Boreskov Institute of Catalysis Fritz Haber Institute of the Max Planck Society

5th Russian-German Seminar "Bridging the Gap between Model and Real Catalysis"

Synchrotron Radiation in Catalysis

June 23 - 26, 2019 Novosibirsk, Russia

Scientific Program

Novosibirsk-2019

Organised by

Boreskov Institute of Catalysis, Novosibirsk, Russia

&

Fritz Haber Institute of the Max Planck Society, Berlin, Germany





Scientific Committee	
Prof. Dr. Valerii I. Bukhtiyarov	Boreskov Institute of Catalysis, Novosibirsk, Russia
Prof. Dr. Robert Schlögl	Fritz Haber Institute of the Max Planck Society, Max Planck Institute for Chemical Energy Conversion, Berlin, Germany
Prof. Dr. Alexander Yu. Stakheev	Zelinsky Institute of Organic Chemistry, RAS, Moscow, Russia
Prof. Dr. Ekaterina.S. Lokteva	Lomonosov Moscow State University, Moscow, Russia

Organizing Committee

Prof. Dr. Valerii I. Bukhtiyarov	Boreskov Institute of Catalysis, Novosibirsk, Russia
Dr. Axel Knop-Gericke	Fritz Haber Institute of the Max Planck Society, Berlin, Germany
Dr. Marina V. Bukhtiyarova	Boreskov Institute of Catalysis, Novosibirsk, Russia
Dr. Vasily V. Kaichev	Boreskov Institute of Catalysis, Novosibirsk, Russia

Secretariat

Dorothea Damm	Fritz Haber Institute of the Max Planck Society, Berlin, Germany	
Marina S. Suvorova	Boreskov Institute of Catalysis, Novosibirsk, Russia	

Language

English is the official language of the seminar

Scientific program

The scientific program of seminar includes plenary lectures (40 min) and oral presentations (20 min).

The main topics are:

- in situ and operando studies of model and real catalysts
- advanced synchrotron methods in catalysis
- electrocatalysis

Abstract submission and publication

Authors of all contributions are invited to submit one or two page abstracts (A4) in English. Tables, artworks and references will be accepted within this limit. The text should be typed 1.25 line spaced with 2.5 cm all around margins. Please use Calibri 12 pt. References should be cited in the order of occurrence in the text as numbers in square brackets [1]. Please use the example of abstract on the conference site <u>http://conf.nsc.ru/rgs-2019/en</u>.

Venue and Accommodation

The Seminar will take place in Boreskov Institute of Catalysis and a conference-centre of the <u>Morozovo hotel</u> (Novosibirsk region, Rechkunovskaya recreation area -1.

Accommodation is arranged by the Organizing Committee at the **Morozovo hotel**.

Accommodation 23-26 June 2019 (STANDARD, single/twin) is included in registration fee. Please send an application for accommodation after notification of acceptance.

Transportation

Novosibirsk Airport "Tolmachevo" is located about 30 km from Akademgorodok. The representatives of the Organizing Committee will meet participants at the Airport in the morning, 23 June and provide transportation to the hotel by a special transport (the representatives will have the transparencies with the 5th Russian-German Seminar on Catalysis logo). The transfer from Boreskov Institute to the Morozovo hotel will be organized.

Entry visa to Russia

All foreign participants of the Seminar need a valid passport and an entry visa to Russia (passport should be valid 6 months after Seminar – at least until 1st of January, 2020).

Detailed information is given at the site.

Registration and fee

Those who plan to attend the Seminar are kindly requested to register at the <u>website</u> before 1 April 2019. Authors are also requested to send their abstracts and registration form as attached Word-files by e-mail: <u>suvorova@catalysis.ru</u>.

For Russian participants: 10 000 Rubles

For foreign participants: 200 Euro

The registration fee covers all Conference documentation and materials, accommodation, meals, Welcome reception, refreshments.

For foreign participants:

To receive an invoice for the registration fee payment, please fill in the form on the site and send it to Organizing Committee (Marina Suvorova e-mail: <u>suvorova@catalysis.ru</u>).

For Russian participants:

Russian participants can transfer the registration fee after receiving Notification of acceptance of report.



