SPIN CHEMISTRY MEETING 2019

Conference Program

18-22 August 2019

Saint Petersburg, Russia

SPIN CHEMISTRY MEETING 2019

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Sponsors

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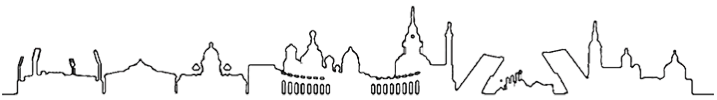
ADANI from ideas to solutions

HYPERSPIN



Welcome to the 16th Spin Chemistry Meeting 2019, in St. Petersburg, Russia!

Spin Chemistry meeting is a well-established forum gathering scientists from all over the world to discuss progress in magnetic field effects on chemical processes, chemically induced spin hyperpolarization and related phenomena. Previous Spin Chemistry Meetings have taken place in Tomakomai, Japan (1991); Konstanz, Germany (1992); Chicago, USA (1994); Novosibirsk, Russia (1996); Jerusalem, Israel (1997); Emmetten, Switzerland (1999); Tokyo, Japan (2001); Chapel Hill, USA (2003); Oxford, UK (2005); San Servolo, Italy (2007); St Catharines, Canada (2009); Noordwijk, The Netherlands (2011); Bad Hofgastein, Austria (2013); Kolkata, India (2015); Schluchsee, Germany (2017).

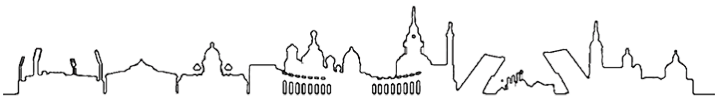
This conference will cover the main areas of spin chemistry, including:

- **Magnetic field effects in chemistry and biology**
- **Hyperpolarized nuclear magnetic resonance**
- **Hyperpolarized electron paramagnetic resonance**
- **Novel material and spintronics**
- **Theory and spin dynamics**
- **New experimental methods**

SCM-2019 intends to promote interactions and synergies between different areas of spin chemistry. To facilitate participation of young scientists in this activity, tutorials on spin chemistry will be organized prior to main SCM-2019 event.

We wish you fruitful conference and enjoyable stay in St. Petersburg!

Konstantin Ivanov (Co-chairman) **Leonid Kulik** (Co-chairman)



SPIN CHEMISTRY MEETING 2019

Committees

Local Organizing Committee

- Prof. Konstantin Ivanov, co-chairman
- Prof. Leonid Kulik, co-chairman
- Dr. Dmitri Stass, secretary
- Lionella Sukhinina, accountant
- Prof. Renad Sagdeev
- Prof. Alexandra Yurkovskaya
- Prof. Sergey Tarasenko
- Prof. Nikita Lukzen
- Dr. Denis Sosnovsky
- Alexander Popov
- Dr. Andrey Anisimov
- Dr. Kirill Baryshnikov

Program Committee

- Prof. Konstantin Ivanov
- Prof. Leonid Kulik
- Prof. Renad Sagdeev
- Prof. Yuri Molin
- Prof. Alexandra Yurkovskaya
- Prof. Sergey Tarasenko
- Prof. Peter J. Hore
- Prof. Jan Behrends
- Prof. Kiminori Maeda
- Prof. Jörg Matysik
- Prof. Stefan Weber

International SCM Committee

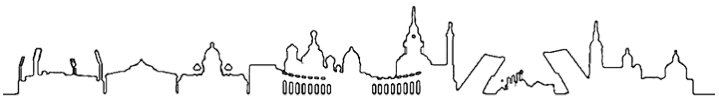
- Samita Basu (Kolkata, India)
- Jan Behrends (Berlin, Germany)
- Art van der Est (St Catharines, Canada)
- Malcolm Forbes (Bowling Green, USA)
- Günter Grampp (Graz, Austria)
- Peter Hore, Chairman (Oxford, UK)
- Konstantin Ivanov (Novosibirsk, Russia)
- Yasuhiro Kobori (Kobe, Japan)
- Leonid Kulik (Novosibirsk, Russia)
- Jörg Matysik (Leipzig, Germany)
- Kiminori Maeda (Saitama, Japan)
- Marilena di Valentin (Padua, Italy)
- Michael Wasielewski (Evanston, USA)
- Stefan Weber (Freiburg, Germany)
- Markus Wohlgenannt (Iowa, USA)

