Prof. Igor V. Koptyug

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Date and place of birth: May 7, 1963, Novosibirsk, Russia *Nationality:* Russian
Home address: 12 Zhemchuzhnaya St., apt. 23, Novosibirsk 630090, Russia
Marital and family status: Married, 3 children

a. Professional Preparation

Novosibirsk State University, Novosibirsk, Russia	Physics	B.S., 1983
Novosibirsk State University, Novosibirsk, Russia	Chemical Physics	M.S., 1985
Institute of Chemical Kinetics and Combustion, Novosibirsk, Russia	Chemical Physics	Ph.D., 1991
Columbia University, New York, NY (Postdoc)	Spin chemistry, NMR, ESR	1991-1995

b. Appointments

2017 – Deputy Director, International Tomography Center, SB RAS, Novosibirsk, Russia
2015 –Chief Research Scientist (part-time), Novosibirsk State University, Novosibirsk, Russia.
2010 - Head of Laboratory, International Tomography Center, SB RAS, Novosibirsk, Russia
2010 – Scientific Director, Joint Department of Tomography, Institute of Cytology and Genetics, SB RAS and ITC SB RAS, Novosibirsk, Russia
2006 – Professor, Catalysis, International Tomography Center, SB RAS, Novosibirsk, Russia
2003 - Doctor of Sciences (Dr. Sci.) degree in catalysis, Boreskov Institute of Catalysis, SB RAS, Novosibirsk, Russia.
1997 – 2001 – Scientific Secretary, Scientific Council of the International Tomography Center, SB RAS, Novosibirsk, Russia
1995-2009 - research group head, International Tomography Center, SB RAS, Novosibirsk, Russia

c. Awards

The Russian Academy of Sciences Award for the series of studies "Nanostructuring of an active component as a method to control catalytic properties of supported metal catalysts in hydrogenation and oxidation reactions", 2016.

Commemorative medal "For the work to the benefit of Novosibirsk city", Novosibirsk City Mayor, Novosibirsk, Russia, 2013.

Commemorative medal "For contribution to the development of the Novosibirsk Region", Government of the Novosibirsk Region, Russia, 2012.

The Russian Academy of Sciences Award for the series of studies «Using the principles of green chemistry in the fundamental and applied research for sustainable development", 2011.

Diploma from the Russian Academy of Sciences for the substantial contribution to the development of academic science in Russian Federation, 2007.

The award "Best review published in Russian Chemistry Reviews in 2003", 2004.

First degree diploma from the administration of the Novosibirsk region for the outstanding achievements of young scientists in the nomination "Chemistry and materials science", 2003

Official acknowledgment from the President of the Russian academy for many years of fruitful scientific research in the Academy for the benefit of science, 1999.

d. Publications (in total, 198 publications in peer review journals and monographs/book chapters)
The list of publications for the last 3 years is attached.

e. Synergistic Activities

1. Vice-Secretary General (2005-2013), Vice-President (since 2013-2017), Advisor (since 2017), Division of Spatially Resolved Magnetic Resonance, Groupment AMPERE.
2. Member of the Thesis Defense Council D 003.012.01, Boreskov Institute of Catalysis, Novosibirsk, Russia.
3. Invited Professor, Ecole Normale Superieure, Lyon, France, 2018.
4. Invited Professor, Ecole Normale Superieure, Paris, France, 2016.
5. Invited Professor, Pierre and Marie Curie University, Paris – 2003.
6. Invited talks at international magnetic resonance and catalysis conferences on a regular basis.
7. Participation in the organization of National and International conferences and schools as a member of the Organizing and Program committees.
8. Reviewed grant proposals for NSF, Wellcome Trust (UK), NSERC (Canada), NWO (The Netherlands), KU Leuven (Belgium), The Foundation for Polish Science (Poland); reviewed papers for Science, Nature Communications, JACS, Angewandte Chemie, ChemComm and other international journals.
9. Editorial board member of Scientific Reports.

