiosensitisers [1,2]. The radiosensitising effect of metal NPs is commonly related to strong irradiation-induced emission of secondary electrons, which activate hydrolysis of the surrounding aqueous medium and thus increase the yield of hydroxyl radicals (OH•) and other reactive oxygen species that may produce damage to tumor cells.

Radiosensitising NPs are usually synthesized with an organic coating to reduce toxicity, improve stability in physiological conditions and target specific biological sites. A large number of possible coating molecules form a vast landscape of "metal core - organic coating" combinations. Many different parameters can be varied to optimize the radiosensitising properties of NPs (e.g., the size, shape and composition of a metal core; thickness, composition and density of the coating) which makes it challenging to systematically explore each of them experimentally.

This talk will present a recently developed theoretical and computational approach to analyze formation and transport of secondary electrons and hydroxyl radicals after irradiation of coated metal NPs with ions [3]. This methodology accounts for the detailed atomistic structure of the coating material around the metal core, which was simulated by means of the MBN (Meso-Bio-Nano) Explorer software [4,5]. It also takes into account the important low-energy and many-body phenomena such as collective electron excitations (the surface and volume plasmons) in the metallic core. It was shown previously that these collective excitations of delocalized electrons in small metallic NPs are the source of intense emission of low-energy electrons [6]. Results for the case study of a gold NP coated with polyethylene glycol (PEG) and irradiated with 0.1 - 10 MeV/u carbon ions will be presented.

One of the further developments of this methodology concerns the analysis of ion irradiation induced fragmentation of coated metal NPs. Collisions with the NPs of experimentally relevant sizes can be efficiently explored by means of modern computational methods based on molecular dynamics. Recent implementations in MBN Explorer, such as the reactive interatomic force fields [7] and the Irradiation Driven Molecular Dynamics (IDMD) approach [5,8], provide tools for modeling of collisions, wherein the dynamics of MBN systems is accompanied by random, local quantum transformations (e.g., breakage and formation of covalent bonds, charge transfer, etc.) induced in the system during the collision process. The application of these methods for modeling of irradiation induced processes will be briefly outlined.

REFERENCES

[1] K. Haume et al., *Cancer Nanotechnol.* **7**, 8 (2016)

[2] A.V. Solov’yov (ed.), *Nanoscale Insights into Ion-Beam Cancer Therapy* (Springer International Publishing, Cham, Switzerland, 2017)
[3] K. Haume, P. de Vera, A. Verkhovtsev, E. Surdutovich, N.J. Mason, A.V. Solov’yov, *Eur. Phys. J. D* **72**, 116 (2018)
[4] I.A. Solov’yov, A.V. Yakubovich, P.V. Nikolaev, I. Volkovets, A.V. Solov’yov, *J. Comput. Chem.* **33**, 2412 (2012)
[5] I.A. Solov’yov, A.V. Korol, A.V. Solov’yov, *Multiscale Modeling of Complex Molecular Structure and Dynamics with MBN Explorer* (Springer International Publishing, Cham, Switzerland, 2017)
[6] A. Verkhovtsev, A.V. Korol, A.V. Solov’yov, *Phys. Rev. Lett.* **114**, 063401 (2015); *J. Phys. Chem. C* **119**, 11000 (2015)
[7] G.B. Sushko, I.A. Solov’yov, A.V. Verkhovtsev, S.N. Volkov, A.V. Solov’yov, *Eur. Phys. J. D* **70**, 12 (2016)
[8] G.B. Sushko, I.A. Solov’yov, A.V. Solov’yov, *Eur. Phys. J. D* **70**, 217 (2016)

ELECTRON ATTACHMENT IN BIOMOLECULAR MODELS OF INCREASING COMPLEXITY

Jaroslav Kočišek, Michal Fárník, Juraj Fedor

Department of Dynamics of Molecules and Clusters, J. Heyrovský Institute of Physical Chemistry
of the CAS, v. v. i., Dolejškova 2155/3, 182 23 Prague 8, Czech Republic
E-mail: kocisek@jh-inst.cas.cz

The understanding of processes in biological systems on the molecular level requires systematic studies of elementary reactions of biomolecules. The most detailed information can be obtained from studies of isolated molecules in the gas phase. However, to apply such information in a description of biological processes requires careful inspection of changes in reaction dynamics induced by a surrounding environment. The presentation overviews our studies of how the environment influences the electron attachment (EA).

One of the most important processes induced by EA in biological systems is the molecular fragmentation at sub-excitation energies via dissociative electron attachment (DEA). In our study of microhydrated uracil and thymine [1], we demonstrated that a water environment can significantly suppress DEA. The suppression, observed also in the pulsed radiolysis study in solution [2], may be caused by caging of the dissociating hydrogen proposed in the recent theoretical study [3]. Such caging is accompanied with a significant energy release to the water as demonstrated in our study of halouracils [4]. This may be important in radiation chemistry, where the interactions of secondary low-energy electrons with molecules or nanoparticles possessing high electron affinity can increase the value of LET (linear energy transfer). But the role of water is not restricted to the passive thermal bath effects. Water can react with anions created by EA and enable charge and hydrogen transfer, which are inaccessible in isolated molecules. This will be demonstrated on our recent results for EA to microhydrated nucleotide deoxycytidine monophosphate (dCMP) [5].

Acknowledgement: This work was supported by Czech Science Foundation grant no. 16-10995Y.

REFERENCES

[1] J. Kočišek, A. Pysanenko, M. Fárník, J. Fedor, JPC Letters 7, 3401 (2016)
[2] J. Ma, F. Wang, S. A. Denisov, A. Adhikary, M. Mostafavi, Sci. Adv. 3, e1701669 (2017)
[3] J. Kohanoff, M. McAllister, G. A. Tribello, B. Gu, J. Phys.: Condens. Matter 29, 383001 (2017)
[4] J. Poštulka, P. Slavíček, J. Fedor, M. Fárník, J. Kocisek, JPC B 121, 8965 (2017)
[5] J. Kočišek, B. Sedmidubská, S. Indrajith, M. Fárník, J. Fedor, JPC B 122, 5212 (2018)

AN EFFECT OF THE SPACE DIMENSION OF ELECTRON FERMI-GAS UPON THE SPIN ORDERING IN CLUSTERS AND NANOPARTICLES

Orlenko E V[1], Orlenko F E [2]

[1]Theoretical Physics Department, Peter the Great St.Petersburg Polytechnic University,
Polytechnicheskaya, 29, 195251, St.Petersburg, Russia
E-mail: eorlenko@mail.ru
[2] Department of Physics, St.Petersburg State Chemical Pharmaceutical Academy,
Professor Popov's St., 197022, St.Petersburg, Russia
E-mail: fadler@mail.ru

The goal of the present research is to analyze a general effect of a dimension size upon the spontaneous polarization in the electron Fermi-gas. The possibility of spontaneous magnetism was discussed theoretically using the Hartree–Fock method, the Landau Fermi-liquid formalism, Heisenberg variation model [1,2] . We perform a general consideration of low dimension fermi-objects, like metallic (or semiconductors) nanoparticles with sizes ν=1,2 and quasi-low dimensions ν*=0,1,2 metallic clusters corresponding to the "pseudo" sizes ν=6,5,4. Thermodynamic properties of the electron Fermi-gas of an arbitrary dimension will be discussed in general consideration. We have developed the general criteria for appearing the spontaneous polarization in the electron Fermi-gas of arbitrary dimension.

We calculated the total energy of the arbitrary dimension system, as well as the exchange contribution per particle using the Hartree–Fock method. The dependence of the energy per particle on the polarization degree of the system has been determined. It isshown that spontaneous polarization exits in the system when a universal parameter of the particles density satisfies the inequality rs ≥rs*. We have analytically developed this parameter in general form:

$$r_s * = \frac{2C_{2\nu}}{C_{1\nu}} \frac{\left(\left(1+\alpha\right)^{\frac{\nu+2}{\nu}} + \left(1-\alpha\right)^{\frac{\nu+2}{\nu}} \right)}{\left(\left(1+\alpha\right)^{\frac{\nu+1}{\nu}} + \left(1-\alpha\right)^{\frac{\nu+1}{\nu}} \right)},$$

which is useful for each type of dimension size. A comparative analysis of one-, two- to six-dimensional systems is performed. We have obtained a general expression for the total energy per particle as a function of the polarization and dimension of the system. According to this expression, the possibility of spontaneous polarization in the system is dependent of the dimension of the system:

$$\frac{E}{N} = \frac{C_{2\nu}}{r_s^2} \left(\left(1+\alpha\right)^{\frac{\nu+2}{\nu}} + \left(1-\alpha\right)^{\frac{\nu+2}{\nu}} \right) - \frac{C_{1\nu}}{r_s} \left(\left(1+\alpha\right)^{\frac{\nu+1}{\nu}} + \left(1-\alpha\right)^{\frac{\nu+1}{\nu}} \right).$$

REFERENCES
[1].F. E. Orlenko, G. G. Zegrya, and E. V. Orlenko, *Tech. Phys.*, **53**, 978 (2008)
[2].F.E. Orlenko, S.I. Chelkak, E.V. Orlenko, G.G. Zegrya, *JETP*, **110** (5), 805 (2010)

Poster Presentations

CHANNELING OF ELECTRONS AND POSITRONS IN PERIODICALLY BENT DIAMOND CRYSTAL

A.V. Pavlov[1,2], K.B. Agapev[2], V.K. Ivanov[2], A.V. Korol[2,3], A.V. Solov'yov[3]

[1]St. Petersburg State Maritime University, Leninsky ave. 101, 198262, St. Petersburg, Russia
[2]Department of Experimental Physics, Peter the Great St. Petersburg Polytechnic University,
Polytechnicheskaya 29, 195251, St. Petersburg, Russia
E-mail: a.pavlov@physics.spbstu.ru
[3]MBN Research Center, Max-von-Laue-Str. 1, 60438, Frankfurt am Main, Germany

Creation of new light sources is an important part of scientific progress. Light sources with photon energy in sub-GeV energy range can open new possibilities for various scientific experiments and technological applications [1]. One of the promising ways of generating such photons relies on propagating ultra-relativistic charged particles through a periodically bent crystals (PBC). In this device, called a Crystalline Undulator (CU) additional emission appears due to the periodicity of the projectile trajectory which follows the shape of periodic bending. To tune the emitted photon energy and intensity one can vary the bending period, λ_u, and amplitude, a. To provide numerical results of high level of predictivity, one must rely on a software package which allows for accurate simulation of the projectile motion in a crystalline environment.

For our purposes, we used the MBN Explorer [2] software package to simulate the crystalline structure and the trajectories of ultra-relativistic particles as well as to calculate spectral and angular distributions of the radiation emitted [3].

The parameters used in the simulations were chosen to match those used in the ongoing experiments at the MAinz MIcrotron (MAMI) facility [4]. Namely, the energy of the projectiles was considered within the range 270-855 MeV. Both electron and positron channeling along oriented diamond (110) was simulated. Channeling properties and emission spectrum were calculated for the straight crystals as well as for the PBCs with different bending amplitudes a = 1.2, 2.5 and 4.0 Å. The bending period was fixed at the value of 5 microns. The crystal thickness along the incident beam direction is 20 microns. Spectral distribution was calculated for several apertures including that of 0.24 mrad which corresponds to the MAMI experimental setup.

Figure 1 shows the emission spectra for electrons (left panels) and positrons (right panels) of different energies, as indicated. The upper row, graphs (a), corresponds to the straight diamond (110) crystal. In this case the spectra are dominated by peaks due to the channeling radiation. Graphs (b) and (c) correspond to PBCs. In this case, the additional peaks appear in the low-energy part of the spectra due to the radiation.

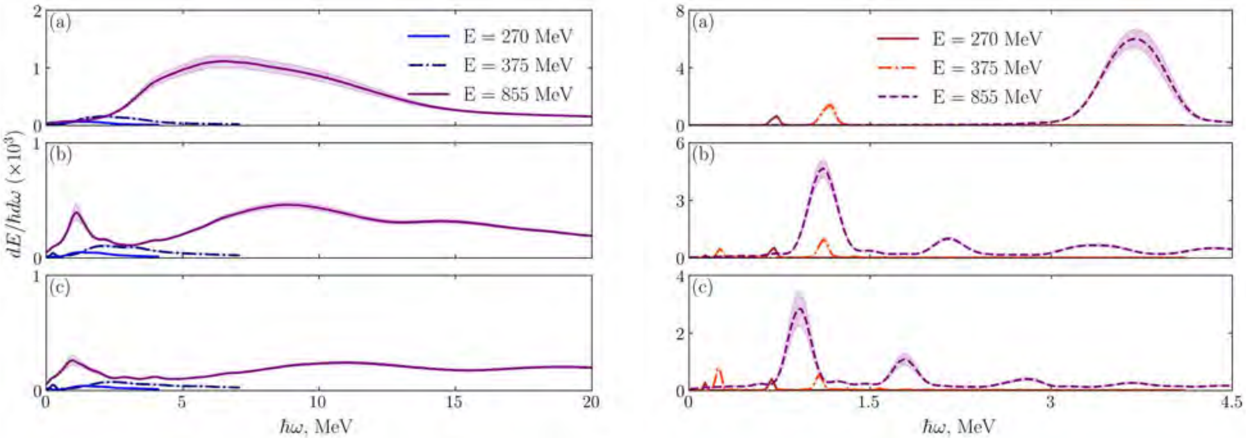


Figure 1. Emission spectra by electrons (left panels) and positrons (right) channeling in straight, (a), and periodically bent, (b) *a*=2.5 Å, (c) *a* = 4.0 Å, diamond (110) crystals. The data refer to the aperture 0.24 mrad.

