

**Russian Academy of Sciences  
Institute of Geology of Ore Deposits, Petrography, Mineralogy, and  
Geochemistry (IGEM) RAS**

**Russian Mineralogical Society, Moscow branch  
Institute of Geochemistry and Petrology, ETH Zurich, Switzerland  
Institute of Geological Sciences, University of Bern, Switzerland  
Paul Scherrer Institute, Switzerland**



## **1<sup>st</sup> Russian-Swiss Seminar**



**«Methods for modelling of geochemical  
processes: algorithms, data prediction,  
experimental validation, and relevant  
applications»**



### **Programme**

**IGEM RAS, Moscow**

**May 17–20, 2011**

## Goal of the Seminar:

**to get together renowned experts on the subject, presently active in Russian and Swiss universities and research institutes**

## Specific Aims:

- To evaluate existing approaches and algorithms for geochemical modelling, to discuss the feasibility of a benchmarking network
- To assess state-of-the-art methods of thermodynamic data prediction and compilation of internally consistent databases for geochemical modelling
- To formulate actual needs for hydrothermal experimental studies for model validation and application to relevant ore-formation systems
- To strengthen contacts, identify common research interests, possible synergies among research groups in view of potential applications for bilateral research projects, concerted actions, networks and workshops

## Organizing Committee

**Chairman:** *Acad. Prof. Nikolay S. Bortnikov*

**Vice-chairmen:** *Prof. Nikolay N. Akinfiyev, Prof. Larryn W. Diamond*

**Secretary:** *Lyudmila A. Koroleva (laqueen@igem.ru)*

**Members:** *Elena F. Bazarkina* *Boris R. Tagirov*  
*Olga Yu. Plotinskaya* *Alexander V. Zotov*

## Program Committee

*Dmitrii V. Grichuk (MSU)* *Peter Alt-Epping (Univ. Bern)*

*Evgenii G. Osadchii (IEM RAS)* *Thomas Wagner (ETHZ)*

*Alexandr V. Zotov (IGEM RAS)* *Dmitrii A. Kulik (PSI)*

## Venue

The seminar will be held at the Institute of Geology of Ore Deposits, Petrography, Mineralogy, and Geochemistry (IGEM) Russian Academy of Sciences (RAS), 117019, Staromonetny per., 35, Moscow, Russia, <http://www.igem.ru> Tel. +7(499) 230-82-31, Fax.+7(495) 951-15-87 E-mail: [laqueen@igem.ru](mailto:laqueen@igem.ru)

The Institute is located between Metro (subway) stations Polyanka and Tretyakovskaya, close to the city centre.

# Scientific Program

## Day 1, May 17, 2011

9:30 – 9:45 **Opening remarks:** Academician N. S. Bortnikov, Chairman of the Seminar

**9:45 – 12:45 Session I** (Chairpersons: Bazarkina E.F., Osadchii E.G.)

### **State of the art in experimental studies of fluid chemistry and ore deposition**

9:45 – 10:15 Keynote: Tagirov B.R., Baranova N.N., Zotov A.V., Akinfiyev N.N., Koroleva L.A., Shikina N.D., Polotnyanko N.A., Khodakovskiy I.L., Shvarov Yu.V. The speciation and transport of palladium in hydrothermal fluids: Experimental modeling and thermodynamic constraints

10:15 – 10:35 Aranovich L.Y., Novikova M.A. Acid-base fractionation in the model Cl-bearing granite

10:35 – 10:55 Bazarkina E.F., Pokrovskiy G.S. X-ray absorption fine structure spectroscopy study of palladium transport by hydrothermal fluids

**10:55 – 11:15 Coffee break**

11:15 – 11:35 Nekrasov S., Bychkov A., Matveeva S.S. The behaviour of gallium in greisens: experimental and natural data

11:35 – 11:55 Zotov A.V., Koroleva L.A. Experimental determination of hydrogen fugacity at supercritical parameters

11:55 – 12:15 Zezev D., Hingerl F., Driesner T. Experimental data and modeling of the properties of mixed electrolyte aqueous solutions

**12:15 – 12:45 Discussion I**

**12:45 – 14:30 Lunch**

**14:30 – 16:30 Session II** (Chairpersons: Diamond L.W., Shvarov Yu. V.)

### **Methods of geochemical modelling: Thermodynamic, kinetic, and reactive mass transport approaches**

14:30 – 15:00 Keynote: Kulik D.A., Kosakowski G. Algorithms and codes for geochemical thermodynamic modelling: Ready for reactive mass transport simulations?