f. Collaborators & Other Affiliations

(i) Current collaborators

Prof. E. Chekmenev, Vanderbilt University Institute of Imaging Science, Nashville, TN; Prof. C. Coperet, ETH, Zurich; Prof. J. Perez-Ramirez, ETH, Zurich; Prof. Boyd M. Goodson, Southern Illinois University, Department of Chemistry and Biochemistry, Carbondale, IL; Prof. V.I. Bukhtiyarov, Prof. V.N. Parmon, Boreskov Institute of Catalysis, Novosibirsk, Russia; Prof. A. Corma, Instituto de Tecnologia Quimica UPV-CSIC, Valencia, Spain; Prof. V.-V. Telkkii, Department of Physics, University of Oulu, Oulu, Finland; Prof. G. Bodenhausen, ENS Paris, France; Prof. Sami Jannin, ENS Lyon, France, Prof. J.-B. Hövener, Kiel University, Germany.

(ii) Graduate and Postdoctoral Advisors

Graduate advisor - Prof. Renad Z. Sagdeev, Director, International Tomography Center, SB RAS, Novosibirsk, Russia; Postdoctoral advisor - Prof. Nicholas J. Turro, William P. Schweitzer Professor of Chemistry, Columbia University, New York, NY.

(iii) Thesis Advisor and Postgraduate-Scholar Sponsor

Anna A. Lysova, research scientist, International Tomography Center (ITC), Novosibirsk, Russia; Kirill V. Kovtunov, research scientist, ITC, Novosibirsk, Russia; Vladimir V. Zhivonitko, research scientist, ITC, Novosibirsk, Russia; Andrey A. Savelov, head of group, ITC, Novosibirsk, Russia; Anatoly V. Matveev, engineer, Schlumberger, Novosibirsk Technological Center, Novosibirsk, Russia; Ivan S. Glaznev, research scientist, Boreskov Institute of Catlaysis, Novosibirsk, Russia; Lyudmila Yu. Ilyina, researcher, Boreskov Institute of Catlaysis, Novosibirsk, Russia.
The total number of graduate students advised: 10; postdoc scholars sponsored: 5

g. **Ongoing Research Support**

Federal budget (Federal Agency for Scientific Organizations) Koptyug (co-PI)
available annually
Utilization of magnetic resonance, optical and mass spectroscopy techniques for the studies of physical and chemical processes in condensed phase
The overall goal of this multi-PI project is to development of instrumental techniques including NMR and MRI
Role: co-PI

Russian Foundation for Basic Research (RFBR) grant Koptyug (PI)
09/2017-08/2020
Magnetic Resonance Spectroscopy and Molecular Imaging of Metabolic Pathways in Cancer
The goal of this project is the development and application of the novel NMR spectroscopy and imaging for the studies of metabolic pathways in cancer with the utilization of hyperpolarization of nuclear spins of key metabolites.
Role: PI

Russian Foundation for Basic Research (RFBR) grant Koptyug (PI)
01/2019-12/2021
Long-lived hyperpolarized molecules for magnetic resonance produced using parahydrogen.
The goal of this project is the development of inexpensive approaches both to the synthesis of contrast agents and to their hyperpolarization with the use of parahydrogen-based techniques (PHIP, SABRE) for a broad range of applications.
Role: PI