Key Dates

1 April 2019	Submission of preliminary registration forms and Abstracts	
15 April 2019	Notification of acceptance	
15 April – 15 May 2019	Payment of fee	
1 June 2019	Distribution of preliminary Scientific Program	
23-26 June 2019	Working days	
26-29 June 2019	Post-tour to Altai	

Contacts

Germany: **Dorothea Damm**, Fritz-Haber-Institut der MPG, Berlin E-mail: <u>damm@fhi-berlin.mpg.de</u> Tel: +49 (0)30 8413 4402, Fax: +49 (0)30 8413 4401

Russia : Marina Suvorova,

Boreskov Institute of Catalysis, Novosibirsk E-mail: <u>suvorova@catalysis.ru</u> Tel: +7 (383) 326-95-84

Schedule

June 23,			June 24,
	Sunday		Monday
	Arrival		Chair: Knop-Gericke A.
		09.30	PL-3 – Savinova
		10.10	PL-4 – Steinrück
		10.50	OP-6 – Behm
		11.10	Coffee-break
			Chair: Steinrück H.
		11.40	OP-7 – Smirnova
		12.00	OP-8 – Abdel-Mageed
		12.20	OP-9 – Saraev
		12.40	OP-10 – Bulavchenko
		13.00	OP-22 – Kaichev
		13.30	Lunch
			Chair: Zubavichus Yan
		15.00	OP-12 – Stotz
		15.20	OP-13 – Sulzman
14:00	Registration	15.40	OP-14 – Bukhtiyarova M.
14:45	Opening Session	16.00	OP-15 – Alekseeva
	Chair: Bukhtiyarov V.	16.20	OP-16 – Pakharukova
15:00	PL-1 – Knop-Gericke	16.40	OP-17 – Shefer
15:40	PL-2 – Zubavichus		
16:20	Coffee-break		
	Chair: van de Krol R.		
16:50	OP-1 – Shmakov		
17:10	OP-2 – Belyakova		
17:30	OP-3 – Nikitina		
17:50	OP-4 – Bukhtiyarov A.		
18:10	OP-5 – Mamatkulov		
19.00	Welcome Party	19.00	Banquet

of the Seminar

	lune 25 lune 26 20				
	June 25 <i>,</i> Tuesday	June 26-29			
	-				
	Chair: Savinova E.				
09.30	PL-5 – van de Krol				
10.10	PL-6 – Kiskinova				
10.50	OP-18 – Kuznetsov				
11.10	Coffee-break				
	Chair: Kiskinova M.				
11:40	OP-19 – Hävecker				
12:00	OP-20 – Kibis				
12:20	OP-21 – Wittkämper				
12:40	OP-11 – Skorupska				
13:00	OP-23 – Balyakin				
13.30	Lunch	Post-tour to Altai			
		26 – departure to Altai			
		27, 28 – Excursion program			
14:30	departure to Boreskov	29 - departure to Novosibirsk			
1 1.50	Institute of Catalysis				
15.00	Excursion to Boreskov				
10.00	Institute of Catalysis				
16.00	PL-7 – Bukhtiyarov V.				
17.00	PL-8 – Schlögl (Video Lecture)				
18.00	Closing Ceremony				
10.00	cioning concinionity				
19.00	Dinner				
10.00		[

PL – Plenary Lecture (40 min) **OP** – Oral Presentation (20 min)

Scientific Program

June 23, Sunday

Morozovo Hotel Conference hall, 4th floor

AFTERNOON SESSION

Chairperson: Prof. Dr. Valerii Bukhtiyarov

14.45 Opening Session

Plenary Lectures

15.00 PL-1

Presenting author: Dr. Axel Knop-Gericke The Electronic Structure of Solid/Liquid Interfaces Relevant for Water Oxidation and Carbondioxide Reduction

1 – MPI for Chemical Energy Conversion, Mülheim, Germany 2 – Fritz-Haber-Institute of the MPG, Berlin, Germany

15.40 PL-2

Presenting author: Prof. Dr. Yan Zubavichus Structural Diagnostics of Catalysts Using X-Ray Synchrotron Radiation: Current Possibilities and Future Prospects Boreskov Institute of Catalysis, Novosibirsk, Russia

16.20 Coffee-break

16.50 OP-1

Presenting author: **Dr. Alexander Shmakov**

<u>Shmakov A.N.</u>, Vinokurov Z.S., Yakushkin S.S., Nesterov N.S., Martyanov O.N.