An interesting feature to be pointed out is the sensitivity of the intensity of the channeling radiation in PBC to the increase of the beam energy. That effect is mostly seen for the 855 MeV positrons: the powerful peak of the channeling radiation in the straight crystal virtually disappears in the PBCs. Theoretical analysis of channeling properties and numerical analysis of trajectories were used to explain that result.

More results of the calculations together with their qualitative and quantitative analysis will be presented at the conference.

The work was supported in part by the Alexander von Humboldt Foundation Linkage Grant and by the HORIZON 2020 RISE-PEARL project. We acknowledge the Peter the Great Saint-Petersburg Polytechnic University Supercomputing Center (www.spbstu.ru) for providing the opportunities for carrying out large-scale computer simulations.

REFERENCES

[1] A.V. Korol, A.V. Solov'yov, W. Greiner. Channeling and Radiation in Periodically Bent Crystals. Springer Verlag, Berlin Heildeberg, second edition, 2014.
[2] I. A. Solov'yov, A. V. Yakubovich, P. V. Nikolaev, I. Volkovets, A. V. Solov'yov. MesoBioNano explorer—a universal program for multiscale computer simulations of complex molecular structure and dynamics. J. Comput. Chem. **33** (2012) 2412–2439.
[3] G. B. Sushko, V. G. Bezchastnov, I. A. Solov'yov, A. V. Korol, W. Greiner, A. V. Solov'yov. Simulation of ultra-relativistic electrons and positrons channeling in crystals with MBN explorer. J. Comput. Phys. **252** (2013) 404–418.
[4] H. Backe, W. Lauth, Nucl. Instrum. Meth. B **355** (2015) 24.

A NEGATIVE ION FORMATION IN VIEW OF EXCHANGE PERTURBATION THEORY METHOD

Alexandr Evstafev[1], Elena Orlenko[1,2]

[1]Department of “Theoretical Physics”, Peter the Great St.Petersburg Polytechnic University,
Polytechnicheskaya, 29, 195251, St.Petersburg, Russian Federation
E-mail: evstafev93@mail.ru
[2]E-mail: eorlenko@mail.ru

By using a formalism of Exchange perturbation theory (EPT) [1,2] in its invariant form we calculate a cross section for the process of formation a negative Helium- ion. The obtained expression for the cross section accounts all exchange contributions with respect to all electrons permutations: $\sigma_{fi} = \frac{2\pi\mu_i}{\hbar^2 k_i}\delta(E_f - E_i)\left|\left\langle \Psi_f^0 \middle| \hat{T} \middle| \Phi_i^{0(0)} \right\rangle\right|^2$, where an initial state ket –vector is $\left|\Phi_i^0\right\rangle = \frac{1}{f_{\mathrm{He}}}\Psi_{\mathrm{He}}(\vec{r}_1,\vec{r}_2)\mathrm{X}_{He}(\xi_1,\xi_2)\frac{1}{(2\pi\hbar)^{3/2}}\exp(i\vec{k}_i\vec{r}_3)\chi(\xi_3)$ and an antisymmetric bra-vector of a final state is $\left\langle\Psi_f\right| = \hat{A}\Phi_f^0(1,2,3) = \hat{A}\psi_{1s}(\vec{r}_1)\psi_{2p}(\vec{r}_2)\psi_{5s}(\vec{r}_3)\chi_1(\xi_1)\chi_2(\xi_2)\chi_3(\xi_3)$

The formalism of the time-dependent exchange perturbation theory is applicable for cases of restructuring colliding particles, such as ion charge exchange or electron capture processes, and takes into account electron permutations among colliding centers. EPT allows representing the computation results of Helium-electron colliding process with electron capture in the analytical form. . Preliminary results are in a good agreement with experimental dates.

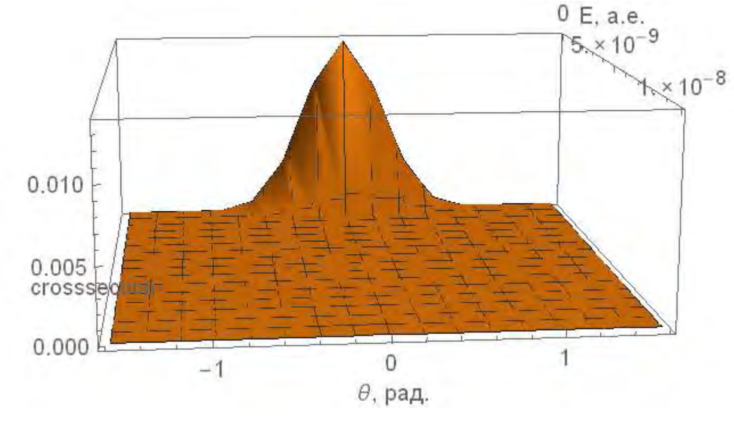


Figure 1: Cross section of the scattering process with an electron capture.

REFERENCES

[1] E.V. Orlenko, A.V. Evstafev, F.E. Orlenko, *JETP*, Vol. **120**, (2) 296 (2015)
[2] E.V. Orlenko, T. Latychevskaia, A.V.Evstafev, F.E. Orlenko, *Theoretical Chemistry Accounts*, **134**, 41 (2015)

FIBRONECTINS ADHESION TO GRAPHENE

Anders Frederiksen, Ilia A. Solov'yov

Department of Physics, Chemistry and Pharmacy, University of Southern Denmark,
Campusvej 55, 5000, Odense, Denmark
E-mail: afred15@student.sdu.dk

The mechanisms of cellular growth has attracted scientists' attention for a long time. In the quest to understand how this complex biological process occurs, recent investigations [1,2] have focused on artificial growth of stem cells atop of inorganic surfaces such as graphene. Stem cells are specifically interesting as these cells are considered being critically important in human embryonic development [1]. It became apparent that certain proteins are likely responsible for holding cells on top of graphene surfaces, fibronectin being one of them [3].

We have investigated the adhesion of fibronectin to graphene through simulations as pictured in Figure 1. The simulations suggest that fibronectin can bind to graphene, with arginine residues being the best contributors. The strength of arginine attraction to the graphene surface was further investigated through single amino acid simulations and the best/ worst amino acid binders were revealed. In order to better understand the amino acid – graphene interaction quantum chemical simulations were carried out. As size is a limiting factor of quantum chemical simulations the system was reduced to a single amino acid on top of a C6-symmetric graphene patch. The quantum chemical simulations confirmed that the adhesion energy of the single amino acids to the graphene is lowered due to the induced polarization forces, and demonstrated that this effect could become substantial and therefore further stabilize fibronectin binding to graphene.

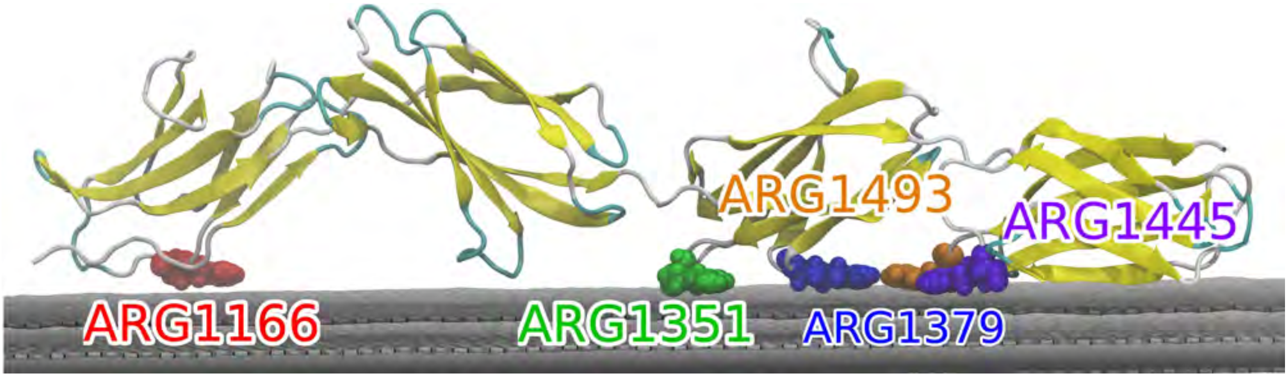


Figure 1: Fibronectin on top of graphene as used in the simulations with the best binding arginines highlighted.

REFERENCES
[1]. D. B. Leahy, I. Aukhil and H. P. Erickson, *Cell Press* **84** (1996)
[2] Kenry et al. *Biomaterials* **155** (2018)
[3] B. Zhang, P. Wei, Z, Zhou and T. Wei, *Advanced Drug Delivery Reviews* **105** (2016)

CROSS SECTIONS AND ELECTRONIC ENERGIES FOR NUCLEOTIDES UPON COLLISION WITH CHARGED CARBON IONS

Andreas Alberg-Fløjborg, Adrian Bøgh Salo, Ilia A. Solovyov

Department of Physics, Chemistry and Pharmacy,
University of Southern Denmark, Campusvej 55, DK-5230 Odense M, Denmark
anfol14@student.sdu.dk

In a recent study [1], it was computationally demonstrated that collisions between a charged carbon ion and a cytosine-guanine (CYT+GUA) nucleotide pair induces a large number of free electrons into the cellular medium. These secondary electrons have been reported to be the major cause to the damage produced during the ion bean cancer therapy treatment, i.e. by forming reactive free radical species or causing DNA single strand breaks (SSB) and double strand breaks (DSB) [2-5].

Here we continue the earlier investigations from [1] and characterize the collision between the charged carbon ion and the CYT+GUA pair, by calculating the collision cross section, the average energy of released electrons and their energy ranges. Specifically, ionization, electronic release, electron capture by the C^{4+}, and the free electrons production cross sections were established. The results show that electrons are produced with energies ranging as high as 129 eV and an average of 21 eV with the mean energy highly dependent on the impact angle. Calculations of the differential cross sections for electrons produced with energies 30-40 eV are comparable with experimental data for protons with energy 1.2 MeV colliding with adenine [6]. Furthermore, calculations of the total ionization cross section are of the same order as the combined ionization cross section of cytosine and guanine upon collision with 0.1 MeV protons [5].

REFERENCES

[1] A. B. Salo, A. Alberg- Fløjborg, and I. A. Solov'yov, Phys. Rev. A 98, 012702 (2018).
[2] E. Surdutovich, O. Obolensky, E. Scifoni, I. Pshenichnov, I. Mishustin, A. V. Solov'yov, and W. Greiner, The European Physical Journal D 51, 63 (2009).
[3] E. Surdutovich and A. V. Solov'yov, Journal of Physics: Conference Series 438 (2012).
[4] E. Surdutovich and A. V. Solov'yov, The European Physical Journal D 68, 353 (2014).
[5] A. Solov'yov, Nanoscale Insights into Ion-Beam Cancer Therapy (Springer, 2017).
[6] Y. Iriki, M. Imai, and A. Itho, Physical Review A 84, 032704 (2011).

FREE ELECTRON PRODUCTION FROM NUCLOTIDES UPON COLLISION WITH CHARGED IONS

Adrian Bøgh Salo, Andreas Alberg-Fløjborg, Ilia A. Solovyov

Department of Physics, Chemistry and Pharmacy,
University of Southern Denmark, Campusvej 55, DK-5230 Odense M, Denmark
anfol14@student.sdu.dk

Ion beam cancer therapy has become increasingly favored worldwide in treatment of certain types of cancer over the last decade [1,2]. Whereas the clinical effects of the therapy are well documented, the understanding of the underlying physical mechanisms is somewhat incomplete. The problem arises due to the multiscale nature of the effects involved in ion beam cancer therapy, as the effects range from quantum mechanical to macroscopic scales [3-6]. The present study investigates the production of free electrons in the vicinity of the Bragg peak [7] through quantum mechanical simulations of the collision between a C^{4+} ion with a cytosine-guanine nucleotide pair taken from a DNA double helix. Time dependent density functional theory was employed using the Octopus 6.0 software [8-10]. The results show that such a collision triggers the release of a large number of electrons into the cellular environment, as only a fraction is captured by the C^{4+} ion; an exemplary process is illustrated in Fig. 1. Furthermore, it is demonstrated that the impact angle and projectile kinetic energy has much more influence on the number of ejected electrons than the impact parameter [11].