Publications of I.V. Koptyug, 2016-2019

1. A.I. Svyatova, K.V. Kovtunov, I.V. Koptyug. Magnetic resonance imaging of catalytically relevant processes, *Rev. Chem. Eng.* (2019); doi: 10.1515/revce-2018-0035.
2. V.V. Zhivonitko, J. Bresien, A. Schulz, I.V. Koptyug. Parahydrogen-induced polarization with a metal-free P-P biradicaloid, *Phys. Chem. Chem. Phys.* (2019); doi: 10.1039/C8CP07625A.
3. N.V. Chukanov, B.M. Kidd, L.M. Kovtunova, V.I. Bukhtiyarov, R.V. Shchepin, E.Y. Chekmenev, B.M. Goodson, K.V. Kovtunov, I.V. Koptyug. A versatile synthetic route to the preparation of 15N heterocycles, *J. Labelled Compd. Radiopharm.* (2018); doi: 10.1002/jlcr.3699.
4. A. Selent, V.V. Zhivonitko, I.V. Koptyug, V.-V. Telkki. Quantifying the adsorption of flowing gas mixtures in porous materials by remote detection NMR, *Microporous Mesoporous Mater.*, **269**, 148(2018); doi: 10.1016/j.micromeso.2017.05.040.
5. V.V. Zhivonitko, I.V. Skovpin, K.C. Szeto, M. Taoufik, I.V. Koptyug. Parahydrogen-induced polarization study of silica-supported vanadium oxo organometallic catalyst, *J. Phys. Chem. C*, **122**, 4891(2018); doi: 10.1021/acs.jpcc.7b12069.
6. A.V. Bukhtiyarov, D.B. Burueva, I.P. Prosvirin, A.Y. Klyushin, M.A. Panafidin, K.V. Kovtunov, V.I. Bukhtiyarov, I.V. Koptyug. Bimetallic Pd-Au/HOPG catalysts: from composition to pairwise parahydrogen addition selectivity, *J. Phys. Chem. C*, **122**, 18588(2018); doi: 10.1021/acs.jpcc.8b06281.
7. K.V. Kovtunov, D. Lebedev, A. Svyatova, E.V. Pokochueva, I.P. Prosvirin, E.Y. Gerasimov, V.I. Bukhtiyarov, C.R. Muller, A. Fedorov, I.V. Koptyug. Robust in situ magnetic resonance imaging of heterogeneous catalytic hydrogenation with and without hyperpolarization, *ChemCatChem*, **11**, 969(2018); doi: 10.1002/cctc.201801820.
8. K. Sorochkina, V.V. Zhivonitko, K. Chernichenko, V.-V. Telkki, T. Repo, I.V. Koptyug. Spontaneous 15N nuclear spin hyperpolarization in metal-free activation of parahydrogen by molecular tweezers, *J. Phys. Chem. Lett.*, **9**, 903(2018); doi: 10.1021/acs.jpclett.7b03433.
9. K.V. Kovtunov, D. Burueva, L. Kovtunova, V. Bukhtiyarov, I. Koptyug. Single-site heterogeneous catalysts: from synthesis to NMR signal enhancement, *Chem. Eur. J.*, **25**, 1420(2018); doi: 10.1002/chem.201803515.
10. O.G. Salnikov, R.V. Shchepin, N.V. Chukanov, L. Jaigirdar, W. Pham, K.V. Kovtunov, I.V. Koptyug, E.Y. Chekmenev. The effects of deuteration of 13C-enriched phospholactate on the efficiency of parahydrogen-induced polarization using magnetic field cycling, *J. Phys. Chem. C*, **122**, 24740(2018); doi: 10.1021/acs.jpcc.8b07365.
11. O.G. Salnikov, L.M. Kovtunova, I.V. Skovpin, V.I. Bukhtiyarov, K.V. Kovtunov, I.V. Koptyug. Mechanistic insight into heterogeneous hydrogenation of furan derivatives with the use of parahydrogen, *ChemCatChem*, **10**, 1178(2018); doi: 10.1002/cctc.201701653.
12. V.V. Zhivonitko, A.I. Svyatova, K.V. Kovtunov, I.V. Koptyug. Recent MRI studies on heterogeneous catalysis, *Annu. Rep. NMR Spectrosc.*, **95**, 83(2018); doi: 10.1016/bs.arnmr.2018.06.001.
13. N.V. Chukanov, O.G. Salnikov, R.V. Shchepin, K.V. Kovtunov, I.V. Koptyug, E.Y. Chekmenev. Synthesis of unsaturated precursors for parahydrogen-induced polarization and molecular imaging of 1-13C-acetates and 1-13C-pyruvates via side arm hydrogenation, *ACS Omega*, **3**, 6673(2018); doi: 10.1021/acsomega.8b00983.
14. A.N. Pravdivtsev, I.V. Skovpin, A.I. Svyatova, N.V. Chukanov, L.M. Kovtunova, V.I. Bukhtiyarov, E.Y. Chekmenev, K.V. Kovtunov, I.V. Koptyug, J.-B. Hovener. Chemical exchange reaction effect on polarization transfer efficiency in SLIC-SABRE, *J. Phys. Chem. A*, **122**, 9107(2018); doi: 10.1021/acs.jpca.8b07163.