Organizers

- International Tomography Center, Siberian Branch of the Russian Academy of Science (Novosibirsk)

- Voevodsky Institute of Chemical Kinetics and Combustion, Siberian Branch of the Russian Academy of Science (Novosibirsk)

- Ioffe Physical-Technical Institute, Russian Academy of Sciences (St. Petersburg)

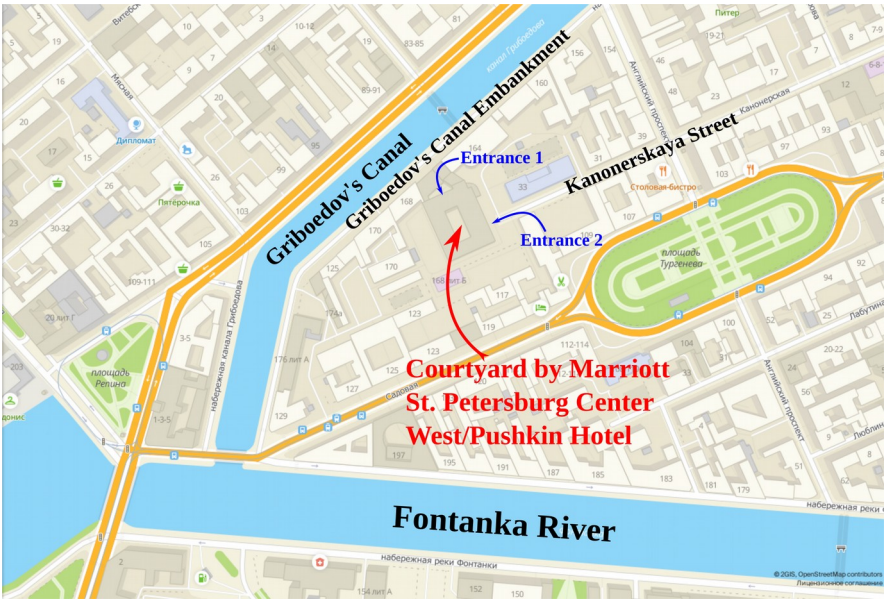


Conference Venue

Courtyard by Marriott St. Petersburg Center West/Pushkin Hotel

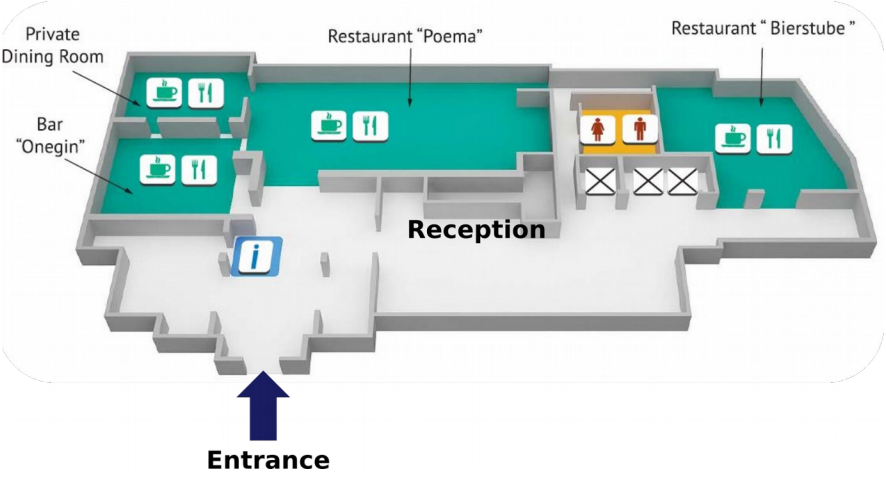
166 Griboedov's Canal, via 33 Kanonerskaya Street, St. Petersburg