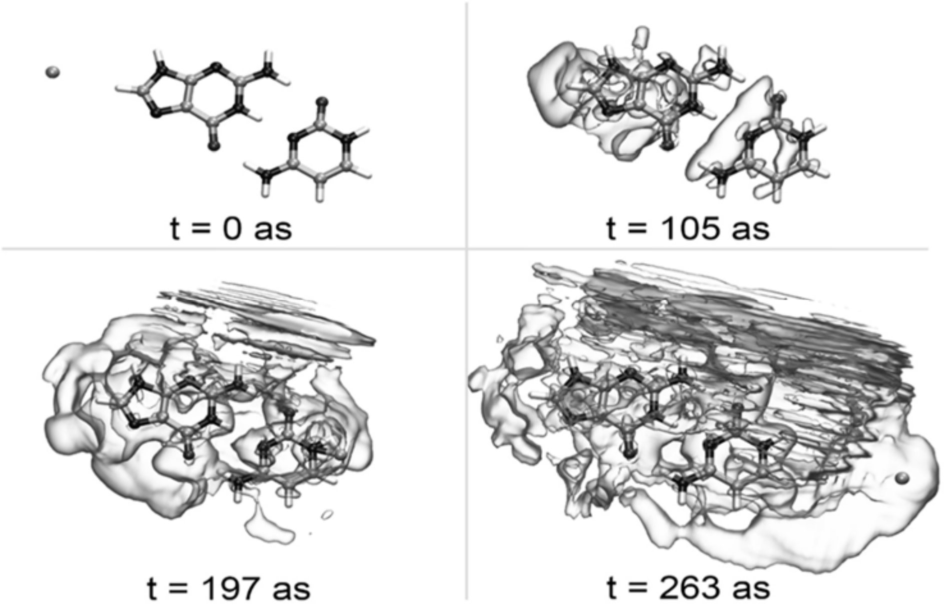


Figure 1: Visualization of the collision between a C^{4+} ion and a cytosine-guanine nucleotide pair. The transparent cloud represents an increase in the local electronic density.

REFERENCES

[1] W. P. Levin, H. Kooy, J. S. Loe_er, and T. F. DeLaney, British Journal of Cancer 93, 849 (2005).

[2] U. Amaldi and G. Kraft, Reports on Progress in Physics 68, 1861 (2005).

[3] E. Surdutovich and A. V. Solov'yov, Journal of Physics: Conference Series 438 (2012).

[4] A. Verkhovtsev, E. Surdutovich, and A. V. Solov'yov, \Predictive assessment of biological damage due to ion beams," in Nanoscale Insights into Ion-Beam Cancer Therapy, edited by A. V. Solov'yov (Springer International Publishing, Cham, 2017) pp. 359{377.

[5] A. Solov'yov, Nanoscale Insights into Ion-Beam Cancer Therapy (Springer, 2017).

[6] A. Verkhovtsev, E. Surdutovich, and A. V. Solovyov, Scienti_c reports 6 (2016).

[7] W. Bragg, The London, Edinburgh, and Dublin Philosophical Magazine and Journal of Science 8, 726 (1904).

[8] M. Marques, A. Castro, G. F. Bertsch, and A. Rubio, Computer Physics Communications 151, 60 (2003).

[9] A. Castro, M. Oliveira, C. Rozzi, X. Andrade, F. Lorenzen, M. Marques, E. Gross, and A. Rubio, Physica Status Solidi B 243, 2465 (2006).

[10] X. Andrade, D. Strubbe, A. Larsen, M. J. T. Oliveira, J. Alberdi-Rodriguez, A. Varas, I. Theophilou, N. Helbig, M. Verstraete, L. Stella, F. Nougueira, A. Aspuru-Guzik, A. Castro, M. A. L. Marques, and A. Rubio, Physical Chemistry Chemical Physics 17, 31371 (2015).

[11] A. B. Salo, A. Alberg-Fl_jborg, and I. A. Solov'yov, Phys. Rev. A 98, 012702 (2018).

AN ADIABATIC POTENTIAL OF THE HE-H INTERACTION

Barilov Andrey[1], Orlenko Elena[2]

[1]Department of Physical Electronics, Peter the Great St. Petersburg Polytechnic University,
Polytechnicheskaya St. 29, 195251, St. Petersburg, Russia
E-mail: andreybarilov@gmail.com
[2]Theoretical Physics Department, Peter the Great St. Petersburg Polytechnic University
Polytechnicheskaya St. 29, 195251, St. Petersburg, Russia
E-mail: eorlenko@mail.ru

We present a formalism of the Exchange perturbation theory (EPT) [1, 2] that accounts for the general identity principle of electrons that belong to the different atomic centers. The set of anti-symmetrized wave functions is non-orthogonal; nevertheless, it possesses a completeness property. A special invariant form of an Hamiltonian that describes an unperturbed system and for perturbation operator is developed with respect to interatomic electrons permutations. It makes possible to obtain properly antisymmetric corrections to the antisymmetrized wave functions of zeroth approximation. A perturbation theory has two small parameters, they are: the overlap degree of the wave functions and the small parameter of the interatomic interaction (perturbation). The EPT formalism has a standard form of an invariant perturbation theory that accounts for intercentre electron permutations among overlapping non-orthogonal states. As an example of the EPT formalism application, we consider an adiabatic potential of the Hydrogen-Helium interaction.

We have developed an analytical expression for the H-He potential in the form:

$$U(R) = E_i^1 = \left\langle \Psi \middle| V_{p=0} \middle| \Phi^{p=0} \right\rangle = \frac{4}{3f_0(R)}\left(K(R) - A_{23}(R)\right);$$

$$K = \left(\varphi_{He}(1)\varphi_{He}(2)\psi_H(3)\left| -\frac{2}{r_{He3}} - \frac{1}{r_{H1}} - \frac{1}{r_{H2}} + \frac{2}{R} + \frac{1}{r_{23}} + \frac{1}{r_{13}} \right| \varphi_{He}(1)\varphi_{He}(2)\psi_H(3)\right)$$

$$A_{23}(R) = \left(\varphi_{He}(1)\varphi_{He}(3)\psi_H(2)\left| -\frac{2}{r_{He3}} - \frac{1}{r_{H1}} - \frac{1}{r_{H2}} + \frac{2}{R} + \frac{1}{r_{23}} + \frac{1}{r_{13}} \right| \varphi_{He}(1)\varphi_{He}(2)\psi_H(3)\right)$$

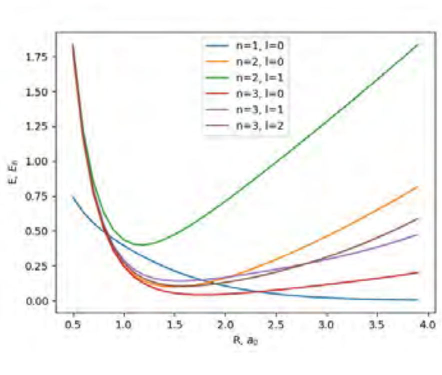


Figure 1: Analytically calculated potential He-H for the ground and excited states of Hydrogen.

REFERENCES

[1] Orlenko, E.V.; Latychevskaya, T.; Evstafev, A.V. ; Orlenko, F.E. *Theor Chem Acc* **134**, 5, 28 (2015)

[2] Orlenko, E.V. ; Evstafev, A.V. ; Orlenko, F.E. *JETP,* **120**, 296 . (2015)

INITIAL RADIATION DNA DAMAGE OBSERVED IN PREMATURELY CONDENSED G2 CHROMOSOMES OF HUMAN LIMPHOCYTES AND ANALYTICAL MODEL OF ION TRACKS

A. Kowalska[1], E. Nasonova[2] , K. Czerski[3] , P. Kutsalo[2] , E. Krasavin[2]

[1]Faculty of Marine Engineering, Maritime University of Szczecin,
Wały Chrobrego 1-2,70-500, Szczecin, Poland
E-mail: a.kowalska@am.szczecin.pl
[2]Joint Institute for Nuclear Research,
Joliot-Curie 6, 141980, Dubna, Russia
E-mail: nasonova@jinr.ru
[3]Institute of Physics, University of Szczecin,
Wielkopolska 15,70-451, Szczecin, Poland
E-mail: konrad.czerski@usz.edu.pl

DNA double-strand breaks (DSB) represent initial events of DNA damage of crucial significance in the formation of structural changes in chromosomes i.e. chromosome aberrations (CA) induced by ionizing radiation. So called dose-response curves of CA usually have a linear-quadratic shape [1] and can be easily applied for estimation of the clinically important relative biological effectiveness (RBE). It has been already shown that the quadratic term may result from two different effects. The most important effect is of a biological origin and can be connected with very efficient DNA repair mechanisms leading to CA, which strongly depend on the local ionization density and thus on the radiation quality [2].. The second associated with physical processes – arises from overlapping ion tracks at high ion fluencies, which locally leads to higher doses and a stronger biological response [3]. Recently, we have proposed a new analytical model which can connect the experimentally estimated parameters of the dose-effect curves with the physical features of ion-tracks [4].

To distinguish between the biological and physical components of the dose-effect curves the knowledge about initial DNA breakage taking place immediately after exposure to ionizing radiation and before the repair mechanisms start to act is of essential importance. In the present work we have adopted the premature chromosome condensation (PCC) technique to study the initial DNA damage. We have studied G2-chromatid breaks in human lymphocytes as well as isochromatid-type breaks (excess fragments) at two different times: directly after irradiation (t_0) and 12 hours later (t_{12}). The lymphocyte samples have been exposed to 150 MeV and spread out Bragg peak (SOBP) proton beams, 22 MeV/u ^{11}B ions and for comparison to ^{60}Co γ rays.

We have determined dose-response curves for both types of breaks as well their statistical frequency distributions. We have shown that t_0 G2-chromatid breaks follow linear-quadratic dependence for all studied cases. This finding has been used to estimate the physical contribution of overlapping ion tracks to curvature of the response curves in the frame of previously developed model, and the results have been compared to data obtained for CA. Additionally, we have concluded increased production of isochromatid-type breaks with the increasing LET value of applied irradiation to be a signature of densely ionizing track structure. Moreover, we have found that distributions of G2-break frequency (at the t_0 and t_{12}) follow Poisson statistics for both proton beams and ^{60}Co γ rays while those obtained for boron ions are over-dispersed.

REFERENCES

[1] Lea D.E., *Actions of radiations on living cells* (Cambridge University Press, Cambridge, 1955)

[2] M. Scholz , G. Kraft, *Advances in Space Research* **18**, 5-14 (1996)

[3] B.D. Loucas ,M. Durante, S.M. Bailey, M.N. Cornforth, *Radiation Research* **179**,9-20 (2013)

[4] A. Kowalska , K Czerski , E. Nasonova, P. Kutsalo, E. Krasavin, *European Physical Journal* D, **71**, 12 332 (2017)

MOLSPIN – MOLECULAR SPIN DYNAMICS SOFTWARE

Claus Nielsen[1], Ilia A. Solov'yov[1]

[1]Department of Physics, Chemistry and Pharmacy, University of Southern Denmark,
Campusvej 55, 5230, Odense M, Denmark
E-mail: clausnielsen@sdu.dk

Magnetic field effects have been measured in various processes involving radical pairs [1-4], and such magnetic field effects, modelled by the radical pair mechanism, have provided the basis for a popular hypothesis for magnetoreception in migratory song birds [5]. The spin dynamics of radical pairs exposed to radiofrequency radiation have also been associated with changes in the production of reactive oxygen species within a biological cell [3,4], an effect that is potentially harmful. In order to investigate such phenomena from a theoretical point of view one needs to employ complex computations, and many groups have developed tools for performing specific types of such calculations. Rather than having to create a new tool for every new type of calculation, however, MolSpin is a general software tool that is designed to handle any type of spin dynamics calculation; this includes but is not limited to solving the Liouville-von Neumann equation to obtain the time-evolution of the density operator, calculating quantum yields (e.g. MARY curves [6] or orientational dependence [5,7]), semi-classical methods [8-10] and perturbation methods [11,12]. Even when a needed calculation method is not yet implemented, MolSpin is designed with a high emphasis on extensibility that makes it easy to implement new or extend existing functionality. For all the heavy calculations MolSpin relies on the Armadillo library [13], which in turn makes use of high-speed math libraries such as OpenBLAS or Intel MKL. Distributed memory parallelization using OpenMPI will be supported in the future, but is not implemented yet.

REFERENCES

[1] K. Maeda et al., *Nature* **453**, 387-309 (2008)
[2] S. Engels et al., *Nature* **509**, 353-356 (2014)
[3] R. J. Usselman *et al*., *Scientific Reports* **6**, 38543 (2016)
[4] R. J. Usselman *et al*., *PLOS ONE* **9**, e93065 (2014)
[5] P. J. Hore and H. Mouritsen, *Annual Review of Biophysics* **45**, 299-344 (2016)
[6] U. E. Steiner and T. Ulrich, *Chemical Review* **89**, 51-147 (1989)
[7] J. B. Pedersen *et al.*, *Scientific Reports* **6**, 36709 (2016)
[8] K. Schulten and P. G. Wolynes, *The Journal of Chemical Physics* **68**, 3292-3297 (1978)
[9] D. E. Manolopoulos and P. J. Hore, *The Journal of Chemical Physics* **139**, 124106 (2013)
[10] A. M. Lewis *et al*., *The Journal of Chemical Physics* **141**, 044111 (2014)
[11] J. M. Canfield *et al*., *Chemical Physics* **182**, 1-18 (1994)
[12] J. M. Canfield *et al*., *Chemical Physics* **195**, 59-69 (1995)
[13] C. Sanderson and R. Curtin, *Jorunal of Open Source Software* **1**, 26 (2016)

COMPARATIVE STUDY ON CALCULATED PROPERTIES OF PLATINUM-BASED MOLECULES

Daniel Süß, Stefan E. Huber, Andreas Mauracher

Institute of Ion Physics and Applied Physics, University of Innsbruck
Technikerstraße 25/3, 6020 Innsbruck, Austria
E-mail: daniel.suess@uibk.ac.at

Platinum-based molecules are among the most leading substances administered in the course of anticancer chemotherapy [1]. For the numerical description of molecular processes involving these molecules (especially in the relevant biomolecular environment) a procedure which seems satisfying with respect to a suitable balance between computational efficiency and accuracy at the electronic structure level remains elusive. In this contribution we present key findings resulting from a comparison of various density functionals and ab-initio methods concerning their performance with respect to geometric and energetic properties of platinum-containing compounds. These properties include bond length, binding energy, electron affinity and heat of formation.