15:00 – 15:20 Mironenko M.V., Zolotov M.Yu. A kinetic-thermodynamic model for irreversible water-rock interactions: approaches and a program implementation

15:20 – 15:40 Alt-Epping P., Diamond L.W. Multiphase flow and multicomponent reactive transport models with applications to geothermal systems and the sequestration of CO<sub>2</sub> in deep aquifers

15:40 – 16:00 Malkovsky V.I., Pek A.A., Aleshin A.P. Modeling of deposit formation through precipitation of ore component on movable thermal barrier by the example of uranium deposits Streltsovskoye+Antey

**16:00 – 16:30 Discussion II**

## **Day 2, May 18, 2011**

**9:30 – 11:30 Session III** (Chairpersons: Wagner T., Khodakovskiy I.L.)

### **Prediction of thermodynamic properties of aqueous species in a wide range of temperatures and pressures**

9:30 – 10:00 Keynote: Plyasunov A.V. Some comments about models for predicting the standard-state and excess properties of electrolytes at high T and P.

10:00 – 10:20 Akinfiyev N.N. Low density hydrothermal fluids: approaches to predict thermodynamic properties of aqueous species

10:20 – 10:40 Bastrakov E.N., Shvarov Yu.V. FreeGs thermodynamic database project: where to?

10:40 – 11:00 Yeriomin O.V. Calculation of standard thermodynamic potentials for zeolites of Na-Al-Si-O-H system

**11:00 – 11:30 Discussion III and Coffee break**

**11:30 – 13:00      Session IV (Chairpersons: Borisov M.V., Tagirov B.R.)**

**Selected model applications to ore formation systems in various  
geochemical environments**

11:30 – 12:00      Keynote: Wagner T. Application of geochemical and isotopic modeling to ore-forming systems

12:00 – 12:20      Esipenko G., Pristavko V. A., Morozova S. G. Method of the Virtual Emmons' Ore Geochemical Shoot: Zoning, parageneses, spectrum and structure of Maiskoe Lode geochemical field assemblages (Central Chukotka)

12:20 – 12:40      Kigai I.N. Some ways for experimental and theoretical studies to meet a current state of knowledge on ore associations with magmatites and related fluids of different redox state

12:40 – 13:00      Kol'tsov A.B. Numerical modeling of thermobarogradient metasomatic processes

**13:00 – 15:00      Lunch**

16:00 – 18:30      Guided Kremlin tour (including the Treasure-house and the Armoury Chamber)

**Day 3, May 19, 2011**

**9:30 – 11:30      Session IV (continued)**

9:30 – 9:50      Li E. Yu., Grichuk D. V., Shilobreeva S. N., Chareev D. A. An experimentally verified thermodynamic model of interactions in the system [basalt-SO<sub>2</sub>-O<sub>2</sub>-(S<sub>2</sub>)]

9:50 – 10:10      Lipatnikova O.A., Grichuk D.V. Thermodynamic modeling of heavy metals forms in bottom sediments of the Ivankovsky Reservoir

10:10 – 10:30      Petrov V.A., Poluektov V.V., Ustinov S.A. Fluid migration within the stress-temperature field: geostructural evaluative approach

10:30 – 10:50 Sushentsova B.Yu., Grichuk D.V., Shilobreeva S.N.  
Thermodynamic simulation of silicate interaction with gases of C-O-H system:  
model verification and prediction

**10:50 – 11:20 Coffee break**

11:20 – 11:40 Volkova M.M., Borisov M.V., Bychkov D.A. Sources of ore  
components and formation models of North Osetiya Pb-Zn vein deposits

11:40 – 12:00 Yeriomina O.V., Yurgenson G.A. About thermodynamic  
equilibria of sulfate-carbonate solutions under anaerobic conditions

12:00 – 12:20 Zykin N.N. The nature of ore-forming solutions according to  
data of water oxygen and hydrogen isotope composition of fluid inclusions

12:20 – 12:40 Vikentyev I.V., Karpukhina V.S., Prokof'ev V.Ju. Models of  
ore-magmatic hydrothermal systems for the VHMS deposits of the Urals

**12:20 – 12:50 Discussion IV**

**12:50 – 15:00 Launch**

**15:30 – 17:00** Guided visit to the Fersman mineralogical museum

*(Museum world-wide collections include more than 135'000 items. Among them  
natural crystals, geodes, druses and other kinds of mineral treasures. Articles made  
of stones by jewelers 18 - 20 centuries. Gemstones. Meteorites and much more.)*

**17:30 Closing party**

## **Day 4, May 20, 2011**

**9:30 – 11:30 Closing discussion** (Moderator: *Diamond L.W.*)

- A. Conclusions on state of the art and knowledge gaps
- B. Ideas on model benchmarking and verification
- C. Identification of common research interests and groups
- D. Possible topics for SNF-RFBR joint proposals
- E. Preparation and publication of the Seminar Proceedings

11:30 – 13:00 Optional meeting of a workgroup on benchmarking codes  
and thermodynamic databases.