

## RUSSIAN-GERMAN SEMINAR

within the framework of the implementation of the "Russian-German Roadmap for Cooperation in Education, Science, Research and Innovation" and the development of mutually beneficial cooperation in new promising areas.

### Digital Materials

**Date and time: December 6, 2021, 10.00 - 14.00 (Moscow time)**

**Venue: NUST MISIS, Science Cluster: "The Point of Birth of Innovations"**  
**Moscow, Leninsky Prospekt, 6, bld. 7,**

**Working language:** English

**Participation format:** full-time/online

**Format:** seminar

**9:30– 10:00**      **Registration of participants and guests of the event**  
**Welcome coffee**

**10:00 – 10:20**      **Opening (*Welcome words*)**

**Andrey Polyakov, Head of Science Department,** National University of Science and Technology "MISIS"

**Svetlana Shevereva,** Representative of the Ministry of Science and Higher Education of the Russian Federation

**10:20 – 13:30**      **Panel discussion**

***Moderators:***

***Russian side:*** **Pavel Sorokin,** Dr., Laboratory "Inorganic Nanomaterials", National University of Science and Technology "MISIS"

***German side:*** **Yury Lysogorskiy,** Dr. Research Group Leader  
Data-Driven Methods for Atomistic Simulations  
Department of Atomistic Modelling and Simulation  
Ruhr-Universität Bochum





*Questions for discussion:*

- Material design – the future in numbers
- Digital doubles
- Digital solutions in materials science
- Big Data - development and main directions
- Artificial intelligence
- The use of artificial intelligence in the design of materials.
- Achieving targeted synthesis of materials with specified properties

*Reports and discussion:*

- **Ilya Eremin** - Ruhr-Universität Bochum  
Topic: «**Collective phenomena in quantum matter**»
- **Alexandra Khvan** – Director of SRC «Thermochemistry of materials», National University of Science and Technology “MISIS”,  
Topic: «**Third generation CALPHAD**»
- **Vladimir Sokolovsky** – Prof. Chelyabinsk State University  
Topic: «**Theoretical approaches to investigate magnetocaloric heusler alloys**»
- **Olga N. Miroshkina** - PostDoc in the Collaborative Research Centre/Transregio (CRC/TRR) 270, University of Duisburg-Essen  
Topic: «**Rational design of narrow-hysteresis materials: Cross-coupled magnetocaloric materials**»
- **Sergey Levchenko** – Center for Energy Science and Technology, Skoltech  
Topic: «**Cheminformatics in catalysis research**»





- **Sergey Erokhin** Laboratory "Inorganic Nanomaterials of National University of Science and Technology "MISIS",  
Topic: **"An example of successful material design. The solution to the long-standing problem of controlling the chirality of carbon nanotubes»**
- **Yury Lysogorskiy** - Dr. Research Group Leader Data-Driven Methods for Atomistic Simulations  
Department of Atomistic Modelling and Simulation  
Ruhr-Universität Bochum  
  
Topic: **«Data-driven platform for the interatomic potentials development and validation»**
- **Andrey V. Matveev** – Ph. D., Head of the Laboratory of Deep Machine Learning in Physical Methods, Novosibirsk State University  
Topic: **«Artificial intelligence for imaging data analysis in Materials Science: microscopy and behind»**
- **Alexander Shapeev** – Associate Professor, Skoltech  
Topic: **«Artificial intelligence for accelerating and automating atomistic simulations »**

**13:30 – 14:00** Press approach / group photo  
**Coffee break**