High Energy X-Ray Synchrotron In Situ and Operando Diagnostics of Heterogeneous Catalysts

Boreskov Institute of Catalysis, Novosibirsk, Russia

17.10 OP-2

Presenting author: Dr. Olga Belyakova <u>Belyakova O.A.¹</u>, Zubavichus Ya.V.¹, Vasil'kov A.Y.², Naumkin A.V.² The Study of Au/Ni Bimetallic Nanoparticles Using a Combination of XAFS, XRD and SAXS/ASAXS Synchrotron Techniques

1 – Boreskov Institute of Catalysis, Novosibirsk, Russia 2 – A.N.Nesmeyanov Institute of Organoelement Compounds RAS, Moscow, Russia

17.30 OP-3

Presenting author: Nadezhda Nikitina

Pichugina D.A., <u>Nikitina N.A.</u>, Kuz'menko N.E.

On the Mechanism of CO Oxidation on Gold Nanocluster: Ligand and Doping Effects

M.V. Lomonosov Moscow State University, Moscow, Russia

17.50 OP-4

Presenting author: **Dr. Andrei Bukhtiyarov**

Bukhtiyarov A.V.¹, Prosvirin I.P.¹, Mamatkulov M.¹, Yudanov I.V.^{1,2}, Klyushin A.Yu.³, Knop-Gericke A.³, Neyman K.M.^{4,5}, Bukhtiyarov V.I.¹ CO Oxidation on the Model Pd-Au/HOPG Catalysts: NAP XPS and MS Study

1 –Boreskov Institute of Catalysis, Novosibirsk, Russia 2 – Institute of Chemistry and Chemical Technology SB RAS, Federal Research Center "Krasnoyarsk Scientific Center SB RAS", Krasnoyarsk, Russia

3 – Fritz-Haber-Institute der Max Planck Society, Berlin, Germany 4 – Departament de Ciència de Materials i Química Física and Institut de Quimica Teòrica i Computacional, Universitat de Barcelona, Barcelona, Spain

5 — ICREA (Institució Catalana de Recerca i Estudis Avançats), Barcelona, Spain

18.10 OP-5

Presenting author: Dr. Mikhail Mamatkulov

Mamatkulov M.I.¹, Yudanov I.V.^{1,2}, Neyman K.M.^{3,4}

Atomic Ordering in Bimetallic Pd-Au Nanoparticles: Computational Study of Pd Surface Segregation in Reactive Environment

1 – Boreskov Institute of Catalysis, Novosibirsk, Russia

2 – Institute of Chemistry and Chemical Technology SB RAS,

Krasnoyarsk, Russia

3 – Universitat de Barcelona, Barcelona, Spain

4 – Institució Catalana de Recerca i Estudis Avançats (ICREA), Barcelona, Spain

19.00 Welcome Party

June 24, Monday

Morozovo Hotel Conference hall, 4th floor

MORNING SESSION

Chairperson: Dr. Axel Knop-Gericke

Plenary Lectures

09.30 PL-3

Presenting author: **Prof. Dr. Elena Savinova Electrocatalysis at the Molecular Level: from Electrochemical Methods to In Situ Spectroscopies** *UMR 7515 CNRS - University of Strasbourg, Strasbourg, France*

10.10 PL-4

Presenting author: Prof. Dr. Hans-Peter Steinrück

Surface Science of Low Vapor Pressure Liquids

Physical Chemistry, University Erlangen-Nürnberg, Erlangen, Germany

15.40 OP-6

Presenting author: **Prof. Dr. Rolf Jürgen Behm** Wiese K.¹, Rezvani A.¹, Ali M. Abdel-Mageed¹, Klyushin A.², Knop-Gericke A.², Schlögl R.², <u>Behm R.J.¹</u> **Insights into Fundamental Aspects of Au Catalysis from Operando and In Situ Spectroscopy: Methanol Synthesis on Au/ZnO as a Key Example** *1 – Institute of Surface Chemistry and Catalysis, Ulm University, Ulm, Germany 2 – Fritz-Haber-Institute, Department of Inorganic Chemistry, Berlin, Germany*