For validation purposes, our hitherto exploratory study is restricted to a set of molecules for which reasonably accurate experimental data exist. Our choice of density functionals is based on earlier comparative studies concerning relative accuracies of different functionals (see e.g. Refs [2,3]) and on the typical usage of some density functionals (like B3LYP [4]) lacking often in validation of their suitability for the specific system under investigations. Eventual shortcomings in the accuracy with respect to non-metal containing biomolecules are monitored by using an additional test set consisting of such compounds. Moreover, we vary the portion of Hartree-Fock exchange energy used in some of the considered hybrid density functionals in order to explore possible gains in accuracy for the specific systems under investigations here.

REFERENCES

[1] S. Dasari, and P. B. Tchounwou, Cisplatin in cancer therapy: molecular mechanisms of action; Eur. J. Pharmacol. 740 (2014) 364. DOI: 10.1016/j.ejphar.2017.07.025
[2] M. Kokoschka, J. Galgonek, J. Vondrasek, P. Hobza, Computational methods for the description of pharmacologically relevant platinum complexes – molecular structure and bond dissociation; Phys. Chem. Chem. Phys. 18 (2016) 4051. DOI: 10.1039/c5cp03391h
[3] Y. Minenkov, E. Chermak, L. Cavallo, Troubles in the Systematic Prediction of Transition Metal Thermochemistry with Contemporary Out-of-the-Box Methods; J. Chem. Theo. Comp. 12 (2016) 1542. DOI: 10.1021/acs.jctc.5b01163
[4] A. D. Becke, Density-functional thermochemistry. III. The role of exact exchange; J. Chem. Phys. 98 (1993) 5648. DOI: 10.1063/1.464913

VARIABLE ELECTRON TRANSFER PATHWAYS IN AMPHIBIAN CRYPTOCHROME

Emil Sjulstok[1], Gesa Lüdemann[2], Tomas Kubar[2], Marcus Elstner[2] & Ilia A. Solov'yov[1]

[1]Department of Physics Chemistry and Pharmacy, University of Southern Denmark,
Campusvej 55, 5230, Odense, Denmark
E-mail: Sjulstok@gmail.com
[2] Institute of Physical Chemistry, Karlsruhe Institute of Technology,
Hermann-von-Helmholtz-Platz 1, 76131, Karlsruhe, Germany

Cryptochromes are flavoproteins, involved in light-dependent signaling pathways of several vital biological processes, such as the regulation of the hypocotyl growth in plants and entrainment of circadian rhythm in animals. Cryptochromes were also proposed to act as sensors for the geomagnetic field and assists many animals, such as migratory birds, in long-range navigation [1].

Cryptochrome proteins are activated by absorption of light, leading to formation of radical pairs through three sequential electron transfers between a flavin adenin dinucleotide (FAD) cofactor and a conserved triad of tryptophan amino acids [2]. Through mutations of the tryptophan triad it has been shown that the electron transfer can occur via. other amino acids in amphibian cryptochrome. In this study, we use tight-binding DFT [3] to explore the possible, variable electron transfer pathways in amphibian cryptochrome.

REFERENCES

[1] Johnsen, S & Lohmann, K. (2008) Magnetoreception in animals. Physics Today 61, 29–35
[2] Solov’yov, I. A, Domratcheva, T, Moughal Shahi, A. R, & Schulten, K. (2012) Decrypting cryptochrome: Revealing the molecular identity of the photoactivation reaction. JACS 134, 18046–18052.
[3] Kubař, T. & Elstner, M. (2013) Efficient algorithms for the simulation of non-adiabatic electron transfer in complex molecular systems: application to DNA Phys. Chem. Chem. Phys. 15 5794-5813

LONG-TIMESCALE DYNAMICS IN HYDROGEN-BONDED CLUSTERS: STUDY OF VIBRATIONALLY EXCITED $(HBr)_n$ CLUSTERS

Katerina Grygoryeva[1,2], Jozef Rakovský[1], Ondřej Votava[1], and Michal Fárník[1]

[1]J. Heyrovský Institute of Physical Chemistry of the CAS, v. v. i.
Dolejškova 2155/3, 182 23 Prague 8, Czech Republic
E-mail: kateryna.grygoryeva@email.cz
[2]University of Chemistry and Technology, Prague
Technická 5, 166 28 Praha 6, Czech Republic

Hydrogen bonding is recognized as one of the vital interactions defining structural and dynamical behavior of many systems in physics, chemistry and biology [1]. Its properties can be conveniently studied on hydrogen halide (HX) clusters, which exhibit hydrogen bonding of variable strength decreasing in the row HF–HCl–HBr–HI from almost covalent to nearly van der Waals interactions [2]. Hydrogen halides are relatively simple diatomic molecules, which facilitates the theoretical treatment of their clusters at high ab initio level. Thus $(HX)_2$ dimers served as benchmark systems for ab initio quantum mechanical calculations contributing to the development of the hydrogen bond theory [3,4].

One of intriguing questions to be answered concerns the flow of energy in these clusters. Specifically, how does vibrational excitation affect the cluster, and what are its relaxation pathways? In this work, we investigate the effect of vibrational excitation on hydrogen bromide clusters $(HBr)_n$ and on their photodissociation dynamics [5]. In particular, we excite one quantum of HBr stretching vibration at wavelengths corresponding to HBr molecules located in various clusters. For comparison, we also excite bare molecules. Free molecules and molecules in clusters are then photodisociated by a UV-laser pulse; their H-fragments are ionized and their velocities are recorded using a Velocity map imaging (VMI) method. VMI images recorded at different delays between IR and UV laser pulses suggest a presence of fast relaxation dynamics in vibrationally excited clusters; however, it cannot be quantified in our experiment with ns resolution. Nevertheless, these images also show a much longer dynamics happening on a slower time-scale: hundreds of nanoseconds.

ACKNOWLEDGMENTS:

This work has been supported by the Czech Science Foundation project No.: 17-04068S and by Praemium Academieae of the Czech Academy of Sciences 2017.

REFERENCES

[1] G. A. Jeffrey and W. Saenger, Hydrogen Bonding in Biological Structures, 2nd ed. Springer-Verlag Berlin Heidelberg (1994)
[2] Z. Latajka and S. Scheiner, *Chem. Phys.*, **216**, 37 (1997)
[3] S. Davis, D. T. Anderson, and D. J. Nesbitt, *J. Chem. Phys.*, **105**, 6645 (1996)
[4] D. J. Nesbitt, S. Davis, and D. T. Anderson, Recent theoretical and experimental advances in hydrogen bonded clusters, Kluwer Academic Publishers, 26 (2000)
[5] K. Grygoryeva, J. Rakovský et al., *J. Chem. Phys.*, **149**, 000000 (2018)

PS-12

ELECTRON AND PHOTON DRIVEN CHEMISTRY OF PYRUVIC ACID IN CLUSTERS

Katerina Grygoryeva[1,2], Andriy Pysanenko[1], and Michal Fárník[1]

[1]J. Heyrovský Institute of Physical Chemistry of the CAS, v. v. i.
Dolejškova 2155/3, 182 23 Prague 8, Czech Republic
E-mail: kateryna.grygoryeva@email.cz
[2]University of Chemistry and Technology, Prague
Technická 5, 166 28 Praha 6, Czech Republic

Pyruvic acid (PA) represents the simplest α-oxoacid and is widely found in the natural environment as well as in living organisms. Moreover, PA has been detected in carbonaceous meteorites, which suggests its involvement in prebiotic processes [1]. Especially its photochemistry has been extensively studied and it has been found to largely depend on the molecular environment: the gas-phase photochemistry of PA reduces the system's complexity, while the presence of water leads to the generation of more complex products (e. g. [2,3] and references therein). In this study, we aim at molecular-level details that could help us understand the influence of solvent on the reactivity of pyruvic acid.

In this work, we use clusters as a model system for solvation. Specifically, we generate large water clusters (mean cluster size ~400 molecules) and pick up several PA molecules on these ice nanoparticles. The clusters are then detected by time-of-flight mass spectrometry with electron (70 eV) or photon (193 nm) ionization [4,5]. Electrons ionized the more abundant water molecules with higher probability which led to the evaporation of PA molecules and yielded protonated $(H_2O)_nH^+$ clusters. In some cases, protonated fragments with one PA molecule $PA\cdot(H_2O)_nH^+$ were generated (Figure 1). However, no fragments with more than one PA molecule were observed suggesting that the binding of a PA molecule to a protonated cluster $(H_2O)_nH^+$ is stronger than the PA–PA bonding. In the photoionization experiment, PA acted as a chromophore and its reactivity after photon absorption led to the generation of lactic acid and possibly covalently bound larger species. These and more findings obtained in this study provide a valuable insight into pyruvic acid interactions with other PA molecules and water, and into its electron and photon driven chemistry.

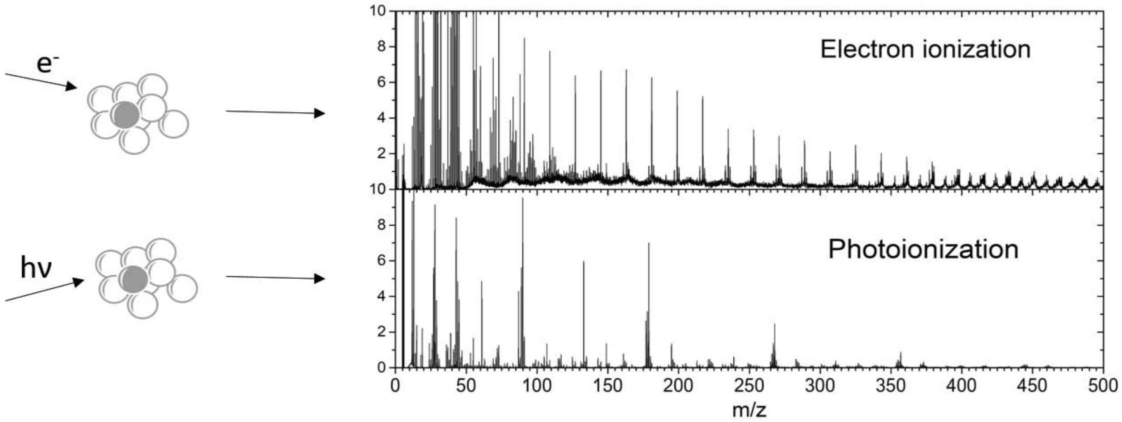


Figure 1: Comparison of spectra of water clusters with PA after electron and photon ionization

ACKNOWLEDGEMENTS:

This work has been supported by the Czech Science Foundation project No.: 17-04068S and by Praemium Academieae of the Czech Academy of Sciences 2017.

REFERENCES

[1] G. Cooper, C. Reed et al., *Proc. Natl. Acad. Sci.*, **108**, 14015 (2011)
[2] A. E. Reed Harris, J. F. Doussin et al., *J. Phys. Chem. A*, **120**, 10123 (2016)
[3] R. J. Rapf, R. J. Perkins et al., *J. Phys. Chem. A*, **121**, 4272 (2017)
[4] J. Kočišek, J. Lengyel, and M. Fárník, *J. Chem. Phys*. **138**, 124306 (2013)
[5] P. Rubovič, A. Pysanenko et al., *J. Phys. Chem. A*, **120**, 4720 (2016)

ELECTRON-INDUCED SINGLE AND DOUBLE STRAND BREAKS IN DNA DETERMINED BY USING THE DNA ORIGAMI TECHNIQUE

Kenny Ebel[1,2], Ilko Bald[1,2]

[1]Institute of Chemistry – Physical Chemistry, University of Potsdam,
Karl-Liebknecht-Str. 24-25, 14476, Potsdam, Germany
[2]Department 1 – Analytical Chemistry and Reference Materials, BAM Federal Institute of Materials
Research and Testing, Richard-Willstätter Str. 11, 12489, Berlin Germany
E-mail: keebel@uni-potsdam.de
E-mail: bald@uni-potsdam.de

Secondary low-energy electrons (LEEs) belong to the most important intermediates in DNA radiation damage. Strand breaks in the DNA backbone can be initiated by resonant electron attachment at different electron energies.[1] Recent experiments suggest that single (SSBs) and double strand breaks (DSBs) depend on the nucleotide sequence and its length, which is exploited for tumor radiation therapy. A novel approach using DNA origami templates carrying different oligonucleotide target sequences provides access to efficient and systematic determination of electron induced DNA strand break cross sections.[2] Here we present the strand break cross sections for polyAn (n = 4, 8, 12, 16, 20) DNA-strands at different electron energies (5-10 eV).[3,4]

For biological systems, the investigation of double strand breaks is more relevant than single strand breaks. Therefore, we present first results on the modification of DNA origami templates with double stranded target sequences and their irradiation with electron energies in the range 5-10 eV.