There are two entrances to Courtyard by Marriott West Pushkin Hotel: one from Griboedov's Canal, the other from Kanonerskaya Street

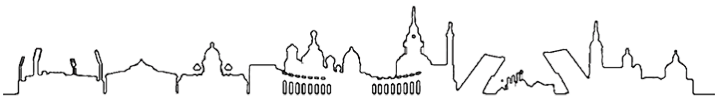


Floorplans

Ground floor



First Floor



SPIN CHEMISTRY MEETING 2019

Conference Sessions

All conference sessions will be held in Courtyard by Marriott West Pushkin Hotel (166 Griboedov's Canal, St. Petersburg).

Tutorials On Spin Chemistry

The tutorial will be held in Tolstoy A Hall (first floor).

Oral Presentations

Oral sessions will be held in Tolstoy Hall (first floor). Contributors may run their presentation on their own laptop or use a laptop provided at the conference site.

Posters

Poster sessions will be held in the evenings of August 19 and 20 in Tolstoy Hall B. Fixing materials will be provided. Posters need to be on display by 20:30 August 19 and must be removed by 16:30, August 22, the latest.

Food And Drinks

Coffee-breaks will be served at the area near Tolstoy Hall.

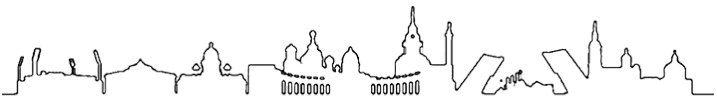
Lunches, dinners and conference banquet are included in the registration fee. They will be served in Poema Restaurant (ground floor).

Boat Trip

The excursion will start at 17:10, August 21, from the conference venue. First, the participants will be guided to the pier of Fontanka River. Please be ready to go by foot about 500 m. The boats will leave from the pier at 17:30. They will navigate through canals of St. Petersburg and Neva River. Food and drinks will be available on board.

Name Tags

Members of the local organizing committee will wear **red name tags**. Regular participants will have **blue name tags** and accompanying persons will wear **green name tags**.



Conference Program

AUGUST 18

Registration at the conference site from 10:00 until evening of August 19

10:20 **Spin Chemistry Tutorials**: Opening

10:30 **Konstantin Ivanov** (Novosibirsk, Russia), Spin dynamics and density matrix formalism

12:00 Coffee-break

12:30 **Peter Hore** (Oxford, UK), Magnetic field effects in chemistry

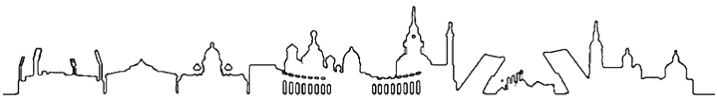
14:00 Lunch

15:30 **Hans-Martin Vieth** (Berlin, Germany), Chemically induced hyperpolarization of nuclear spins

17:00 Coffee-break

17:30 **Kiminori Maeda** (Saitama, Japan), Chemically induced hyperpolarization of electron spins

19:30 Welcome party



SPIN CHEMISTRY MEETING 2019

AUGUST 19

9:00 **Opening** / *K. Ivanov, L. Kulik, P. J. Hore*

Hyperpolarized EPR / *M. Wasielewski*

9:10 **Stefan Weber** (Freiburg, Germany), Something old, something new, something borrowed, something blue: EPR and NMR detection of spin-correlated radical pairs in blue-light photoreceptors

9:50 **Claudia Avalos** (Lausanne, Switzerland), Stable radicals tethered to pentacene studied using time resolved EPR and transient absorption spectroscopy

10:10 **Motoko Asano** (Gunma, Japan), Spin-polarization in the charge transfer excited state of Copper (I) complexes

10:30 **Matvey Fedin** (Novosibirsk, Russia), Electron spin polarization in compact chromophore dyads studied by time-resolved EPR

10:50 Coffee-break

Magnetic field effects / *P. J. Hore*

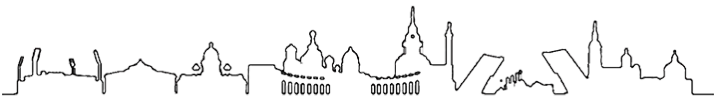
11:20 **Henrik Mouritsen** (Oldenburg, Germany), The quantum robin: biological evidence for radical-pair-based magnetic field effects in cryptochromes of migratory birds