11.10 Coffee-break

ORAL SESSION

Chairperson: Prof. Dr. Hans-Peter Steinrück

11.40 OP-7

Presenting author: Dr. Nadezhda Smirnova

<u>Smirnova N.S.</u>¹, Khramov E.V.², Stolyarov I.P.¹, Cherkashina N.V.¹, Baeva G.N.³, Bragina G.O.³, Yakushev I.A.¹, Mashkovsky I.S.³, Vargaftik M.N.¹, Stakheev A. Yu.³

The Investigation of Thermal Decomposition of Heterobimetallic PtZn(CH₃COO)₄ Acetate Complex in Reductive Conditions by *In Situ* XAFS

1 – N.S. Kurnakov Institute of General and Inorganic Chemistry, Russian Academy of Sciences, Moscow, Russia

2 – National Research Center «Kurchatov Institute», Moscow, Russia 3 – N.D. Zelinsky Institute of Organic Chemistry, Russian Academy of Sciences, Moscow, Russia

12.00 OP-8

Presenting author: Ali M. Abdel-Mageed

<u>Ali M. Abdel-Mageed</u>¹, Fauth C.¹, Rungtaweevoranit B.², Yaghi O.M.², Behm R.J.¹

On the Electronic and Geometric Structure of a Single Atom Cu/UiO-66 Catalyst during CO Oxidation: An Operando FTIR and XAFS Study

1 – Institute of Surface Chemistry and Catalysis, Ulm University, Ulm, Germany

2 – Department of Chemistry, University of California, Berkeley, California, USA

12.20 OP-9

Presenting author: Dr. Andrey Saraev

<u>Saraev A.A.</u>¹, Tsapina A.M.¹, Selivanova A.V.¹, Fedorov A.V.¹, Vorokhta M.², Šmíd B.², Kaichev V.V.¹

NAP XPS Study of CO Oxidation over CuFeAl Nanocomposite Catalysts

- 1 Boreskov Institute of Catalysis, Novosibirsk, Russia
- 2 Charles University, Prague, Czech Republic

12.40 OP-10

Presenting author: **Dr. Olga Bulavchenko** <u>Bulavchenko O.A.^{1,2}</u>, Vinokurov Z.S.^{1,2}, Afonasenko T.N.¹, Tsyril'nikov P.G.³, Saraev A.A.^{1,2}, Kaichev V.V.^{1,2}, Tsybulya S.V.^{1,2} **In Situ XRD and XPS Study of the Reduction Process of Mixed Mn-Zr Oxide Catalysts of CO Oxidation**

1 – Boreskov Institute of Catalysis, Novosibirsk, Russia

2 – Novosibirsk State University, Novosibirsk, Russia

3 – Center of New Chemical Technologies BIC, Omsk, Russia

13.00 OP-22

Presenting author: Dr. Vasily Kaichev

Kaichev V.V.^{1,2}, Chesalov Yu.A.^{1,2}, Saraev A.A.^{1,2}, Tsapina A.M.¹

In Situ Study of Dehydrogenation of Propane over Vanadia-Titania Catalysts

1 – Boreskov Institute of Catalysis, Novosibirsk, Russia

2 – Novosibirsk State University, Novosibirsk, Russia

13.30 Lunch

AFTERNOON SESSION

Chairperson: Prof. Dr. Yan Zubavichus

15.00 OP-12

Presenting author: Dr. Eugen Stotz

<u>Stotz E.</u>¹, Hävecker M.^{1,2}, Valsco-Velez J.J.^{1,2}, Knop-Gericke A.^{1,2}, Schlögl, R.^{1,2}

Modular Concept for Catalysis Research at BESSY from an Engineer Point of View

1 — Fritz-Haber-Institute of the Max-Planck-Society, Berlin, Germany 2 — Max-Planck-Institute for Chemical Energy Conversion, Mülheim, Germany