15. O. Salnikov, K. Kovtunov, P. Nikolaou, L. Kovtunova, V.I. Bukhtiyarov, I.V. Koptyug, E.Y. Chekmenev. Heterogeneous parahydrogen pairwise addition to cyclopropane, *ChemPhysChem*, **19**, 2621(2018); doi: 10.1002/cphc.201800690.
16. B.E. Kidd, J.L. Gesiorski, M.E. Gemeinhardt, R.V. Shchepin, K.V. Kovtunov, I.V. Koptyug, E.Y. Chekmenev, B.M. Goodson. Facile removal of homogeneous SABRE catalysts for purifying hyperpolarized metronidazole, a potential hypoxia sensor, *J. Phys. Chem. C*, **122**, 16848(2018); doi: 10.1021/acs.jpcc.8b05758.
17. D.B. Burueva, K.V. Kovtunov, A.V. Bukhtiyarov, D.A. Barskiy, I.P. Prosvirin, I.S. Mashkovsky, G.N. Baeva, V.I. Bukhtiyarov, A.Y. Stakheev, I.V. Koptyug. Selective single-site Pd-In hydrogenation catalyst for production of enhanced magnetic resonance signals using parahydrogen, *Chem. Eur. J.*, **24**, 2547(2018); doi: 10.1002/chem.201705644.
18. N.V. Chukanov, O.G. Salnikov, R.V. Shchepin, A. Svyatova, K.V. Kovtunov, I.V. Koptyug, E.Y. Chekmenev. 19F hyperpolarization of 15N-3-19F-pyridine via signal amplification by reversible exchange, *J. Phys. Chem. C*, **122**, 23002(2018); doi: 10.1021/acs.jpcc.8b06654.
19. K.V. Kovtunov, E.V. Pokochueva, O.G. Salnikov, S. Cousin, D. Kurzbach, B. Vuichoud, S. Jannin, E.Y. Chekmenev, B.M. Goodson, D.A. Barskiy, I.V. Koptyug. Hyperpolarized NMR: d-DNP, PHIP, and SABRE, *Chem. Asian J.*, **13**, 1857(2018); doi: 10.1002/asia.201800551.
20. D.B. Burueva, I.V. Skovpin, V.V. Zhivonitko, O.G. Salnikov, A.S. Romanov, K.V. Kovtunov, I.V. Koptyug. Application of parahydrogen for mechanistic investigations of heterogeneous catalytic processes, Russ. Chem. Bull., 66, 273(2017); doi: 10.1007/s11172-017-1728-5.
21. L.B. Bales, K.V. Kovtunov, D.A. Barskiy, R.V. Shchepin, A.M. Coffey, L.M. Kovtunova, A.V. Bukhtiyarov, M.A. Feldman, V.I. Bukhtiyarov, E.Y. Chekmenev, I.V. Koptyug, B.M. Goodson. Aqueous, heterogeneous para-hydrogen-induced 15N polarization, *J. Phys. Chem. C*, **121**, 15304(2017); doi: 10.1021/acs.jpcc.7b05912.
22. V.A. Lisitskiy, H. Khan, T.V. Popova, A.S. Chubarov, O.D. Zakharova, A.E. Akulov, O.B. Shevelev, E.L. Zavjalov, I.V. Koptyug, M.P. Moshkin, V.N. Silnikov, S. Ahmad, T.S. Godovikova. Multifunctional human serum albumin-therapeutic nucleotide conjugate with redox and pH-sensitive drug release mechanism for cancer theranostics, *Bioorg. Med. Chem. Lett.*, **27**, 3925(2017); doi: 10.1016/j.bmcl.2017.05.084.
23. V. Rontu, A. Selent, V. Zhivonitko, G. Scotti, I. Koptyug, V.-V. Telkki, S. Franssila. Efficient catalytic microreactors with atomic layer deposited platinum nanoparticles on oxide support, *Chem. Eur. J.*, **23**, 16835(2017); doi: 10.1002/chem.201703391.
24. D.A. Barskiy, O.G. Salnikov, A.S. Romanov, M.A. Feldman, A.M. Coffey, K.V. Kovtunov, I.V. Koptyug, E.Y. Chekmenev. NMR spin-lock induced crossing (SLIC) dispersion and long-lived spin states of gaseous propane at low magnetic field (0.05 T), *J. Magn. Reson.*, **276**, 78(2017); doi: 10.1016/j.jmr.2017.01.014.
25. K.V. Kovtunov, B.E. Kidd, O.G. Salnikov, L.B. Bales, M.E. Gemeinhardt, J. Gesiorski, R.V. Shchepin, E.Y. Chekmenev, B.M. Goodson, I.V. Koptyug. Imaging of biomolecular NMR signals amplified by reversible exchange with parahydrogen inside an MRI scanner, *J. Phys. Chem. C*, **121**, 25994(2017); doi: 10.1021/acs.jpcc.7b10549.
26. R.V. Shchepin, D.A. Barskiy, A.M. Coffey, M.A. Feldman, L.M. Kovtunova, V.I. Bukhtiyarov, K.V. Kovtunov, B.M. Goodson, I.V. Koptyug, E.Y. Chekmenev. Robust imidazole-15N2 synthesis for high-resolution low-field (0.05 T) 15N hyperpolarized NMR spectroscopy, *ChemistrySelect*, **2**, 4478(2017); doi: 10.1002/slct.201700718.
27. D.B. Burueva, A.S. Romanov, O.G. Salnikov, V.V. Zhivonitko, Y.-W. Chen, D.A. Barskiy, E.Y. Chekmenev, D.W.-H. Hwang, K.V. Kovtunov, I.V. Koptyug. Extending the lifetime of

