

**Scientific programme of IWSN-2021:  
International Workshop on  
Synchrotron and Neutron Radiation**

**6-7 December, 2021, Rostov-on-Don**

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**IWSN-2021: International  
Workshop on Synchrotron and  
Neutron Radiation**

*Programme Committee*

Prof. Alexander V. Soldatov  
(Russia)

Prof. Vladimir Dmitriev (France)

Prof. Silvia Bordiga (Italy)

Prof. Nobuhiro Kosugi (Japan)

Prof. Ilias K. Savvas (Greece)

Dr.Habil. Kristina Kvashina  
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Dr.Yulia Podkovyrina Chair

Yulia Polaykova - Co-Chair

Dr. Aram Bugaev

Dr. Alexander Guda

Dr. Oleg Polozhentsev

# PROGRAMME

6-7 December, 2021, Rostov-on-Don

## December 6, Monday

	<b>Opening Ceremony</b>
10:00-10:10	<b>Prof. Alexander Soldatov</b> (Rostov-on-Don, Russia) Welcome Address <a href="https://zoom.us/j/84457169866?pwd=cUdscTFQS3JsOVNtWWIrQmhJZDM0QT09">https://zoom.us/j/84457169866?pwd=cUdscTFQS3JsOVNtWWIrQmhJZDM0QT09</a> (password 809805)
10:10-11:30	<b>Dr. Mikhail Rychev</b> (Hamburg, Germany/Moscow, Russia) Russia on the European landscape of using large-scale facilities <a href="https://zoom.us/j/83979326532?pwd=LzVBL0M4UDJIUGNtRIFYZIREL0t6QT09">https://zoom.us/j/83979326532?pwd=LzVBL0M4UDJIUGNtRIFYZIREL0t6QT09</a> (password 117961)
<b>Section: In situ/Operando characterization</b> <b>Chairman: Dr. Yulia Podkovyrina</b>	
10:30-11:10	<b>Prof. Silvia Bordiga</b> (Turin, Italy) In situ spectroscopies for determination of active sites in zeolites <a href="https://zoom.us/j/89023895802?pwd=djldqN2F3UWlUaDZscXVxcHE3M1NpUT09">https://zoom.us/j/89023895802?pwd=djldqN2F3UWlUaDZscXVxcHE3M1NpUT09</a> (password 298822)
11:10-11:40	<b>Prof. Luneau Dominique</b> (Lyon, France) The metal-radical approach in molecular magnetism Coordination chemistry and nitronyl nitroxide free radical <a href="https://zoom.us/j/87636120650?pwd=QmhMOElvQmk0R0prL3JlSHIGQklCOT09">https://zoom.us/j/87636120650?pwd=QmhMOElvQmk0R0prL3JlSHIGQklCOT09</a> (password 272538)
11:40-12:00	<b>Alina Skorynina</b> (Rostov-on-Don, Russia) High-pressure operando investigation of Pd-MOFs for CO <sub>2</sub> hydrogenation <a href="https://zoom.us/j/81123925252?pwd=QllUdytCRFE5OFpQQ3paOUFPSmRUdz09">https://zoom.us/j/81123925252?pwd=QllUdytCRFE5OFpQQ3paOUFPSmRUdz09</a> (password 174459)
12:00-12:10	<i>Coffee break</i>