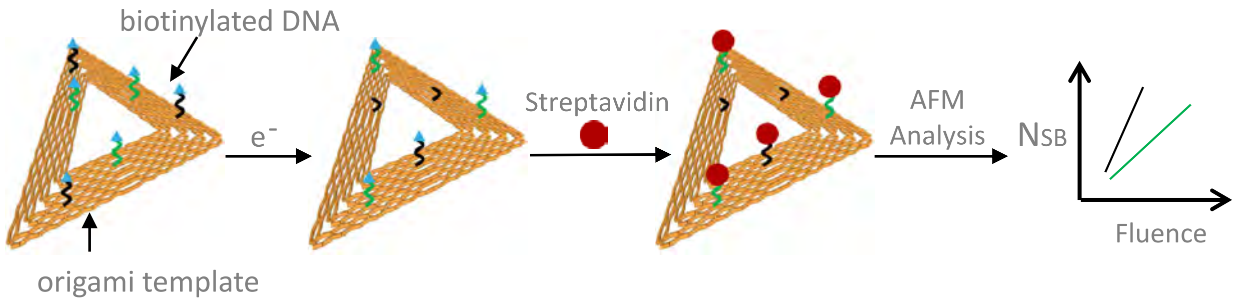


Figure 1: Scheme of the DNA origami technique to determine absolute cross-sections for irradiation-induced DNA strand breaks. DNA target strands are placed onto DNA origami platforms. After irradiation and rinsing the intact target strands are labelled with streptavidin to visualize them in AFM images. Analysis of AFM images obtained at various irradiation conditions yields absolute cross-sections for strand breaks.

REFERENCES
[1] I. Baccarelli *et. al.* 2011 *Phys. Rep.* **508** 1.
[2] A. Keller *et. al.* 2012 *ACS Nano* **6** 4392.
[3] J. Rackwitz *et. al.* 2016 *Angew. Chem. Int. Ed.* **55** 10248-10252.
[4] R. Schürmann *et. al.* 2017 *J. Phys. Chem. B* **121** 5730-5734.

A NEW ION MOBILITY STAGE FOR A TANDEM MASS SPECTROMETER

Klaas Bijlsma, Jan Mulder, Ronnie Hoekstra, Thomas Schlathölter

Zernike Institute for Advanced Materials, University of Groningen,
Nijenborgh 4, 9747AG, Groningen, the Netherlands
E-mail: k.i.j.bijlsma@student.rug.nl

A powerful tool for studying interactions of gas-phase biomolecular ions with radiation is a combination of electrospray ionization (ESI) and tandem mass spectrometry [1]. However, even for target molecular ions of well determined m/z, often many different molecular conformations contribute. We are currently developing an ion mobility spectrometer (IMS) that can be interfaced with our tandem mass spectrometer, to separate 3D conformational states of molecular ions.

Traveling wave ion mobility spectrometry (TW-IMS, developed by the Smith group [2]) is a relatively new technology which has several advantages over a drift tube, a device that is traditionally used for IMS. With TW-IMS, a block-wave voltage signal propagates along the ion track. The resulting dynamic local electric field pushes the ions forward, without the need of a large voltage difference over the whole pathlength. Mobility separation takes place because high mobility ions can keep up with the wave, while lower mobility ions will roll back over a top and fall behind.

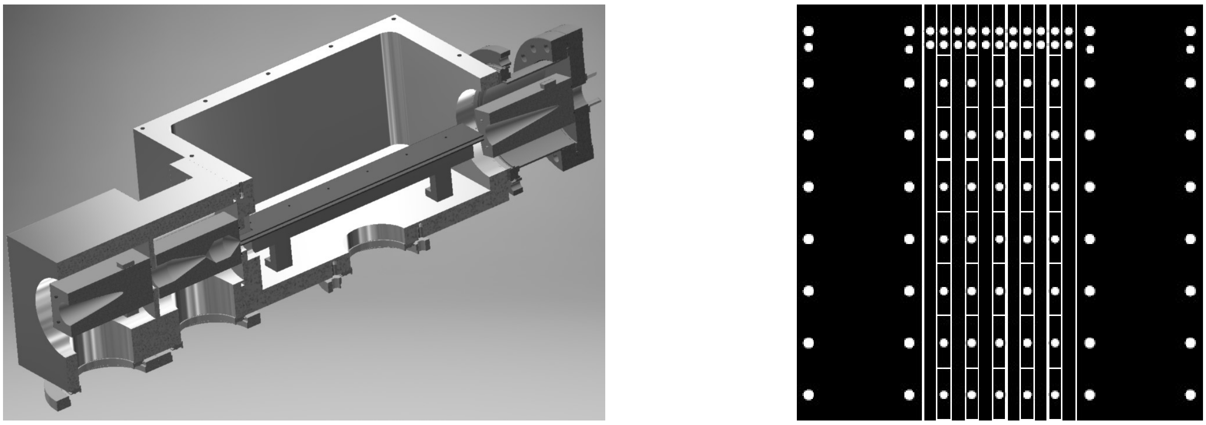


Figure 1: Current state of design, subject to change. Left: Half section view of vacuum system with ion funnels and two closely spaced printed circuit boards (PCBs). Right: A section of the PCB with DC and RF electrodes.

Inspired by the design in [2], the electrodes for the DC wave potentials, as well as electrodes for confining RF potentials will be fabricated on a printed circuit board, with the advantage of being low-cost, compact and easily adjustable.

REFERENCES

[1] S. Bari, O. Gonzalez-Magaña, G. Reitsma, J. Werner, S. Schippers, R. Hoekstra and T. Schlathölter, *The Journal of Chemical Physics* **134,** 024314 (2011)

[2] A. M. Hamid, Y. M. Ibrahim, S. V. Garimella, I. K. Webb, L. Deng, T.-C. Chen, G. A. Anderson, S. A. Prost, R. V. Norheim, A. V. Tolmachev and R. D. Smith, *Analytical Chemistry* **87**, 11301–11308 (2015)

DNA ORIGAMI FORKS FOR SINGLE MOLECULE SERS

Kosti Tapio[1], Arm Mostafa[1], Ilko Bald[1,2]

[1]University of Potsdam, Department of Physical Chemistry, Karl-Liebknecht-Str. 24-25, 14476, Potsdam, Germany.
E-mail: kostapio@uni-potsdam.de
[2]BAM Federal Institute for Materials Research and Testing, Richard-Willstätter-Str. 11, 12489, Berlin, Germany.

The nanotechnology allowed for breakthroughs in different fields e.g. medical diagnostics, food industry and pharmaceutical industry [1,2]. In all of these fields, Surface Enhanced-Raman Spectroscopy (SERS) has been successfully utilized, promising label-free detection and multiplexing of several analytes. However, there is still a demand for new innovations that allow production of universal, cost efficient and simple to use SERS probes. Such innovations would include methods to precisely position molecules and nanoparticles to manifest new hybrid-structures or metamaterials with unique and customizable optical properties.

In this context, the bottom-up approaches have gained huge attraction due to their superior resolution and scalability. Among the different bottom-up materials, one of the leading candidates is DNA due to its versatile self-assembly, the simplicity of its preparation and functionalization properties [3]. Especially promising has been the use of DNA based structures as scaffolds to fabricate optical and electrical nanodevices [4,5,6], where metallic nanoparticles and biomolecules can be patterned with few nanometer precision.

Our overall aim is to develop DNA structures that can act as platforms for precise placement of arbitrary biomolecules and nanoparticles. One such platform could be a tuning fork structure shown in Figure 1. This structure contains a bridge between the arms of the fork and several sticky-ends extension for two nanoparticles. The bridge can be modified to include or to capture a desired biomolecule and two metallic nanoparticles can be hybridized on both sides of the fork to create a nanoparticle dimer, where the biomolecule can be positioned in the hotspot of the dimer. This could be then used in SERS to detect a single, arbitrary biomolecule, e.g., fluorophores and proteins.

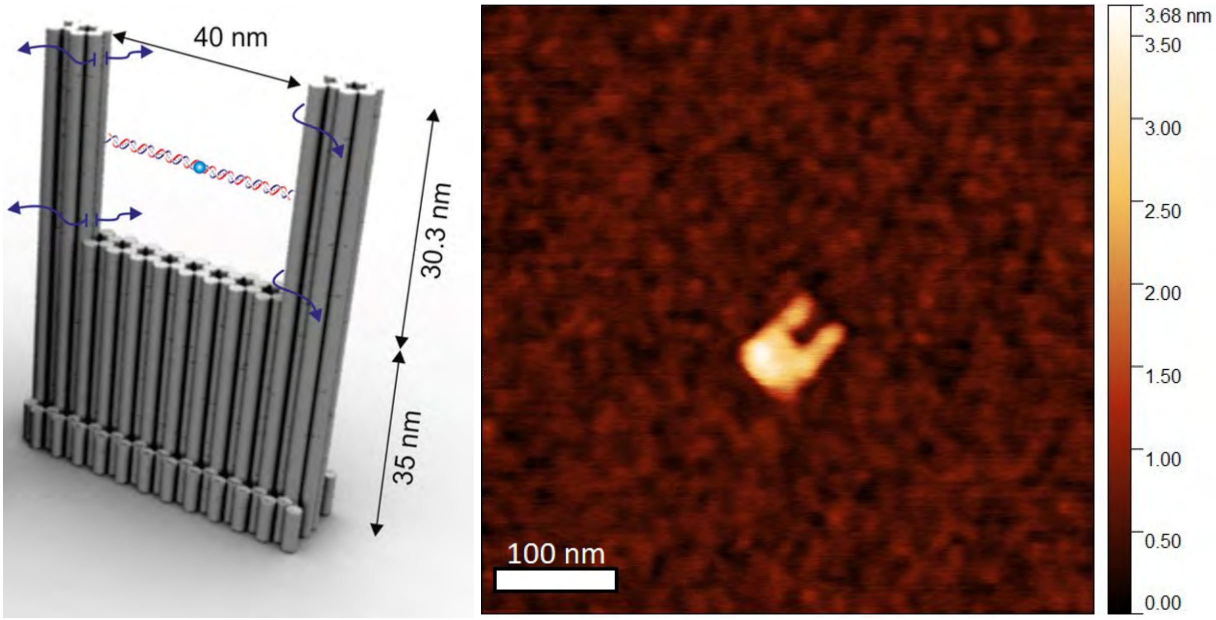


Figure 1: Right: Schematic view of the DNA origami Fork structure. The fork design includes a bridge for a biomolecule attachment (the dot in the middle of the bridge) and sticky-ends (the protruding arrows) for nanoparticle hybridization. Left: AFM image of a Fork structure a silicon surface.

REFERENCES
[1] X. Xie *et. al.* , *Crit. Rev. Food Sci. Nutr.* , 1-14 (2017)
[2] B. Sharma *et. al.*, *Materialstoday* **15**, 16-25 (2012)
[3] N.C. Seeman, *Nature* **421**, 427-431 (2003).
[4] C. Heck *et. al.*, *ACS Photonics* **4**, 1123-1130 (2017)
[5] K. Tapio *et. al.*, *Nano Lett.* **16**, 6780-6786 (2016)
[6] A.V. Pinheiro *et. al.* , *Nat. Nanotechnol.* **6**, 763-772 (2011)

DETERMINATION OF THE MICROSCOPIC DOSE-DAMAGE RELATION FOR RADIATION OF DIFFERENT LINEAR ENERGY TRANSFER.

Marc Benjamin Hahn[1,2], Tihomir Solomun[1], Heinz Sturm[1,3]

[1]Bundesanstalt für Materialforschung und Prüfung, Unter den Eichen 87, 12205 Berlin, Germany.
E-mail: marc-benjamin.hahn@bam.de
[2]Freie Universität Berlin, Institut für Experimentalphysik, Arnimallee 14, 14195 Berlin, Germany.
[3]Technical University Berlin, Pascalstr. 8-9, 10587 Berlin, Germany.

The determination of the microscopic dose-damage relationship for DNA in an aqueous environment is of a fundamental interest for dosimetry and applications in radiation therapy and protection. We combine geant4 particle-scattering simulations in water with calculations concerning the movement of biomolecules to obtain the energy deposit in the biologically relevant nanoscopic volume.[1] We juxtaposition these results to the experimentally determined damage to obtain the microscopic dose-damage relationship at a molecular level. This approach is tested for an experimentally challenging system concerning the direct irradiation of plasmid DNA (pUC19) in water with electrons as primary particles.[2] Here a microscopic target model for the plasmid DNA based on the relation of lineal energy and radiation quality is used to calculate the effective target volume. It was found that on average fewer than two ionizations within a 7.5-nm radius around the sugar-phosphate backbone are sufficient to cause a single strand break, with a corresponding median lethal energy deposit being E1/2=6±4 eV.[1] The presented method is applicable for ionizing radiation (e.g., γ rays, x rays, and electrons) and a variety of targets, such as DNA, proteins, or cells.

REFERENCES

[1] Hahn, M. B., Meyer, S., Kunte, H.-J., Solomun, T. & Sturm, H. Measurements and simulations of microscopic damage to DNA in water by 30 keV electrons: A general approach applicable to other radiation sources and biological targets. *Phys. Rev. E* **95,** 052419 (2017).

[2] Hahn, M. B. *et al.* Direct electron irradiation of DNA in a fully aqueous environment. Damage determination in combination with Monte Carlo simulations. *Phys. Chem. Chem. Phys.* **19,** 1798–1805 (2017).