12:00 **Victor Bezchastnov** (Heidelberg, Germany), Anisotropic response of cryptochrome radicals to a weak magnetic field

12:20 **Tatiana Domratcheva** (Heidelberg, Germany), Formation and decay of magnetosensory radical pairs in animal cryptochrome

12:40 **Christiane Timmel** (Oxford, UK), Demonstration of a chemical compass in microtesla magnetic fields: a proof of principle for radical pair magnetoreception in birds

13:10 Lunch until 14:30



AUGUST 19

Theory and spin dynamics / *K. Ivanov*

14:30 **David Manolopoulos** (Oxford, UK), Master equations for spin dynamics

15:10 **Thomas Fay** (Oxford, UK), Relaxation in radical pair reactions – improvements on phenomenological approaches

15:30 **Timothy Field** (Hamilton, Canada), Dynamical theory of spin noise and relaxation - beyond extreme narrowing

15:50 **Daniel Kattnig** (Exeter, UK), On magnetic field effects in triads of radicals

16:20 Coffee-break

Hyperpolarized NMR / *R. Sagdeev*

16:50 **Gerd Buntkowsky** (Darmstadt, Germany), Hyperpolarization with parahydrogen

17:20 **Olga Morozova** (Novosibirsk, Russia), Inter- and intramolecular reduction of transient histidine radical by tyrosine and tryptophan: TR CIDNP study

17:40 **Stephan Knecht** (Darmstadt, Germany), The role of low concentrated intermediates in Signal Amplification by Reversible Exchange (SABRE) hyperpolarization

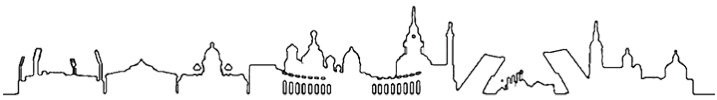
18:00 **Kirill Kovtunov** (Novosibirsk, Russia), Parahydrogen based hyperpolarization in heterogeneous catalysis

18:20 **Ivan Skovpin** (Novosibirsk, Russia), NMR and MRI of SLIC-SABRE hyperpolarized biomolecules

18:40 **Hans-Heinrich Limbach** (Berlin, Germany), Bonding and mobility of hydrogen to and near transition metals

19:00 Dinner

20:30 **Poster session 1**



SPIN CHEMISTRY MEETING 2019

AUGUST 20

New experimental methods / *Y. Kobori*

9:00 **Michael Wasielewski** (Evanston, USA), Photodriven quantum teleportation of an electron spin state in a covalent donor-acceptor-radical system

9:40 **Mark Oxborrow** (London, UK), MASAR cooling of an electromagnetic mode using photo-excited pentacene dissolved in solid para-terphenyl

10:00 **Hao Wu** (London, UK), Room-temperature pulsed or continuous-wave pentacene maser?

10:20 **Jonathan Woodward** (Tokyo, Japan), Microspectroscopy of flavin-based radical pairs

10:50 Coffee-break

Magnetic field effects / *U. Steiner*

11:20 **Tetsuro Kusamoto** (Okazaki, Japan), Magnetoluminescence in photostable radicals

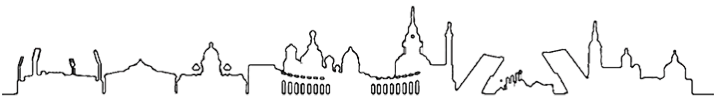
11:50 **Malcolm Forbes** (Bowling Green, USA), Steady state and time resolved EPR investigations of structured (non-Newtonian) fluids

12:10 **Tomoaki Yago** (Saitama, Japan), Low magnetic field effects on triplet pairs

12:30 **Kiminori Maeda** (Saitama, Japan), Probing and controlling transient radical pairs by static and AWG based RF fields in low field regime

