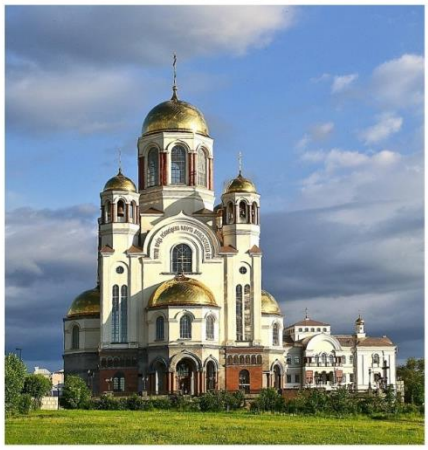
HTMC XVI

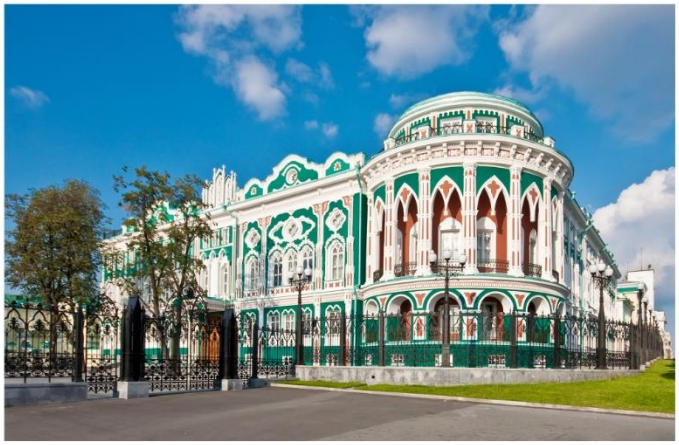
16th IUPAC High Temperature Material Chemistry Conference (HTMC-XVI)

July 2 – 6, 2018, Ekaterinburg, Russia

BOOK OF ABSTRACTS







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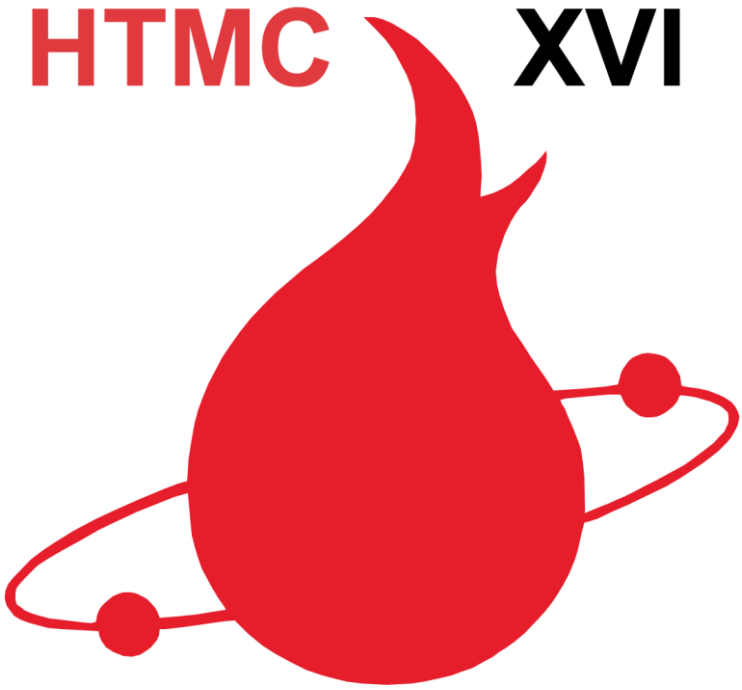

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This Book of Abstracts contains brief information on up-to-date research works in various fields of high temperature materials chemistry such as thermodynamics, theory and modeling, phase structure, ionic and electronic transport phenomena, and covered wide class of natural and synthetic materials for various applications: nuclear energy, aerospace, metallurgical processes. Together with the traditional items the new topic concerning materials for advanced sources of energy has been added.

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Preface

The focus of HTMC-16 meeting is to bring together people from the fields of chemistry, materials science, earth and planetary science, metallurgy, who are working in the area of high temperature phenomena in solid and liquid materials. High temperature materials are of permanent significance for science and industry, especially in recent years.

The list of main topics of the Conference is traditional. It has been reproduced from the previous Conferences held in Orleans, France (2016), Beijing, China (2012) and earlier. It includes important aspects of high temperature material chemistry such as thermodynamics, theory and modeling, phase structure, ionic and electronic transport phenomena, and covered wide class of natural and synthetic materials for various applications, such as, nuclear energy, aerospace, metallurgical processes.
Together with the traditional items the new topic concerning materials for advanced sources of energy has been added to the forthcoming 16th Conference. Design of materials for the energy sources application become a hot topic in a modern material science, but commercialization of renewable energy sources are limited mainly due to the poor durability and quick degradation of their constituents.

The following sessions will take place:

A: High temperature thermodynamic measurements; VBN

B: Theory and modeling of high temperature materials;

C: Melts, ceramics, glasses and amorphous materials;

D: Transport, ionic and electronic conductivity, grain boundaries, interfaces and surfaces;

E: Phase structure and metallurgical processes, corrosion;

F: Earth and planetary materials at high pressures and temperatures;

G: Materials for nuclear energy applications;

H: Materials for aerospace applications;

I: Materials for advanced sources of energy.

There are no parallel sessions and all oral reports are separated into three groups: Plenary talks (Plenary – 35 min), Invited talks (Inv. – 25 min) and Oral reports (O – 15 min).

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BP18

THERMODYNAMIC MODELING OF Zn-S AND Zn-Se ALLOYS

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Semiconductor compounds of the A^2B^6 group are promising materials to creation of unique instruments of optics, optoelectronics, acoustoelectronics, nanoelectronics, laser technology, detecting ionizing radiations. For example, zinc selenide crystals are increasingly applied in the infrared, LED, and fiber optic technology as the detectors of X-rays and elementary particles. Crystals of zinc chalcogenides (ZnSe and ZnS) doped with ions of transition metals (Fe^{2+}, Co^{2+}, Cr^{2+}) are promising materials for creating active media of tunable solid-state lasers.

For growing crystals it is necessary to know the properties of these materials in liquid and solid states. It should be noted that physical and chemical properties of A^2B^6 compounds and alloys are investigated good enough in solid state. However, for liquid phase the information is lack. This is due to the great difficulties in working with these substances: high melting points, high pressures of own vapors, chemical aggressiveness of the gas phase and melts, toxicity. The lack of data constrains the development of all technologies for obtaining these materials, which, in turn, limits the possibilities of their practical application. Thus, the study of the physical and chemical properties of ZnSe and ZnS is still an actual problem.

In the present work, using the TERRA software, the thermodynamic characteristics and equilibrium composition of the condensed and gas phases formed during the equilibrium heating of ZnSe and ZnS in a wide range of temperatures (300-3000 K) at the common pressure of $P = 10^5$ Pa in an argon atmosphere were studied. The effect of temperature and impurity content on the properties of Zn-Se and Zn-S melts has been studied. Temperature dependences of the content of condensed and gas phases and thermodynamic state parameters for each of the systems studied over a wide temperature range have been constructed.