PHOTODYNAMIC INACTIVATION OF BACTERIA USING CARBON DOTS

M. Zühlke[1], T.T. Meiling[1], P. Roder[1], D. Riebe[1],T. Beitz[1], I. Bald[1,2], H.-G. Löhmannsröben[1],
T. Janßen[3], M. Erhard[3], A. Repp[3]

[1]Physical Chemistry, University of Potsdam,
Karl-Liebknecht-Str. 24-25, 14476 Potsdam, Germany
E-mail: mzuehlke@uni-potsdam.de

[2]BAM Federal Institute for Materials Research and Testing,
Richard-Willstätter-Str. 11, 12489 Berlin, Germany

[3]RIPAC-LABOR GmbH
Am Mühlenberg 11, 14476 Potsdam, Germany

The increasing development of antibiotic resistance in bacteria has been a major problem for years, both in human and veterinary medicine. Prophylactic measures, such as the use of autogenous vaccines, are of great importance in reducing the use of antibiotics in livestock. These vaccines are mainly produced on the basis of formaldehyde inactivation. However, the latter damages the recognition elements of the bacterial membrane and thus could reduce the immune response in the animal. An alternative inactivation method developed in this work is based on gentle photodynamic inactivation using carbon dots (CD) at wavelengths $\lambda > 300$ nm.

The photodynamic inactivation was characterized on the non-virulent laboratory strain *Escherichia (E.) coli* K12 using self-synthesized CD [1]. For a gentle inactivation, the CDs must be absorbed by the *E. coli*-cell. The photoinduced formation of the reactive oxygen species only takes place inside the bacterium, which means the outer membrane is not damaged. The loading of the CD into *E. coli* was examined using fluorescence microscopy. The complete loading of the bacterial cells could be achieved in less than 10 minutes. These studies revealed a reversible uptake process so it allows the removal of the potentially toxic CD after irradiation before using as an autogenous vaccine.

The success of photodynamic inactivation was verified by viability assays on agar. In our self-made flow photoreactor, the fastest successful irradiation of the bacteria could be carried out in 34 s. Therefore, the photodynamic inactivation based on CD is very effective. The membrane integrity of the bacteria after irradiation was verified by slide agglutination and atomic force microscopy (AFM). The method developed on the laboratory strain *E. coli* K12 could then be successfully applied to the important avian pathogens *Bordetella avium* and *Ornithobacterium rhinotracheale.*

REFERENCES

[1] Meiling, T. T. et al. White carbon: Fluorescent carbon nanoparticles with tunable quantum yield in a reproducible green synthesis. Sci. Rep. 6, 28557; doi: 10.1038/srep28557 (2016)

PS-18

LOW ENERGY ELECTRON DRIVEN CHEMISTRY FOR THE ADVANTAGE OF EMERGING NANO-FABRICATION METHODS (ELENA); A MARIE SKŁODOWSKA-CURIE INNOVATIVE TRAINING NETWORK

Oddur Ingólfsson *et al.*

[1]Department of Chemistry and Science Institute, University of Iceland, Dunhagi 3, 107 Reykjavik, Iceland. E-mail: odduring@hi.is

ELENA; Low energy ELEctron driven chemistry for the advantage of emerging NAno-fabrication methods, is a Marie Skłodowska-Curie, Innovative Training Network. The network focuses on the, fundamental, electron driven processes underpinning two emerging nano-fabrication methods; Focused Electron Beam Induced Processing FEBIP [1,2,3] (with emphasis on deposition FEBID) and Extreme Ultraviolet Lithography (EUVL) [4,5]. Exploitation of these methods has the potential to improve the manufacturing process of existing devices, improve the performance of specific nano-devices through better material control and higher spatial resolution in their fabrication, and enable the fabrication of new devices. Improved EUVL can provide cost efficient high-volume microchip production for the fabrication of more-advanced integrated circuits housing higher component densities than is currently achievable [6]. FEBID on the other hand is ideally suited for direct, one step production of high aspect ratio components and may be integrated in the production of functional devices where the 3D shape of components is critical [1].

For FEBID the objectives of ELENA embrace the development of new precursor molecules for ultimate composition control of the deposits and for the development of *in situ* purification protocols. Hence, a core objective of ELENA is the design and development of protocols for precursor molecules that lead to purer deposits and higher resolution.

For EUV resists the objective is to gain better control over the low energy induced chemistry within these resists and to use that chemistry to control adverse and limiting factors such as the mean free path of low energy electrons and acid diffusion within the resist. Hence, to control the low energy electron induced chemistry within the resists to improve the performance of EUVL with regards to resolution, sensitivity and line width roughness (RLS).

This is only achievable by understanding the low energy electron induced chemistry involved and by acknowledging this chemistry in the design of new FEBID precursors and EUVL resist material.

In the current contribution the objectives of ELENA and the means to achieve these are discussed.

REFERENCES
[1] I. Utke, *et al. J. Vac. Sci. Technol., B* **26**, (4), 1197 (2008)
[2] W. F. van Dorp *et al. J. Appl. Phys. **104**,* 081301 (2008).
[3] S. Randolph *et al. Crit. Rev. Solid State Mater. Sci.* **31**, (3), 55 (2006)
[4] Saša Bajt *et al. Surf. Sci. Rep.* **63,** 73-99(2008)
[5] B. Wu *et al. J. Vac. Sci. Technol. B* **25**(6), 1743-1761 (2007)
[6] C. Wagner *et al. Ind. Persp. Nature Photonics,* **4**, 24 (2010)

Acknowledgments: This project has received funding from the European Union's Horizon 2020 research and innovation programme under the Marie Skłodowska-Curie grant agreement No 722149

NANOSCALE DEFORMATIONS OF THE DNA DOUBLE HELIX

Sergey N. Volkov

Laboratory of Biophysics of Macromolecules, Bogolyubov Institute for Theoretical Physics,
Natl. Acad. of Sci. of Ukraine, Kiev 03143, Ukraine
E-mail: snvolkov@bitp.kiev.ua

The accuracy of the genetic information transfer in living cells largely depends on the peculiarities and variability of the DNA structure. Due to the polymorphism of the double helix, DNA can change the shape and conformation of the macromolecule under the influence of some external factors. In this case, the arising deformations usually have nanoscale dimensions and are accompanied by conformational transformations of the macromolecule, but without destroying the double-stranded structure as a whole. Such deformations of DNA provide a wide range of tools in the regulation and realization of genetic activity of the macromolecule. Last times, the study of DNA deformations at the nanoscale has acquired also practical significance in materials science because of the production of DNA nanomaterials with the desired properties.

Despite the great interest, theoretical studies of conformational dependent deformations in DNA cause certain difficulties. Due to the large displacements of structural elements from their equilibrium positions these deformations cannot be understood in terms of usually used elastic models. In the same time, all-atomic description cannot fully explain the mechanism of the complex processes of DNA deformations, because of the large number of atoms and degrees of freedom in the structure of the macromolecule. In the report it is shown, that the mechanism of polymorphic macromolecule deformations can be understood and described on the level of a two-component approach. In this instance one component of the model (external) describes the deformation of the macromolecule, as in the model of the elastic rod. Another component (internal) describes the changes in the conformation of the macromolecule monomer units. Under DNA deformations study both components are regarded as coupled on the pathway of a conformational transformation. For a more detailed description of DNA deformations, the model can be supplemented by taking into account other double helix components interrelated to the dominant one.

The developed approach gives a consistent interpretation of the observed deformability of DNA regulatory fragments, such as A-tract, TATA-box, CpG-steps. It is shown that considered localized deformations are by their nature static conformational solitons, which can be induced in definite fragments of the DNA chain and remain stable with suitable boundary conditions in a double helix. The study of the mechanisms of threshold deformations of DNA macromolecules (unzipping and overstretching) have showed that these deformations of DNA should pass in two stages. First, at a certain critical value of the external force acting on the external component, bistable conformation forms in the structure of macromolecule due to the components coupling. This, in turn, stimulates the appearance in the DNA chain of domains with two different conformations of monomers. Secondly, under favorable boundary conditions, the conformational induced deformation acquires the possibility of propagation along the macromolecule in the form of a domain wall, which provides a threshold effect of the deformation. The calculated values of the various contributions to the threshold deformations of DNA are consistent with the observed data and allow one to explain why DNA overstretching is realized as conformational transition within the double helix or as a force induced double helix melting.

THE INFLUENCE OF 5-BROMOURACIL IN DNA STRAND BREAKAGE

Stefanie Vogel[1,2], Robin Schürmann[1], Kenny Ebel[1], Christian Heck[1], Ilko Bald[1,3].

[1]University of Potsdam, Institute of Chemistry, Karl-Liebknecht-Str. 24-25,
14476, Potsdam, Germany, stvogel@uni-potsdam.de
[2]School of Analytical Sciences Adlershof, Humboldt-University Berlin,
Unter den Linden 6, 10099, Berlin, Germany, stvogel@uni-potsdam.de
[3]Department 1 – Analytical Chemistry and Reference Materials, BAM Federal Institute of Materials
Research and Testing, Richard-Willstätter Str. 11, 12489, Berlin, Germany, bald@uni-potsdam.de

DNA is one of the most important biological molecules and its interaction with ionizing radiation is of ongoing interest as the mechanisms of energy deposition, deactivation and the resulting destruction of DNA are still mostly unclear. In this work, the sequence-specific DNA damage induced by VUV photons on the single-molecule level is studied. Oligonucleotides can be specifically designed to contain a modification with the radiosensitizer 5-bromouracil. This can be subsequently attached to DNA nanostructures and adsorbed on a VUV transparent substrate, which can be irradiated in an Argon filled chamber by a well-defined VUV beam. VUV induced bond dissociations can be visualized by AFM, quantified, and plotted against the photon fluence to determine a cross section for single strand breaks for a DNA sequence at a certain irradiation energy (see Fig. below) [1, 2].

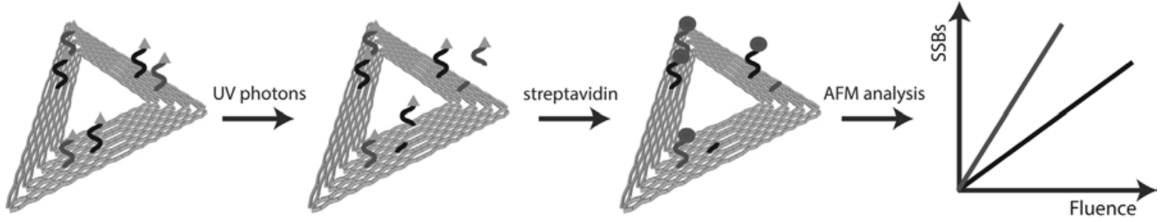


Figure 1: Scheme for DNA strand break detection. Two different DNA sequences are attached to the DNA nanostructure, which can experience a strand break under UV photon radiation. The strand break detection is realized by labelling the intact DNA strand with streptavidin and an analysis via AFM.

To investigate the detailed pathway of the photon-induced damage, identical DNA targets are irradiated under the same experimental conditions (photon energies and fluxes), but isolated in an ion trap. This allows for the determination of the ionization threshold for a specific oligonucleotide. The experiment can be performed by coupling a linear ion trap, fitted with an electrospray ionization source (ESI), to the synchrotron beamline and applying tandem mass spectrometry [3].

In the presented research, short oligonucleotides are modified with 5-bromouracil and the strand breakage with respect to the adjacent nucleobases is determined. The same DNA sequences were studied with tandem mass spectrometry to determine the ionization thresholds of the different DNA sequences for direct comparison. Through this, a clear dependency of the strand breakage on the DNA sequence composition can be identified and a connection to the ionization threshold can be drawn.

REFERENCES
[1] A. Keller *et al., Sci. Rep*. **4**, 7391 (2014).
[2] S. Vogel *et al.,* J. *Phys. Chem. Lett.* **6***,* 4589 (2015).

IN-LINE MONITORING OF GROWTH OF NANO-SCALED PARTICLES IN CONCENTRATED LIQUID DISPERSIONS BY PHOTON DENSITY WAVE SPECTROSCOPY

Stephanie Schlappa[1], Marvin Muenzberg[1], Oliver Reich[1], Roland Hass[1]

[1]Physical Chemistry - innoFSPEC,
University of Potsdam,
Am Mühlenberg 3, 14476 Potsdam, Germany
stepschlappa@uni-potsdam.de

Photon Density Wave (PDW) spectroscopy determines the absolute optical properties of a turbid liquid material without a need for calibration. As it is applicable especially at highest turbidities [1], complex multiple light scattering materials can be investigated without dilution. This is of particular interest for particle sizing in materials which are prone to size changes during dilution. Common methods like dynamic or static light scattering require single scattering and hence dilution of the material under investigation. Furthermore, as PDW spectroscopy currently allows for a time resolution of approx. 2 min^{-1} and can be operated with fiber-optical probes [2], it allows for in-line measurements during chemical, physical, or biological processing of turbid liquid materials. To date only a limited number of process analytical technologies, suitable for high concentrations of highly light scattering particles, exist. PDW spectroscopy [3-6] separately quantifies light absorption and light scattering in multiple scattering liquid dispersions of particles, droplets, or biological cells. Applicable in systems where the absorption coefficient μ_a is significantly smaller than the reduced scattering coefficient μ_s' PDW spectroscopy can be applied to monitor optical changes of such dispersions and for sizing of the dispersed structures in the nano- and micrometer regime. The PDW spectrometer utilized here is self-built [7].

Currently, techniques for in-line process monitoring in liquid dispersions are typically either hindered by the optical diffraction limit (e.g. video microscopy [8]), are restricted in the upper addressable particle concentration, and/or are biased by particle flow (e.g. diffusing wave spectroscopy or fiber-optical quasi-elastic light scattering [8-10]).However, for dispersions containing nano- or micrometer sized particles with volume fractions $\varphi > 0{,}4$, PDW spectroscopy is one of the very few suitable techniques, yet widely unknown. It enables particle sizing in such highly concentrated dispersions in a diameter range of approx. 50 nm – 500 µm.