12:50 **Yoshio Teki** (Osaka, Japan), Photostable non-luminescent pentacene–radical derivative and luminescent radical-excimer: Counters in unique excited-state spin dynamics of pi-radicals

13:20 Lunch until 14:30



AUGUST 20

Hyperpolarized NMR / *J. Matysik*

14:30 **Malcolm Levitt** (Southampton, UK), Entangling spins & space: Spin isomers, endofullerenes, hyperpolarization and long-lived states

15:10 **James Eills** (Mainz, Germany), Polarization transfer in [1-13C]fumarate using constant-adiabaticity field sweeps

15:30 **Yuliya Mindarava** (Ulm, Germany), Hyperpolarization of 13C nuclear spins with Nitrogen-Vacancy center in diamond

15:50 **John Blanchard** (Mainz, Germany), Nuclear spin hyperpolarization in zero to ultralow magnetic fields

16:20 Coffee-break

Materials / *S. Tarasenko*

16:50 **Jan Behrends** (Berlin, Germany), Triplet and quintet states in disordered and crystalline singlet-fission materials

17:30 **Pritam Mukhopadhyay** (New Delhi, India), Synthesis and stabilization of arylenediimide-based planar and twisted radical anions

17:50 **Andreas Sperlich** (Würzburg, Germany), Optically and electrically excited intermediate electronic states in donor:acceptor based OLEDs

18:10 **Jean-Philippe** Ansermet (Lausanne, Switzerland), Probing spin-dependent charge transfer at electrodes using magnetic resonance

18:30 **Alexei Chepelianskii** (Paris-Saclay, France), Spin properties of biexciton state formed through singlet fission

19:00 Dinner

20:30 **Poster session 2**

SPIN CHEMISTRY MEETING 2019

AUGUST 21

Prof. I'Haya memorial session / *Y. Tanimoto*

9:00 **Hisao Murai** (Shizuoka, Japan), Professor. Y. J. I'Haya Memorial lecture - Kick-off of 'Spin Chemistry Meeting'

9:30 **Ulrich Steiner** (Konstanz, Germany), Complete electronic repository of all Spin Chemistry Meetings

Hyperpolarized EPR / *K. Möbius*

9:50 **Marilena di Valentin** (Padua, Italy), Light-induced pulsed EPR dipolar spectroscopy: the spin-polarized triplet state probe

10:20 **Olesya Krumkacheva** (Novosibirsk, Russia), Triplet fullerenes as prospective spin labels for nanoscale distance measurements by pulsed dipolar EPR

10:40 **Rane Vinayak** (Mumbai, India), Designing covalently linked radical-chromophore dyads with a large magnitude of electron spin polarization

11:00 Coffee-break

Hyperpolarized EPR / *M. di Valentin*

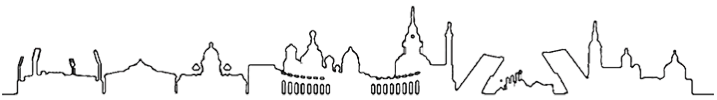
11:30 **Klaus Moebius** (Berlin, Germany), Protein machinery enabling Life without Water: High-field EPR studies of protein/matrix H-bond interactions

12:00 **Art van der Est** (St. Catharines, Canada), Triplet electron transfer and spin polarization in a Palladium porphyrin–fullerene conjugate

12:20 **Alexander Popov** (Novosibirsk, Russia), Out-of-phase ELDOR study of charge separation in organic photovoltaic composites

12:40 **Yasuhiro Kobori** (Kobe, Japan), Molecular geometries and motions driving quintet multiexcitons via singlet fissions

13:00 Lunch until 14:30



AUGUST 21

Theory and spin dynamics / *A. van der Est*

14:30 **Kev Salikhov** (Kazan, Russia), Paradigm shift of spin exchange in solutions of paramagnetic particles

15:00 **Yuri Kandrashkin** (Kazan, Russia), EPR study of photoexcited orthogonal Bodipy dyads

15:20 **David Mims** (Würzburg, Germany), Extreme on-resonance quantum coherence effect on the charge recombination in rigidly linked radical ion pairs with predominant triplet spin gate

