International Conference "Dynamics of Systems on the Nanoscale"

DySoN Conference 2018

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





FINAL ANNOUNCEMENT

Scope

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 <u>isacc-portal.org</u>). 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.

Important Dates

Distribution of the first announcement Distribution of the second announcement Deadline for early-bird registration Deadline for abstract submission Deadline for hotel reservation December 15, 2017 April 03, 2018 August 01, 2018 August 01, 2018 August 07, 2018

Dyson 2018 Program

Monday, 08th October 2018

	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
14 ⁴⁵ - 15 ¹⁵	Amitava Adhikary, Oakland University, USA
	Electron-induced site specific formation and reaction of aminyl radicals in azido-amino
	acids
$15^{15} - 15^{45}$	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
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16 ⁴⁵ - 17 ¹⁰	<u>nanoscale</u> Oddur Ingolfsson, University of Iceland, Reykjavik, Iceland Dissociative electron attachment as potential means for cross-linking of self-assembled
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Tuesday, 09th October 2018

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	Morning session I: Thermal, optical and magnetic properties of nanosystems
9 ³⁰ - 10 ⁰⁰	Andrey V. Solov'yov, MBN Research Center, Frankfurt am Main, Germany
	<i>Dynamics of Meso-Bio-Nano (MBN) systems as seen from computational approach with MBN Explorer</i>
00 20	
$10^{00} - 10^{30}$	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
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
	<u>Afternoon session I: Cluster and biomolecular ensembles, complexes, nanostructured</u> <u>materials</u>
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
	<u>biodamage</u>
$9^{30} - 9^{55}$	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
11 ³⁰ - 11 ⁵⁵	Morning session II: Interaction of radiation with biosystems: mechanisms and applications 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
	Afternoon Session I: Biomedical applications of radiation
14 ³⁰ - 15 ⁰⁰	Eugene Surdutovich , Oakland University, Rochester, USA Multiscale approach to the physics of ion-beam cancer therapy
15 ⁰⁰ - 15 ³⁰	Steffen Greilich, 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

9 ³⁰ - 10 ⁰⁰	Morning session I: Electron & spin transport in molecular systems Ulrich Kleinekathöfer, Jacobs University Bremen, Germany
20	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
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
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	Alexey Verkhovtsev, German Cancer Research Center (DKFZ), Heidelberg, Germany Irradiation induced processes with radiosensitizing nanoparticles
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
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

	Morning session I: Biological systems and application of nanoparticles
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
11 ³⁰ - 11 ⁵⁵	Morning session II: Structure and dynamics of clusters, nanoparticles and biomolecules 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	Rodolphe Antoine , Université de Lyon1, Lyon, France New routes to enhance emission properties of gold nanoclusters
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
$\frac{13^{00} - 13^{30}}{13^{30} - 14^{30}}$	Final Discussion and Conference Closing Lunch and Departure

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 <u>link</u> 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.

<u>From Airport Berlin-Tegel:</u> 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 €

<u>From Berlin Main Station</u>: Take the regional train RE 1 (25 min) or S-Bahn S7 (40 min) to Potsdam Main Station (Ticket "Berlin ABC").

<u>From Potsdam Main Station:</u> 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 <u>www.bahn.de</u> or <u>www.vbb.de</u>.

Potsdam can be reached by car from the A10 and the A115 Highway.

Registration

The number of rooms reserved at the hotels for conference participants is limited. We advise the participants to register for the conference and the hotel at the earliest convenience.

Late registration is still possible under the following conditions: Conference Fee: 500 € Undergraduate and PhD students: 350 €

The fee includes the book of abstracts, coffee breaks, lunches, the conference reception, a sightseeing tour and the conference dinner. The payment to the order of "DySoN 2018" can be made

By bank transfer to Bank Account Name: Bank name: Branch Address: IBAN: BIC:

MBN Research Center gGmbH Deutsche Bank Hauptstr. 561462 Koenigstein Germany DE15500700240137588000 DEUTDEDBFRA

Please quote your NAME and DYSON on the transfer.

Please ensure there are NO charges to us.

Abstract Submission

Late abstracts for poster presentations should be submitted electronically as soon as possible. Please send your abstracts to <u>dyson.conference@gmail.com</u> with the title "DySoN 2018 Abstract". The abstracts are to be supplied by the authors typewritten in camera-ready form in A4 format (210x297 mm). The length of the abstract should not exceed two pages. The abstract template with more detailed preparation guidelines is available for download <u>here</u>. Please note that we accept files in the MS Word document format. Upon abstract submission, please indicate whether the abstract is intended for an oral contribution (invited or contributed), or a poster presentation.

Accommodation

Please book accommodation directly with the <u>Hotel Steigenberger</u>, <u>Potsdam</u>, <u>Germany</u>, see also the <u>link on the</u> <u>Conference site</u>. If a cheaper accommodation is required, we recommend the B&B hotel close to Potsdam Main Station.

Official Invitation and Visa

Conference participants are advised to check the passport and visa requirements for travel to Germany.

Conference Language

The language of the conference is English.

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

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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)