MISIS

International Summer School on

Computational Materials Design

12-19 July

National University of
Science and Technology
MISIS

- **CALPHAD**
- **Ab initio calculations**
- **Data analysis. Python**
- **Cluster work**
- **Kinetics**
- **Molecular dynamics**

COSTS

Summer school fee is **250 EUR** for the one-week program which includes 34 hours of lectures and practical work and 14 hours of individual work.

THINK BRIGHT!

International summer school on computational materials design

The aim of the summer school is to provide students with an introduction to the use of thermodynamic, kinetic and ab initio modelling to solve real problems in multicomponent chemical systems (such as: materials, development, casting and solidification, heat treatment, extraction, refining, welding, brazing and soldering) and to illustrate just how easy thermodynamics can be applied in industry.

Program

Subject	Total hours	Lectures and practical work	Individual work
Computational and experimental thermodynamics and phase diagrams	14	12	2
Modelling of kinetic processes	4	4	0
Ab initio calculations	8	6	2
Basics of the modern clusters work	6	4	2
LAMMPS Modelling	8	4	4
Data analysis. Python	8	4	4
Total	48	34	14

Requirements for students:

4th year bachelors, MA students specialized in Materials science, Inorganic Chemistry, Physical Chemistry, Physics in Material science.

PhD students from related fields of Materials Science, Chemistry and Physics.

Students should have knowledge in:

Basic knowledge of Materials Science and Physical Chemistry

Basic understanding of Thermodynamics and Phase Diagrams