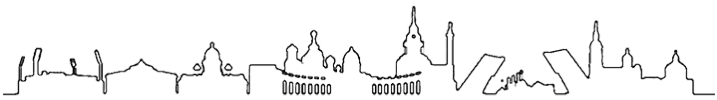
15:40 **Takeji Takui** (Osaka, Japan) Practical quantum algorithms for quantum chemical calculations on quantum computers

16:10 **Valerii Zapasskii** (St. Petersburg, Russia), Spin noise spectroscopy in progress

16:50 Coffee-break

17:10 Cultural program, boat trip

20:00 Conference banquet



SPIN CHEMISTRY MEETING 2019

AUGUST 22

Hyperpolarized NMR / *S. Weber*

9:00 **Jorg Matysik** (Leipzig, Germany), The solid-state photo-CIDNP effect: New results and developments

9:40 **Yonghong Ding** (Leipzig, Germany), Field-cycling solution NMR reveals 1H, 13C and 15N photochemically induced dynamic nuclei polarization in cysteine-lacking LOV domains

10:00 **Alexey Kiryutin** (Novosibirsk, Russia), Proton relaxometry of long-lived spin order

10:20 **Dennis Kurzbach** (Vienna, Austria), Signal-improved real-time NMR spectroscopy of proteins by hyperpolarized water

10:40 Coffee-break

New experimental methods / *L. Kulik*

11:10 **Gurumurthy Rajalakshmi** (Hyderabad, India), Optical detection of spins

11:30 **Andrey Anisimov** (St.Petersburg, Russia), The ODMR of vacancy spin centers in silicon carbide

11:50 **Oksana Koplak** (Chernogolovka, Russia), Microwave remote reading of logic states of spin valve

12:10 **Stuart Mackenzie** (Oxford, UK), Optical cavity-based spectroscopy for the sensitive detection of magnetic field effects

12:30 **Gerd Kothe** (Freiburg, Germany), Creation and detection of scalable nuclear spin qubits in hyperpolarized molecular solids

12:50 Lunch until 14:30

AUGUST 22

Magnetic field effects / *G. Grampp*

14:30 **Yoshifumi Tanimoto** (Hiroshima, Japan), Magnetic field effects in chemistry, physics and biology

15:00 **Kirill Baryshnikov** (St. Petersburg, Russia), Magnetic susceptibility of point crystal defects subjected to the Jahn-Teller effect

15:20 **Nikolay Polyakov** (Novosibirsk, Russia), Possibilities of spin chemistry in the study of chiral systems

15:40 **Dongkyum Kim** (Gwangju, Republic of Korea), Magnetic field effect of exciplex fluorescence on a highly designable peptoid scaffold

16:00 Coffee-break

Materials / *J. Behrends*

16:30 **Anna Rodina** (St. Petersburg, Russia), Optical access to the surface spins in colloidal nanocrystals

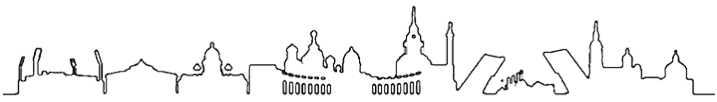
17:00 **Mikhail Fonin** (Konstanz, Germany), Robust magnetism of prototypical Fe4 molecular magnets on functional surfaces

17:20 **Roman Morgunov** (Chernogolovka, Russia), Spin controlled oxidation and dislocation mobility under hyperfine and/or external magnetic fields in the 29Si enriched crystals

17:40 **Tomoaki Miura** (Niigata, Japan), Charge carrier and spin dynamics in organic semiconductor thin films studied by simultaneous measurement of transient optical absorption and photocurrent signals

18:00 **Vladimir Dyakonov** (Würzburg, Germany), Optically and electrically addressable spin states in 2D and 3D organic and inorganic semiconductors

18:40 Closing of the conference



Posters

P01 **Aleksandra Ageeva** (Novosibirsk, Russia), Use of spin effects to study the nature of phototoxicity of ketoprofen and ketoprofen-based dyads

P02 **Sergei Anishchik** (Novosibirsk, Russia), Electric and magnetic field effects in the luminescence from X-irradiated CVD diamonds

