

SPONSORS REGISTRATION PROGRAM COMMITTIES TRAVEL

The APDIC World Round Robin Seminar and Summer School is a seminar organized by <u>APDIC</u>. As it was declared in the first seminar, "<u>APDIC</u> has valuable human resources who are expert in assessing, calculating and determining a phase diagram. One of the new activities we decided to launch is to offer a series of educational seminars on phase diagrams to industry people and students. This is the basic idea of World Round Robin Seminar (WRRS). The lecturers selected among us and requested by us are all well known experts in the fields, and they provide a systematic knowledge of phase diagrams starting from the fundamentals of how to read a phase diagram to up-to-date application in designing new materials such as functional and electric applications."

For more information about <u>APDIC</u> and WRRS seminars see <u>here</u>. Information about registration and organization fee see <u>here</u>

Торіс	Speaker	Country
Fundamentals (4 th of July)		
Phase equilibrium calculation by Cluster Variation Method	Prof. Tetsuo Mohri	Japan
Phase Diagrams	Prof. Rainer Schmid- Fetzer	Germany
Thermodynamic Data	Dr. Alan Dinsdale	Russia
Microstructure Characterization ab initio	Prof. Igor Abrikosov	Russia/Sweden
Problems with thermodynamic assessments	Dr. Ales Kroupa	Czech Republic
Experimental thermodynamics	Prof. Herbert Ipser	Austria
Applications (5 th of July)		
Applications of computational thermodynamics to steelmaking and processing	Dr. Andre Costa e Silva	Brazil
Calphad as a tool for steel development and processing	Dr. Bengt Hallstedt	Germany
Pyro-metallurgical	Prof. Pekka Taskinen	Finland
Nuclear Materials	Dr. Christine Gueneau	France
Fertilizers	Prof. Irina Uspenskaya	Russia
Solders and Brazes	Prof. Herbert Ipser	Austria
Phase equilibria, phase diagrams and phase stabilities in materials for green energy harvesting	Prof. Jean-Claude Tedenac	Russia/France
Application of the CALPHAD method for ferritic boiler steels	Dr. André Schneider	Germany
Thermodynamic Modeling of Aqueous Solutions – Mission impossible?	Dr. Sippola Hannu	Finland

Preliminary program of the seminar

Software and experimental equipment exhibition and summer school

1. Thermo-Calc Software User Group Meeting and Summer School (<u>Thermo-Calc Software</u>) Dictra and Prisma software Presentation and workshop

2. CompuTherm User Group Meeting and Summer School (CompuTherm LLC)

Presentation and workshop Pandat software

3. DFT, ab initio. Introduction into the pseudopotential and PAW technique: Generalities. How to run VASP calculations, Parameters.

4. Introduction to phonons using Quantum-Espresso: harmonic theory, frozen phonons, density functional perturbation theory (DFPT), quasi-harmonic phase diagrams, anharmonicity.

5. Ising. Monte Carlo simulations of configurational thermodynamics of alloys: Monte Carlo simulations utilizing effective cluster interactions derived from first principles will be used to model order-disorder phase transitions of real alloys.

We look forward to seeing you at the WRRS in Moscow in July!

Dr. Alexandra Khvan Director of SRC "Thermochemistry of materials" NUST MISIS