hyperpolarized propane gas via reversible dissolution, *J. Phys. Chem. C*, **121**, 4481(2017); doi: 10.1021/acs.jpcc.7b00509.
28. O.G. Salnikov, H.-J. Liu, A. Fedorov, D. Burueva, K.V. Kovtunov, C. Coperet, I.V. Koptyug. Pairwise hydrogen addition in the selective semihydrogenation of alkynes on silica-supported Cu catalysts, *Chem. Sci.*, **8**, 2426(2017); doi: 10.1039/C6SC05276B.
29. D.A. Barskiy, K.V. Kovtunov, E.Y. Gerasimov, M.A. Phipps, O.G. Salnikov, A.M. Coffey, L.M. Kovtunova, I.P. Prosvirin, V.I. Bukhtiyarov, I.V. Koptyug, E.Y. Chekmenev. 2D mapping of NMR signal enhancement and relaxation for heterogeneously hyperpolarized propane gas, *J. Phys. Chem. C*, **121**, 10038(2017); doi: 10.1021/acs.jpcc.7b02506.
30. K.V. Kovtunov, V.V. Zhivonitko, I.V. Skovpin, O.G. Salnikov, I.V. Koptyug. "Catalytic enhancement of NMR sensitivity for advanced spectroscopic and imaging studies in catalysis and life sciences", in: Magnetic nanomaterials: applications in catalysis and life sciences, S.H. Bossmann, H. Wang, eds. 2017, The Royal Society of Chemistry, 142-171.
31. K.V. Kovtunov, L.M. Kovtunova, M.E. Gemeinhardt, A.V. Bukhtiyarov, J. Gesiorski, V.I. Bukhtiyarov, E.Y. Chekmenev, I.V. Koptyug, B. Goodson. Heterogeneous microtesla SABRE enhancement of 15N NMR signals, *Angew. Chem. Int. Ed.*, **56**, 10433(2017); doi: 10.1002/anie.201705014.
32. M.F. Delley, M.-C. Silaghi, F. Nunez-Zarur, K.V. Kovtunov, O.G. Salnikov, D.P. Estes, I.V. Koptyug, A. Comas-Vives, C. Coperet. X-H bond activation on Cr(III),O sites (X = R, H): key steps in dehydrogenation and hydrogenation processes, *Organomet.*, **36**, 234(2017); doi: 10.1021/acs.organomet.6b00744.
33. O.G. Salnikov, D.B. Burueva, E.Y. Gerasimov, A.V. Bukhtiyarov, A.K. Khudorozhkov, I.P. Prosvirin, L.M. Kovtunova, D.A. Barskiy, V.I. Bukhtiyarov, K.V. Kovtunov, I.V. Koptyug. The effect of oxidative and reductive treatments of titania-supported metal catalysts on the pairwise hydrogen addition to unsaturated hydrocarbons, *Catal. Today*, **283**, 82(2017); doi: 10.1016/j.cattod.2016.02.030.
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35. S. Babailov, A. Akulov, M. Moshkin, I. Koptyug. Prospects of paramagnetic lanthanide complexes for magnetic resonance imaging, local thermosensing, *J. Phys. Conf. Ser.*, **886**, 012003(2017); doi: 10.1088/1742-6596/886/1/012003.
36. K.V. Kovtunov, A.S. Romanov, O.G. Salnikov, D.A. Barskiy, E.Y. Chekmenev, I.V. Koptyug. Gas phase UTE MRI of propane and propene, *Tomography*, **2**, 49(2016); doi: 10.18383/j.tom.2016.00112.
37. D.B. Burueva, O.G. Salnikov, K.V. Kovtunov, A.S. Romanov, L.M. Kovtunova, A.K. Khudorozhkov, A.V. Bukhtiyarov, I.P. Prosvirin, V.I. Bukhtiyarov, I.V. Koptyug. Hydrogenation of unsaturated six-membered cyclic hydrocarbons studied by the parahydrogen-induced polarization technique, *J. Phys. Chem. C*, **120**, 13541(2016); doi: 10.1021/acs.jpcc.6b03267.
38. V.V. Zhivonitko, I.V. Skovpin, M. Crespo-Quesada, L. Kiwi-Minsker, I.V. Koptyug. Acetylene oligomerization over Pd nanoparticles with controlled shape: a parahydrogen-induced polarization study, *J. Phys. Chem. C*, **120**, 4945(2016); doi: 10.1021/acs.jpcc.5b12391.