P03 **Lewis Martyn Antill** (Saitama, Japan), Spatiotemporal measurement of cryptochromes for animal magnetoreception

P04 **Nathan Babcock** (Exeter, UK), Interplay between dipolar and hyperfine couplings in model spin systems

P05 **Martin Brodrecht** (Darmstadt, Germany), Amino acid building-blocks for solid-phase peptide synthesis of spin labeled peptides for EPR and DNP applications

P06 **Victoire Dejean** (Oxford, UK), Intrinsic magnetic field effects in viscous flavin solutions

P07 **Matthew Golesworthy** (Oxford, UK), Cavity-enhanced measurement of radical pair-based magnetic field effects

P08 **Jamie Gravell** (Oxford, UK), Magnetic field effects in protein crystals by confocal microscopy

P09 **Kevin Henbest** (Oxford, UK), Magnetically sensitive light-induced reactions in Drosophila Melanogaster cryptochromes

P10 **Noboru Ikeya** (Tokyo, Japan), Magnetic field effect fluorescence microscopy for in vivo and anisotropic field measurements on flavin based radical pairs

P11 **Nana Iwata** (Saitama, Japan), Low field effect on radical pairs confined in the binding pocket of bovine serum albumin

P12 **Yuri Kandrashkin** (Kazan, Russia), Triplet mechanism of electron spin polarization in moderately coupled triplet-doublet rigid complexes as a source of the enhanced $+1/2 \leftrightarrow -1/2$ transitions

P13 **Ken Kato** (Osaka, Japan), Photocurrent behaviour and electrically detected magnetic resonance study of TIPS-pentacene and pentacene–radical derivative

P14 **Shun Kimura** (Tokyo, Japan), Magnetic field effect on the luminescence of stable radicals in a rigid environment

P15 **Alexey Kiryutin** (Novosibirsk, Russia), Ultrafast single-scan TOCSY NMR detection of a PHIP-hyperpolarized protease inhibitor

P16 **Igor Kochman** (St. Petersburg, Russia), Temperature dependence of bands overlap in AlSb/InAs/GaSB/AlSb QCW at microwave absorption in magnetic field

P17 **Marcin Konowalczyk** (Oxford, UK), Cavity enhanced spectroscopy studies of magnetic field effects of proteins

P18 **Leonid Kulik** (Novosibirsk, Russia), Charge separation and recombination in organic photovoltaic blend PCDTBT/PC71BM

P19 **Ivan Kurganskii** (Novosibirsk, Russia), Time-resolved EPR study of BODIPY-carbazole dyads

P20 **Nikita Lukzen** (Novosibirsk, Russia), Multifrequency NMR as an efficient tool to investigate stable heterospin complexes in solutions

P21 **Jiate Luo** (Oxford, UK), Radiofrequency magnetic field effects on magnetoreceptive radical pairs

P22 **Kenta Masuzawa** (Saitama, Japan), Quantum control of radical pairs based on the local optimization theory

P23 **Saki Matsuda** (Kobe, Japan), Mechanism of multiple multiexciton formation and triplet dissociation by singlet fission in thin films

P24 **Taisuke Matsuo** (Saitama, Japan), Low field effect in the photochemical reaction of xanthone and DABCO in a micelle

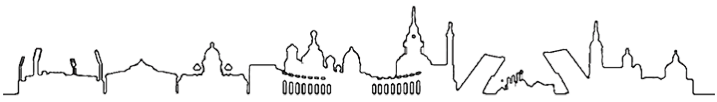
P25 **Olga Morozova** (Novosibirsk, Russia), Indirect NMR detection of formation and decay of guanine cation radical in neutral aqueous solution

P26 **Shinya Oyama** (Kobe, Japan), Photoinduced charge recombination in P3HT:PC70BM blend film studied by TR-EPR

P27 **Thomas Player** (Oxford, UK), Viability of radical pair magnetoreception involving superoxide radicals

P28 **Taichi Sato** (Saitama, Japan), Pulsed MFE measurement of FAD and amino acid mixture