15.20 OP-13

Presenting author: **Frederic Paul Sulzman** <u>Sulzmann F.</u>¹, Carbonio E.³, Jones T.¹, Knop-Gerincke A.², Schlögl R.^{1,2} **Differentiation of Strongly Bound Oxygen on Silver** 1 – Fritz-Haber-Institut der Max-Planck-Gesellschaft, Department of Inorganic Chemistry, Berlin, Germany 2 – Department of Heterogeneous Reactions, Max Planck Institute for Chemical Energy Conversion, Mühlheim an der Ruhr, Germany 3 – Helmholtz-Zentrum Berlin für Materialien und Energie GmbH, BESSY II, Berlin, Germany

15.40 OP-14

Presenting author: Dr. Marina Bukhtiyarova Bukhtiyarova M.V., Prosvirin I.P., Bukhtiyarov A.V., Panafidin M.A. In Situ XPS Study of Selective Methanol Oxidation over Cu Catalysts on the Base of Layered Double Hydroxides

Boreskov Institute of Catalysis, Novosibirsk, Russia

16.00 OP-15

Presenting author: Dr. Mariya Alekseeva

<u>Alekseeva M.V.</u>^{1,2}, Smirnov A.A.^{1,2}, Selischeva S.A.^{1,2}, Shilov I.N.^{1,2}, Fedorov A.V.^{1,2}, Bulavchenko O.A.^{1,2}, Saraev A.A.^{1,2}, Yakovlev V.A.^{1,2} In Situ and Advanced Synchrotron Studies of Catalysts for Bio-Oxygenates Hydroconversion

1 – Boreskov Institute of Catalysis, Novosibirsk, Russia

2 – Novosibirsk State University, Novosibirsk, Russia

16.20 OP-16

Presenting author: Dr. Vera Pakharukova

Application of Pair Distribution Function Analysis to Structural Studies of Supported Catalysts

1 – Boreskov Institute of Catalysis, Novosibirsk, Russia 2 – Novosibirsk State University, Novosibirsk, Russia

16.40 OP-17

Presenting author: **Dr. Kristina Shefer** <u>Shefer K.I.^{1,2}</u>, Moroz E.M.¹

Nanoscale Catalytic Systems Based on Alumina and Aluminum Hydroxides. Reserch Using the PDF Method

1 –Boreskov Institute of Catalysis, Novosibirsk, Russia 2 – Novosibirsk State University, Novosibirsk, Russia

19.00 Banquet

June 25, Tuesday

Morozovo Hotel Conference hall, 4th floor

MORNING SESSION

Chairperson: Prof. Dr. Elena Savinova

Plenary Lectures

09.30 PL-5

Presenting author: Prof. Dr. Roel van de Krol

Van de Krol R., Friedrich D., Eichberger R., Favaro M., Starr D.E. Time-Resolved and Operando Photoemission Studies on Metal Oxide Photoelectrodes

Helmholtz-Zentrum Berlin für Materialien und Energie GmbH, Institute for Solar Fuels, Berlin, Germany

10.10 PL-6

Presenting author: Dr. Maya Kiskinova Microscopic Insights on Properties of Catalysts Using Synchrotron-

Based Methods

Elettra-Sinctrotrone Trieste, Area Science Park, Trieste-Basovizza, Italy

10.50 OP-18

Presenting author: **Prof. Dr. Mikhail Kuznetsov** <u>Kuznetsov M.V.¹</u>, Ogorodnikov I.I.¹, Usachov D.Yu.², Yashina L.V.³ **Photoelectron Diffraction and Holography for Surface Structure Studies** 1 – Institute of Solid State Chemistry, Ural Branch of the Russian Academy of Sciences, Ekaterinburg, Russia 2 – St. Petersburg State University, Dept. of Physics, St. Petersburg, Russia 3 – Moscow State University, Dept. of Chemistry, Moscow, Russia

11.10 Coffee-break

ORAL SESSION

Chairperson: Dr. Maya Kiskinova

11.40 OP-19

Presenting author: Dr. Michael Hävecker

Koch G.^{1,2}, <u>Hävecker M.^{2,3}</u>, Kube P.², Bellini G.³, Trunschke A.³, Stotz E.³, Schlögl R.^{2,3}

The Rich Surface Oxygen Chemistry of Perovskites as Revealed by Synchrotron Based Ambient Pressure X-ray Photoelectron Spectroscopy (AP-XPS)