39. K.V. Kovtunov, D.A. Barskiy, R.V. Shchepin, O.G. Salnikov, I.P. Prosvirin, A.V. Bukhtiyarov, L.M. Kovtunova, V.I. Bukhtiyarov, I.V. Koptyug, E.Y. Chekmenev. Production of pure aqueous 13C-hyperpolarized acetate via heterogeneous parahydrogen-induced polarization, *Chem. Eur. J.*, **22**, 16446(2016); doi: 10.1002/chem.201603974.
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41. B. Vuichoud, E. Canet, J. Milani, A. Bornet, D. Baudouin, L. Veyre, D. Gajan, L. Emsley, A. Lesage, C. Coperet, C. Thieuleux, G. Bodenhausen, I. Koptyug, S. Jannin. Hyperpolarization of frozen hydrocarbon gases by dynamic nuclear polarization at 1.2 K, *J. Phys. Chem. Lett.*, **7**, 3235(2016); doi: 10.1021/acs.jpclett.6b01345.
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46. D.P. Estes, G. Siddiqi, F. Allouche, K.V. Kovtunov, O.E. Safonova, A.L. Trigub, I.V. Koptyug, C. Coperet. C-H activation on Co,O sites: isolated surface sites versus molecular analogs, *J. Am. Chem. Soc.*, **138**, 14987(2016); doi: 10.1021/jacs.6b08705.
47. D.A. Barskiy, A.N. Pravdivtsev, K.L. Ivanov, K.V. Kovtunov, I.V. Koptyug. Simple analytical model for signal amplification by reversible exchange (SABRE) process, *Phys. Chem. Chem. Phys.*, **18**, 89(2016); doi: 10.1039/C5CP05134G.
48. K.V. Kovtunov, D.A. Barskiy, O.G. Salnikov, R.V. Shchepin, A.M. Coffey, L.M. Kovtunova, V.I. Bukhtiyarov, I.V. Koptyug, E. Chekmenev. Toward production of pure 13C hyperpolarized metabolites using heterogeneous parahydrogen-induced polarization of ethyl [1-13C]acetate, *RSC Adv.*, **6**, 69728(2016); doi: 10.1039/C6RA15808K.