P29 **Masaya Sato** (Tokyo, Japan), Establishing shaped pulse RYDMR based fluorescence and transient optical absorption microscopic method



P30 **Petr Semenikhin** (St. Petersburg, Russia), Manifestation of Coulomb blockade of spin exchange upon compensation of doped semiconductor

P31 **Kirill Sheberstov** (Novosibirsk, Russia), Hyperpolarization and long-lived states of the nuclear spins in azobenzene

P32 **Denis Sosnovsky** (Novosibirsk, Russia), Solution-state photo-CIDNP in LOV domains: Role of solid-state mechanisms

P33 **Dmitri Stass** (Novosibirsk, Russia), On algebraic properties of the sub-block of zero field hyperfine Hamiltonian with penultimate total spin projection for arbitrary hyperfine structure, and field dependence of radical pair recombination probability in the vicinity of zero field

P34 **Sergey Tarasenko** (St. Petersburg, Russia), Theory of spin noise at electron paramagnetic resonance

P35 **Felix Torres** (Zurich, Switzerland), Identification of molecular features for the design of new CIDNP active molecules

P36 **Mikhail Uvarov** (Novosibirsk, Russia), Light-induced charge transfer state in the composite DTS(FBTTh2)2:PC71BM

P37 **Ewoud Vaneeckhaute** (Leuven, Belgium), Coherent solvent hyperpolarization using aminosilanes

P38 **Hans-Martin Vieth** (Berlin, Germany), Hyperpolarization and NMR relaxation dispersion at magnetic field from 5nT to 10T

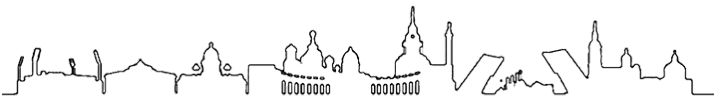
P39 **Laura Katharina Wienands** (Darmstadt, Germany), Investigation of parahydrogen induced hyperpolarisation efficiency of spin labelled amino acid

P40 **Hanming Yang** (Madison, USA), LC-Photo-CIDNP advances enable fast and inexpensive hyperpolarization of biomolecules in solution

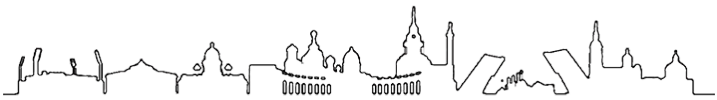
P41 **Alexandra Yurkovskaya** (Novosibirsk, Russia), Detailed mechanism of reaction between aromatic amino acids and triplet-excited benzophenones revealed by time-resolved CIDNP

P42 **Hang Zhou** (Oxford, UK), Exploring surface aggregation and magnetic field effect of biological molecules via polarization-sensitive evanescent wave spectroscopy

P43 **Ivan Zhukov** (Novosibirsk, Russia), Light-induced nuclear hyperpolarization in rigid D-X-A dyads reveals positive sign of exchange interaction and dominance of minor channel in CIDNP formation



For Notes



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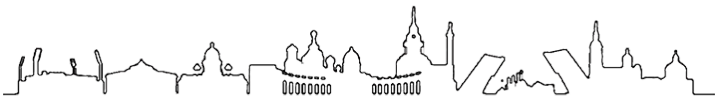

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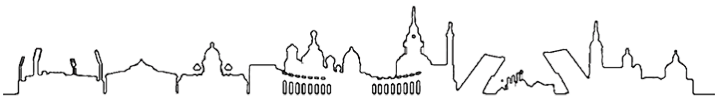

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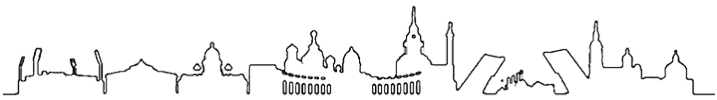

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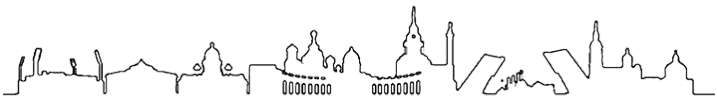

For Notes