1 – TU Berlin, BasCat-BASF Joint Lab, Berlin, Germany 2 – MPI for Chemical Energy Conversion, Mülheim a.d.Ruhr, Germany 3 – Fritz Haber Institute, Berlin, Germany

12.00 OP-20

Presenting author: Dr. Lidiya Kibis

<u>Kibis L.S.</u>^{1,2}, Svintsitskiy D.A.^{1,2}, Derevyannikova E.A.¹, Kardash T.Yu.^{1,2}, Slavinskaya E.M.^{1,2}, Stonkus O.A.^{1,2}, Svetlichnyi V.A.³, Boronin A.I.^{1,2}

In Situ/Ex Situ Study of Model Rh-Doped CeO₂ Catalysts

- 1 Boreskov Institute of Catalysis, Novosibirsk, Russia
- 2 Novosibirsk State University, Novosibirsk, Russia
- 3 Tomsk State University, Tomsk, Russia

12.20 OP-21

Presenting author: Dr. Haiko Wittkämper

<u>Wittkämper H.</u>¹, Raman N.², Grabau M.¹, Maisel S.³, Taccardi N.², Debuschewitz J.², Bauer T.⁵, Wu M.⁴, Haumann M.², Görling A.³,

Spiecker E.⁴, Libuda J.⁵, Wasserscheid P.², Steinrück H.-P.¹, Papp C.¹

Spectroscopic Insights to Rh-Ga Alloys as Model Systems for a Novel Type of Dehydrogenation Catalyst

1 – Friedrich-Alexander-Universität Erlangen-Nürnberg (FAU), Lehrstuhl für Physikalische Chemie II, Erlangen, Germany

2 – Friedrich-Alexander-Universität Erlangen-Nürnberg (FAU), Lehrstuhl für Chemische Reaktionstechnik (CRT), Erlangen, Germany

3 – Friedrich-Alexander-Universität Erlangen-Nürnberg (FAU), Lehrstuhl für Theoretische Chemie, Erlangen, Germany

4 – Friedrich-Alexander-Universität Erlangen-Nürnberg (FAU), Lehrstuhl für Werkstoffwissenschaften, Mikro- und Nanostrukturforschung, Erlangen, Germany

5 – Friedrich-Alexander-Universität Erlangen-Nürnberg (FAU), Lehrstuhl für Katalytische Grenzflächenforschung, Erlangen, Germany

12.40 OP-11

Presenting author: Dr. Katarzyna Skorupska

<u>Skorupska K.</u>, Jone D.T., Mom R., Sulzmann F., Chuang Ch.-H., Melder J., Kurz P., Knop-Gericke A., Schlögl R.

Manganese Oxides under OER

Fritz-Haber-Institut of of the Max-Planck Society, Berlin, Germany

13.00 OP-23

Presenting author: Ilya Balyakin

Balyakin I.A.^{1,2,3}, Rempel A.A.^{1,2,3}

Computer Modeling of CdS-TiO₂ Heterojunctions in Photo Catalyst

1 – Institute of Solid State Chemistry of the Ural Branch of the Russian Academy of Sciences, Ekaterinburg, Russia

2 – Ural Federal University, Ekaterinburg, Russia

3 – Institute of Metallurgy of the Ural Branch of the Russian Academy of Sciences, Ekaterinburg, Russia

13.30 Lunch

AFTERNOON SESSION

- 14.30 Departure to Boreskov Institute of Catalysis
- 15.00 Excursion to Boreskov Institute of Catalysis

Boreskov Institute of Catalysis, Novosibirsk, Russia Conference hall, 3th floor

Plenary Lectures

16.00 PL-7 Presenting author: Prof. Dr. Valerii I. Bukhtiyarov Synchrotron in Catalysis

Boreskov Institute of Catalysis, Novosibirsk, Russia

17.00 PL-8 (Video Lecture)

Presenting author: **Prof. Dr. Robert Schlöegl Material Science of Heterogeneous Catalysts**

Fritz Haber Institute of the Max Planck Society, Berlin, Germany

Max Planck Institute for Chemical Energy Conversion, Mülheim, Germany