12:10-12:40	<p><b>Dr. Aram Bugaev</b> (Rostov-on-Don, Russia) Machine learning for vibrational spectroscopies: How to build a theoretical training set <a href="https://zoom.us/j/86843570714?pwd=RVZzZmR6MEI2VmFiUTISc3czLzkzUT09">https://zoom.us/j/86843570714?pwd=RVZzZmR6MEI2VmFiUTISc3czLzkzUT09</a> (password 688292)</p>
12:40-13:00	<p><b>Bogdan Protsenko</b> (Rostov-on-Don, Russia) In situ FTIR as instrument for characterization of palladium hydride phase <a href="https://zoom.us/j/89706753019?pwd=bkFNSIVueVINeVVxQIBmemRWeENjZz09">https://zoom.us/j/89706753019?pwd=bkFNSIVueVINeVVxQIBmemRWeENjZz09</a> (password 328935)</p>
13:00-14:00	<i>Lunch</i>
<p><b>Section: SR for homogenous and heterogenous catalysis</b> <b>Chairman: Dr. Aram Bugaev</b></p>	
14:00-14:40	<p><b>Prof. Anton Maximov</b> (Moskow, Russia) The contribution of synchrotron research to the development of oil refining and petrochemical industry processes <a href="https://zoom.us/j/81975868837?pwd=NWZJOHIzU2J5RjBPaytuc3RzU2RKZz09">https://zoom.us/j/81975868837?pwd=NWZJOHIzU2J5RjBPaytuc3RzU2RKZz09</a> (232529)</p>
14:40-15:00	<p><b>Dr. Evgeniy Naranov</b> (Moskow, Russia) Hydroformylation and hydrogenation over novel immobilized Rh-containing catalysts <a href="https://zoom.us/j/84491233353?pwd=Y1oxcFRJc2xyajdJaUxoTVd2bDN6UT09">https://zoom.us/j/84491233353?pwd=Y1oxcFRJc2xyajdJaUxoTVd2bDN6UT09</a> (password 878969)</p>
15:00-15:20	<p><b>Dr. Iliia Pankin</b> (Rostov-on-Don, Russia) DFT study of different Cu-oxo species formation in Cu-SSZ-13 catalyst <a href="https://zoom.us/j/87303600647?pwd=anRBdUo3c2dKbmw0Z0lvK3VDdW5FQT09">https://zoom.us/j/87303600647?pwd=anRBdUo3c2dKbmw0Z0lvK3VDdW5FQT09</a> (password 867066)</p>
15:20-15:30	<i>Coffee break</i>
15:30-16:10	<p><b>Prof. Dirk De Vos</b> (Leuven, Belgium) Metal centres in porous materials as catalysts for organic reactions, and structure-activity relationships based on XAS <a href="https://zoom.us/j/87903145428?pwd=KzBQNS83UW11REVLAThS">https://zoom.us/j/87903145428?pwd=KzBQNS83UW11REVLAThS</a></p>

	<a href="#">YlpTck9Zdz09</a> (password 774464)
16:10-16:30	<b>Kwinten Janssens</b> (Leuven, Belgium) Evolution of the active species of homogeneous Ru-based hydrogenation catalysts in ionic liquids <a href="https://zoom.us/j/88247142679?pwd=Nm5NcUJrbnpud1JPT0djN2NBUWYydz09">https://zoom.us/j/88247142679?pwd=Nm5NcUJrbnpud1JPT0djN2NBUWYydz09</a> (password 331059)
16:30-17:00	<b>Lisa Van Emelen</b> (Leuven, Belgium) Cu-MOFs <a href="https://zoom.us/j/83479244650?pwd=cWFsVkNCZnZ6Y2ozMmhkSGlhbFJUUT09">https://zoom.us/j/83479244650?pwd=cWFsVkNCZnZ6Y2ozMmhkSGlhbFJUUT09</a> (password 376141)
17:00	<b>POSTER Session</b>
<b>December 7, Tuesday</b>	
<i>Section: Sorption in porous materials</i> <i>Chairman: Dr.Yulia Podkovyrina</i>	
10:00-10:30	<b>Alexey Ermakov</b> (Moscow, Russia) Porous Microcarriers as a Novel Platforms for Encapsulation, Storage, And Controlled Release of Reactive Oxygen Species <a href="https://zoom.us/j/82989816839?pwd=SHNjVVNPdFlhTkVZa0w0bzNiZDMwZz09">https://zoom.us/j/82989816839?pwd=SHNjVVNPdFlhTkVZa0w0bzNiZDMwZz09</a> (password 268202)
10:30-11:00	<b>Dr.Habil. Kristina Kvasnina</b> (Grenoble, France) Exploring radioactive materials through the high energy synchrotron methods <a href="https://zoom.us/j/81618635087?pwd=eW0lZGRkWVNRRWRtVmFzdXI1bDNPUT09">https://zoom.us/j/81618635087?pwd=eW0lZGRkWVNRRWRtVmFzdXI1bDNPUT09</a> (password 434366)
11:00-11:30	<b>Dr. Mahmoud Mazarji</b> (Rostov-on-Don, Russia) Potential application of metal-organic frameworks in the different remediation technologies <a href="https://zoom.us/j/87524293423?pwd=bHoyNHg1NmV4NU9SSDN6MXIUSGhBUT09">https://zoom.us/j/87524293423?pwd=bHoyNHg1NmV4NU9SSDN6MXIUSGhBUT09</a> (password 946387)
11:30-11:50	<b>Dr. Trushina Daria</b> (Moscow, Russia) Porous calcium carbonate particles - structural aspects and prospects in drug delivery <a href="https://zoom.us/j/81696015768?pwd=L1p4QXNzcyt1eTE0WW15a">https://zoom.us/j/81696015768?pwd=L1p4QXNzcyt1eTE0WW15a</a>