REFERENCES

[1] Münzberg M., Hass R., Khanh N.D.D., Reich O., Limitations of turbidity process probes and formazine as their calibration standard, Anal. Bioanal. Chem. 409:719-728 (2017).

[2] Hass R., Munzke D., Vargas Ruiz S., Tippmann J., Reich O., Optical monitoring of chemical processes in turbid biogenic liquid dispersions by photon density wave spectroscopy, Anal. Bioanal. Chem. 407:2791-2802 (2015).

[3] Bressel L., Hass R., Reich O., Particle sizing in highly turbid dispersions by photon density wave spectroscopy, J. Quant. Spectrosc. Radiat. Transf. 126:122-129 (2013).

[4] Bressel L., Wolter J., Reich O., Particle sizing in highly turbid dispersions by Photon Density Wave spectroscopy: Bidisperse systems, J. Quant. Spectrosc. Radiat. Transf. 162:213-220 (2015).

[5] Fishkin J.B., Fantini S., van de Ven M.J., Gratton E., Gigahertz photon density waves in a turbid medium: Theory and experiments, Phys. Rev. E 53:2307-2319 (1996).

[6] Richter S.M., Shinde R.R., Balgi G.V., Sevick-Muraca E.M., Particle sizing using frequency domain photon migration, Part. Part. Syst. Charact. 15:9-15. (1998).

[7] Hass R., Reich O., Photon Density Wave spectroscopy for dilution-free sizing of highly concentrated nanoparticles during starved-feed polymerization, ChemPhysChem 12:2572-2575 (2011).

[8] H.G. Merkus, *Particle Size Measurements Fundamentals, Practice, Quality* (Springer, Amsterdam, 2009).

[9] Scheffold F., Particle sizing with diffusing wave spectroscopy, J. Dispersion Sci. Technol. 23:591-599 (2002).

[10] Wiese H., Horn D., Single-mode fibers in fiber-optic quasielastic light scattering: A study of the dynamics of concentrated latex dispersions, J. Chem. Phys. 94:6429-6443 (1991).

RADIATION DAMAGE OF G-QUADRUPLEX DNA IN THE GAS-PHASE

Wen Li[1], Xin Wang[1], Wessel Douma[1], Ronnie Hoekstra[1], Marwa Abdelmouleh[2], Michal Ryszka[2], Jimmy Rangama[2], Violaine Vizcaino[2], Jean-Christophe Poully[2],Thomas Schlathölter[1]

[1]Zernike Institute for Advanced Materials, University of Groningen, Nijenborgh 4, 9747 AG, Groningen, Netherlands
[2] CIMAP, UMR 6252 (CEA/CNRS/ENSICAEN/Université de Caen Normandie), Caen, France
E-mail: wen.li@rug.nl

Telomeres are the protective end-caps of human DNA and their role in carcinogenesis is an issue of intense research[1]. It has been suggested that telomere sequences (TTAGGG) also play an important role in radiation action on DNA, as they are for instance predicted to efficiently “trap” excitation energy[2]. In living cells, repeats of TTAGGG and other G-rich sequences form stable 3-dimensional G-quadruplex structures which are though to play a key role in cellular response upon ionizing radiation[3].

We have studied the direct effect of single X-rays or fast heavy ions on gas-phase DNA anions using a combination of radiofrequency ion trapping and mass spectrometry. Various DNA damage processes such as glycosidic bond cleavage leading to base loss but also direct strand breaks are observed for X-ray absorption in short sequences such as dTTAGGG or dTGGGGT. If these sequences are embedded in a G-quadruplex, DNA damage is dramatically reduced. In case of fast heavy ion impact, this reduction is not observed and also complex DNA structures are efficiently damaged.

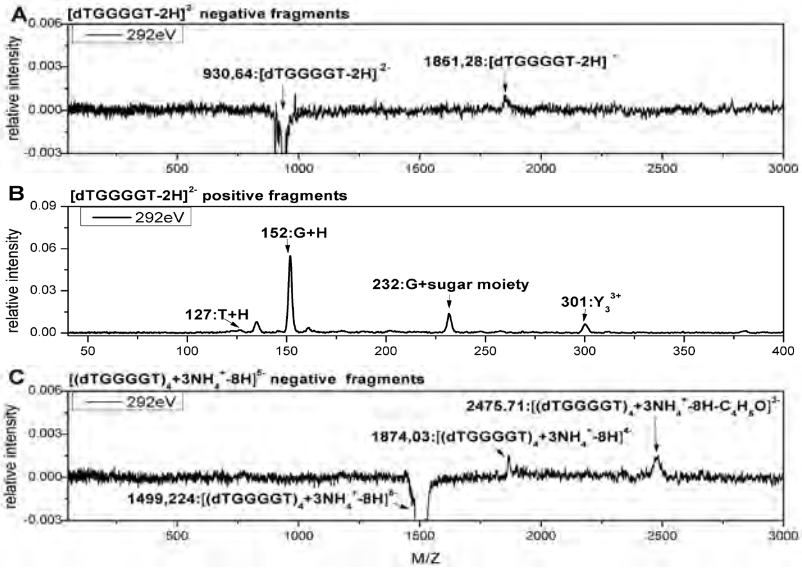


Figure 1: Mass spectrum for TGGGGT monomer (A:negative fragments and B:positive fragments) and G-quadruplex structure $[(dTGGGGT)_4+3NH_4^+-8H]^{5-}$(C).

REFERENCES
[1] Burge, S., et al., *Nucleic Acids Res* **34**, 5402-15 (2006)
[2] E. Cauet, *Journal of Biomolecular Structure & Dynamics* **29**, 557 (2011)
[3] Ambrus, A., et al., *Nucleic Acids Res* **34**(9), 2723-35 (2006)

OPTICAL CHARACTERIZATION OF PARTICLE SIZE DISTRIBUTIONS OF HIGHLY TURBID WAX DISPERSIONS

Wenke Müller[1], Daniela Vasquez[1], Roland Hass[1], Lena Bressel[1]

[1]University of Potsdam, Institute of Chemistry/Physical Chemistry - innoFSPEC
Am Mühlenberg 3, 14476 Potsdam, Germany
E-mail: wemueller@uni-potsdam.de

Particle sizing in turbid dispersions is of fundamental importance in academics as well as in industry. This is especially the case during industrial production of highly turbid dispersions, since optical and mechanical properties and hence quality of these products is strongly influenced by particle size [1]. However, most sizing techniques like Dynamic (DLS) or Static Light Scattering (SLS) are not suitable for such typically highly concentrated products. In contrast, Photon Density Wave (PDW) spectroscopy based on multiple light scattering is able to determine independently and without any calibration or dilution the optical properties, i.e. the absorption coefficient μ_a and the reduced scattering coefficient μ_s', of the highly concentrated dispersions. While the μ_a is related to chemical properties of the sample, μ_s' gives information about the particle size (distribution). Taking additionally into account models for particle interaction, particle sizes can be determined especially at high concentrations. This has been proven many times for mono- and bidisperse systems [1,2]. However, particle sizing in polydisperse systems is still under study.

To understand multiple scattering in polydisperse systems model dispersions are needed, which can be produced with defined size distributions. In this study, wax-water-dispersions were prepared by high-pressure emulsification of the melted wax in water in the presence of an emulsifier and subsequent cooling to room temperature. The size distribution of the wax dispersions was determined in a comparative study by SLS and DLS as well as PDW spectroscopy. Samples measured by SLS and DLS had to be strongly diluted before measurement, whereas PDW spectroscopy could be applied to the highly concentrated sample. While the wax is liquid at high temperatures allowing for emulsification, the droplets should solidify when cooling to room temperature. Hence, at room temperature the particles should be stable against Ostwald ripening and dilution during DLS and SLS measurements. This allows for size analysis with different techniques at high and low particle concentrations without any change of the size distribution.

As one of the important parameters, the influence of the emulsifier-wax ratio on the particle size distribution was analyzed. Highly concentrated, turbid wax dispersions with weight fractions from 20 % to 45 % and emulsifier-wax ratios between 0.2 % and 0.6 % (w/w) were prepared. Thus, dispersions with sizes in the nanometer range were obtained. It was found that higher emulsifier-wax-ratios lead to smaller mean particle sizes, as confirmed by all three sizing methods. Moreover, mean particle sizes do not change with changing wax content, as long as the emulsifier-wax-ratio and other parameters such as homogenization pressure and temperature are kept constant. Further influences on the size distribution were investigated and will be presented.

REFERENCES

[1] L. Bressel, R. Hass, O. Reich, *Journal of Quantitative Spectroscopy & Radiative Transfer* **126**, 122-129 (2013).

[2] L. Bressel, J. Wolter, O. Reich, *Journal of Quantitative Spectroscopy & Radiative Transfer* **162**, 213-220 (2015).

RADIATION ACTION ON GAS-PHASE DUPLEX DNA ANIONS

Wessel Douma[1], Wen Li[1], Xin Wang[1], Ronnie Hoekstra[1], Marwa Abdelmouleh[2], Michal Ryszka[2],
Jimmy Rangama[2], Violaine Vizcaino[2], Jean-Christophe Poully[2],Thomas Schlathölter[1]

[1]Zernike Institute for Advanced Materials, University of Groningen, Nijenborgh 4, 9747 AG,
Groningen, Netherlands
[2] CIMAP, UMR 6252 (CEA/CNRS/ENSICAEN/Université de Caen Normandie), Caen, France
E-mail: F.W. Douma@student.rug.nl

DNA damage is generally considered to be the leading cause of cell death in cancer therapy, and is caused by breakages of both backbones of the DNA duplex. Single-photon induced DNA single-strand breaks have been observed in the gas-phase oligonucleotides [1] and in oligonucleotides supported by DNA-origami [2]. However, there are still many fundamental questions regarding the underlying damage mechanisms on a molecular level, especially for interactions of duplex DNA with protons and heavy ions as compared to X-ray photons.

We investigate the most fundamental interactions between DNA and radiation, by storing deprotonated gas-phase oligonucleotides in a radiofrequency ion trap (shown in figure 1), exposing them to soft X-rays or MeV carbon ions, and characterizing fragmentation using a time of flight mass spectrometer. The DNA anions are produced using an electrospray ionization source, which leaves the molecules intact, and enables control over the charge state of the molecule.

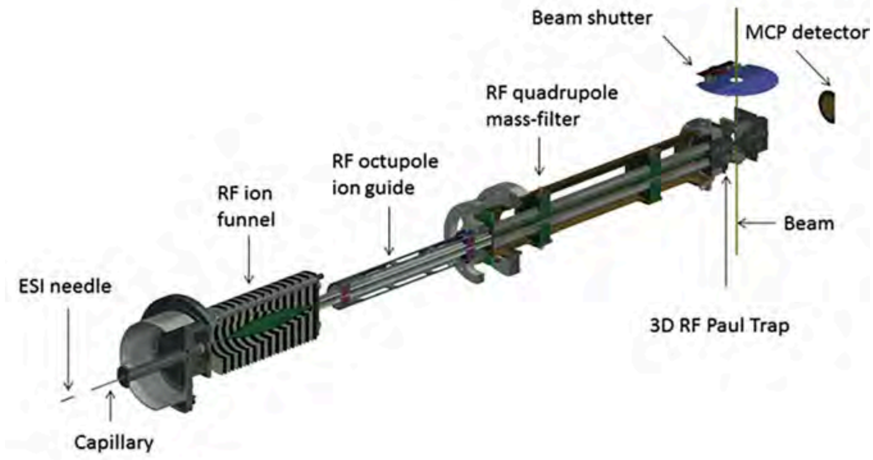


Figure 1: The home-built tandem mass-spectroscopy setup “Paultje”. The length between the 3D RF Paul Trap and the MCP detector is not to scale.

Currently, we are working on answering the question whether a single soft X-ray photon or MeV carbon ion can induce a double strand break in isolated duplex DNA strands. The information that is obtained from these experiments will be compared with theoretical calculations.

REFERENCES

[1] O. Gonzalez-Magana, M. Tiemens, G. Reitsma, L. Boschman, M. Door, S. Bari, P. O. Lahaie, J. R. Wagner, M. A. Huels, R. Hoekstra and T. Schlathölter, *Phys. Rev. A*, **87**, 032702 (2013)

SOFT X-RAY INDUCED CHARGE DYNAMICS IN GAS PHASE OLIGONUCLEOTIDES

Xin Wang[1], Wen Li[1], Wessel Douma[1], Klaas Bijlsma[1], Ronnie Hoekstra[1], Sadia Bari[2], Lucas Schwob[2], Thomas Schlathölter[1]

[1]Zernike Institute for Advanced Materials, University of Groningen, Nijenborgh 4, 9747AG Groningen, The Netherlands
[2]Deutsches Elektronen-Synchrotron, DESY, Notkestr. 85, 22607 Hamburg, Germany
E-mail: xin.wang@rug.nl

In biological systems, the halogenated nucleobase 5-bromouracil (BrU) can replace thymine in DNA sequences. BrU is regularly used as a radiosensitizer in radiotherapy and its interaction with ionizing radiation has been intensively studied on a molecular level [1].