	<a href="#">E1KcVVuZz09</a> (password 898925)
11:50-14:00	<i>Break</i>
12:35-14:00	<i>Lunch</i>
<b>Section: Machine learning and theoretical modeling</b>	
<b>Chairman: Dr.Yulia Podkovyrina</b>	
14:00-14:40	<b>Dr. Alexander Guda</b> (Rostov-on-Don, Russia) Workshop on machine learning in XAS. A good practice in quantitative XANES analysis <a href="https://zoom.us/j/81926284639?pwd=MUVRCg1SaVJzcXVQWV M4eVBrckxwdz09">https://zoom.us/j/81926284639?pwd=MUVRCg1SaVJzcXVQWV M4eVBrckxwdz09</a> (password 221972)
14:40-15:00	<b>Oleg Usoltsev</b> (Rostov-on-Don, Russia) Machine learning application for XANES analysis of Pd nanocatalysts <a href="https://zoom.us/j/85990274949?pwd=UFhYdnJBbTVDRUM3RUx CY05JMDYyUT09">https://zoom.us/j/85990274949?pwd=UFhYdnJBbTVDRUM3RUx CY05JMDYyUT09</a> (password 399775)
15:00-15:10	<i>Coffee-Break</i>
15:10-15:30	<b>Anastasia Smirnova</b> (Moscow, Russia) Nitrogen K-edge simulation and electronic structure investigation for the f-elements organic extractants study <a href="https://zoom.us/j/88404520366?pwd=d2R5dzFDS2wybDJacXNYV HIyRitzdz09">https://zoom.us/j/88404520366?pwd=d2R5dzFDS2wybDJacXNYV HIyRitzdz09</a> (password 860431)
15:30-15:45	<b>Tereshchenko Andrei</b> (Rostov-on-Don, Russia) Applying machine learning algorithms and adaptive sampling approach for predicting binding energy of CO adsorbed on Pd nanoparticles <a href="https://zoom.us/j/85453104083?pwd=UC9kUnQ0eVhHNzlSTINH YWIEUS90QT09">https://zoom.us/j/85453104083?pwd=UC9kUnQ0eVhHNzlSTINH YWIEUS90QT09</a> (password 354679)
15:45-16:00	<b>Elizaveta Kozyr</b> (Turin, Italy) Speciation of Ru Molecular Complexes in Homogeneous Catalytic System: Fingerprint XANES Analysis Guided by Machine Learning <a href="https://zoom.us/j/88159140199?pwd=Q0tJWThhMEFsdHdkSkpOL 29ndjVrUT09">https://zoom.us/j/88159140199?pwd=Q0tJWThhMEFsdHdkSkpOL 29ndjVrUT09</a> (password 748927)

16:00-16:15	<b>Svetlana Shapovalova</b> (Rostov-on-Don, Russia) Characterization of novel valence tautomeric cobalt complex using temperature- and time-resolved XANES studies <a href="https://zoom.us/j/81691919648?pwd=MDM1YTVjWWZJUFBPU2s5K1B2Ly91dz09">https://zoom.us/j/81691919648?pwd=MDM1YTVjWWZJUFBPU2s5K1B2Ly91dz09</a> (password 427459)
16:30	<b><i>POSTER Session</i></b>