We are using BrU-containing gas-phase oligonucleotides to study migration of charge and energy in these systems. In BrU-A(n)G (n=1-5), the Br atom acts as a soft X-ray chromophore whose L-shell can be selectively excited, leaving this end of the molecule positively charged. The A(n) sequence is known to facility charge transport. G has the lowest oxidation potential of the nucleobases and is most likely carrying the photoinduced positive charge when migration is finished.

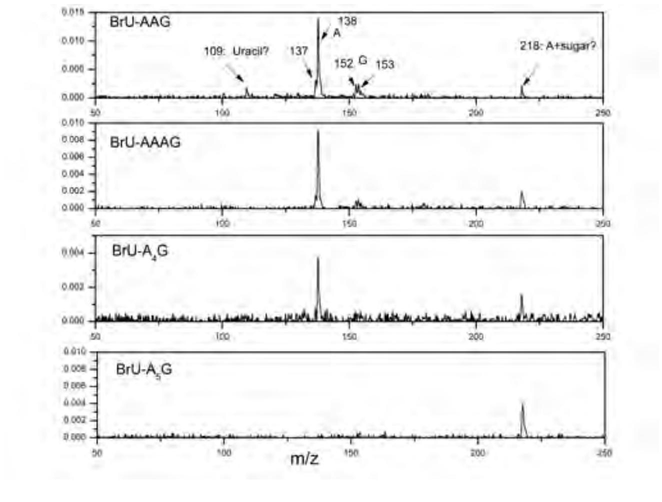


Figure 1: Positive yields of negative BrU-A(n)G (n=2-5) ions colliding with 300 eV photons. With the increasing of the number of A units, several fragmentation channels are closed.

In a first series of experiments, conducted at the synchrotron facility PETRA III (Hamburg), we have studied the influence of the number of A units on the yield of G-containing fragments for photon energies around the C K-edges and the Br L-edge.

REFERENCES

[1] R. Schürmann, T. Tsering, K. Tanzer, S. Denifl, S. V. K. Kumar, I. Bald, Angew. Chem. Int. Ed. 2017, 56, 10952

SELF-ASSEMBLY AND RHEOLOGICAL PROPERTIES OF NANOFLUIDS -A DISSIPATIVE PARTICLE DYNAMICS STUDY-

Yusei Kobayashi[1], Noriyoshi Arai[1,2]

[1]Department of Mechanical Engineering, Kindai University,
3-4-1 Kowakae, 577-8502, Higashiosaka, Japan
E-mail: kobayashiyusei@gmail.com
[2] Research Institute for Science and Technology, Kindai University,
3-4-1 Kowakae, 577-8502, Higashiosaka, Japan
E-mail: arai@mech.kindai.ac.jp

Over the past several decades, extensive research has been conducted to investigate the rheological property of nanofluids with the goal of developing microelectronics, fuel cells, and engine cooling/vehicle thermal management. Here, the self-assembly of nanofluid is an important technique for controlling their rheological properties (e.g., viscosity and thermal conductivity). Self-assembly of nanofluid (nanoparticle) can spontaneously result in a variety morphologies depending on the volume fraction of nanoparticle, the chemical nature of nanoparticle surface, solvent type, and the temperature, among other physical conditions. Hence, the prediction and control of the self-assembly of colloidal nanoparticles is very important and constitute a useful process in materials chemistry and engineering.

Previous studies have already been reported on thermal properties of nanofluids[1]. However, the mechanism of thermal properties has not been clarified so far. We performed molecular simulations to investigate the thermal properties of nanofluids. Here, we attempt to investigate the influence of the addition agent (nanoparticles) properties on the thermal conductivity and viscosity. Three distinct types of nanoparticles were considered: hydrophobic, hydrophilic, and patchy. We observed diverse self-assembled structures between the different nanoparticles designs. Moreover, we found that the thermal conductivity and viscosity behavior depends on the self-assembled phase and the chemical nature of the nanoparticles surface.

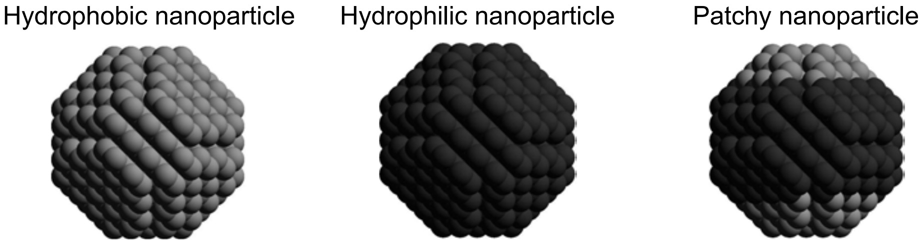


Figure 1: Three kinds of nanoparticle models are employed in this simulation: the hydrophobic uniform nanoparticle, the hydrophilic uniform nanoparticle, and the patchy nanoparticle.

REFERENCES

[1] W. Cui, Z. Shen, J. Yang, S. Wu, and M. Bai, *RSC Advances* **4**, 55580 (2014)

List of Participants

Last Name	First Name	Affiliation	E-mail
Adhikary	Amitava	Oakland University, USA	adhikary@oakland.edu
Antoine	Rodolphe	iLM CNRS and University of Lyon, France	rantoine@lasim.univ-lyon1.fr
Bald	Ilko	University of Potsdam, Germany	bald@uni-potsdam.de
Balykin	Victor	Institute of Spectroscopy, Russian Federation	balykin@isan.troitsk.ru
Bandiera	Laura	INFN, Ferrara, Italy	laura.bandiera451@gmail.com
Bari	Sadia	DESY, Hamburg, Germany	sadia.bari@desy.de
Barilov	Andrey	Peter the Great St.Petersburg Polytechnic University, Russian Federation	andreybarilov@gmail.com
Behmand	Behnaz	Alternative Energies and Atomic Energy Commission, France	behnaz.behmand@cea.fr
Berchignac	Catherine	Laboratoire Aime Cotton, CNRS, France	catherine.brechignac@u-psud.fr
Bergner	Andreas	Innovative Hochschule, Potsdam Transfer, Germany	bergner@uni-potsdam.de
Bijlsma	Klaas	University of Groningen, The Netherlands	k.i.j.bijlsma@student.rug.nl
Broyer	Michel	University of Lyon, France	michel.broyer@univ-lyon1.fr
Calvo	Florent	University Joseph Fourier, France	florent.calvo@univ-grenoble-alpes.fr
Choi	Youngeun	University of Potsdam, Germany	yochoi@uni-potsdam.de
Connerade	Jean-Patrick	Imperial College, UK	jean-patrick@connerade.com
Cortés	Emiliano	Imperial College, UK	e.cortes@imperial.ac.uk
Czerski	Konrad	University of Szczecin, Poland	konrad.czerski@usz.edu.pl

de Vera	Pablo	MBN Research Center, Germany	pablodevego@gmail.com
Denifl	Stephan	University of Innsbruck, Austria	stephan.denifl@uibk.ac.at
Dorn	Alexander	Max-Planck-Institut for Nuclear Physics, Germany	A.Dorn@mpi-k.de
Douma	Wessel	University of Groningen, The Netherlands	f.w.douma@student.rug.nl
Ebel	Kenny	University of Potsdam, Germany	keebel@uni-potsdam.de
Eden	Sam	Open University, Milton Keynes, UK	s.p.eden@open.ac.uk
Ernst	Wolfgang	Graz University of Technology, Austria	wolfgang.ernst@tugraz.at
Farnik	Michal	J. Heyrovsky Institute of Physical Chemistry v.v.i., Czech Republic	michal.farnik@jh-inst.cas.cz
Field	David	University of Aarhus, Denmark	dfield@phys.au.dk
Foldrup	Andreas	University of Southern Denmark, Denmark	anfol14@student.sdu.dk
Frederiksen	Anders	University of Southern Denmark, Denmark	afred15@student.sdu.dk
Friis	Ida	University of Southern Denmark, Denmark	friis@sdu.dk
Gianturco	Franco	The University of Innsbruck, Austria	Francesco.Gianturco@uibk.ac.at
Golding	Jon	Open University, Milton Keynes, UK	jon.golding@open.ac.uk
Gölzhäuser	Armin	University of Bielefeld, Germany	goelzhaeuser@physik.uni-bielefeld.de
Greilich	Steffen	German Cancer Research Center, Germany	s.greilich@dkfz-heidelberg.de
Grygoryeva	Katerina	J. Heyrovský institute of physical chemistry, Czech Republic	kateryna.grygoryeva@jh-inst.cas.cz
Gühr	Markus	University of Potsdam, Germany	mguehr@uni-potsdam.de

Guidi	Vincenco	Ferrara University, Italy	guidi@fe.infn.it
Hahn	Marc Benjamin	Bundesanstalt für Materialforschung und Prüfung, Germany	marc-benjamin.hahn@bam.de
Hilgers	Gerhard	Physikalisch-Technische Bundesanstalt, Germany	gerhard.hilgers@ptb.de
Husen	Peter	University of Southern Denmark, Denmark	phusen@sdu.dk
Ingolfsson	Oddur	University of Iceland, Iceland	odduring@hi.is
Ivanov	Vadim	Peter The Great Saint-Petersburg Polytechnic University, Russian Federation	ivanov@physics.spbstu.ru
Kattnig	Daniel	University of Exeter, UK	D.R.Kattnig@exeter.ac.uk
Khanna	Shiv	Virginia Commonwealth University, USA	snkhanna@vcu.edu
Kleinekathöfer	Ulrich	Jacobs University Bremen, Germany	u.kleinekathoefer@jacobs-university.de
Kobayashi	Yusei	Kindai University, Japan	kobayashiyusei@gmail.com
Kočišek	Jaroslav	J. Heyrovsky Institute of Physical Chemistry v.v.i. , Czech Republic	jaroslav.kocisek@jh-inst.cas.cz
Kopyra	Janina	Siedlce University, Poland	kopyra@ap.siedlce.pl
Korol	Andrei	MBN Research Center, Germany	korol@mbnexplorer.com
Korol	Vasili	University of Southern Denmark, Denmark	korol@sdu.dk
Kumar	S V K	Mumbai, India	svkk@tifr.res.in
Levitan	Vita	University of Southern Denmark, Denmark	vita@bmb.sdu.dk
Li	Wen	University of Groningen, The Netherlands	wen.li@rug.nl

Löhmannsröben	Hans-Gerd	University of Potsdam, Germany	loehm@uni-potsdam.de
Mason	Nigel	Open University, Milton Keynes, UK	nigel.mason@open.ac.uk
Mauracher	Andreas	University of Innsbruck, Austria	andreas.mauracher@uibk.ac.at
Mondal	Shyamal	Saha Institute of Nuclear Physics, India	smondal.xray@gmail.com
Müller	Wenke	University of Potsdam, Germany	wemueller@uni-potsdam.de
Müller-Werkmeister	Henrike	University of Potsdam, Germany	rikemw@uni-potsdam.de
Nakamura	Masato	Nihon University, Funabashi, Japan	mooming@phys.ge.cst.nihon-u.ac.jp
Nielsen	Claus	University of Southern Denmark, Odense, Denmark	clausnielsen@sdu.dk
Orlenko	Elena	Peter the Great St.Petersburg Polytechnic University, Russian Federation	eorlenko@mail.ru
Palmer	Richard	Swansea University, UK	r.e.palmer@swansea.ac.uk
Pavlov	Alexander	Peter the Great St.Petersburg Polytechnic University, Russian Federation	a.pavlov@physics.spbstu.ru
Polozkov	Roman	ITMO University, St. Petersburg, Russian Federation	polozkov@tuexph.stu.neva.ru
Ptasinska	Sylwia	University of Notre Dame, USA	sylwia.ptasinska.1@nd.edu
Razzokov	Jamoliddin	University of Antwerp, Belgium	jamoliddin.razzokov@uantwerpen.be
Schlappa	Stephanie	University of Potsdam, Germany	stepschlappa@uni-potsdam.de
Schlathölter	Thomas	University of Groningen, The Netherlands	t.a.schlatholter@rug.nl
Schürmann	Robin	University of Potsdam, Germany	robinschuermann@yahoo.de
Shinpaugh	Jefferson	East Carolina University, USA	shinpaughj@ecu.edu
Sjulstok	Emil	University of Southern Denmark, Denmark	emilsr@sdu.dk

Solovyeva	Irina	MBN Research Center, Germany	irina@mbnexplorer.com
Solov'yov	Andrey	MBN Reserach Center, Germany	solovyov@mbnresearch.com
Solov'yov	Ilia	University of Southern Denmark, Denmark	ilia@sdu.dk
Suraud	Eric	LPT Univ. Paul Sabatier, France	suraud@irsamc.ups-tlse.fr
Surdutovich	Eugene	Oakland University, USA	surdutov@oakland.edu
Sushko	Gennady	MBN Research Center, Germany	gennady.sushko@gmail.com
Süß	Daniel	University of Innsbruck, Austria	daniel.suess@uibk.ac.at
Tapio	Kosti	University of Potsdam, Germany	kostapio@uni-potsdam.de
Verkhovtsev	Alexey	German Cancer Research Center, Germany	al.verkhovtsev@gmail.com
Vogel	Stefanie	University of Potsdam, Germany	stefanievogel2@gmx.de
Wang	Xin	University of Groningen, The Netherlands	xin.wang@rug.nl
Zühlke	Martin	University of Potsdam, Germany	mzuehlke@uni-potsdam.de