Report of the

Russian National Committee of Thermal Analysis and Calorimetry

on the activities in the field of Phase Diagrams, Experimental Thermodynamics and

Modelling

Compiled by Alexandra V Khvan and Konstantin Gavrichev

The Russian National Committee of Thermal Analysis and Calorimetry was officially established by Russian Academy of Science in October 2016

**I Specific goals of the National Committee of Thermal Analysis and Calorimetry**

- To energize the fields of Phase Diagrams, Experimental Thermodynamics and Modelling throughout Russia and involve more young people into the field
- To coordinate activities in the specified scientific fields. It's obvious that the amount of scientific work required to cover all the materials of interest even within one area is vast, far beyond the scope of a single organization and that is why we are part of global scientific collaboration in order to achieve reasonable results and make a serious step forward.
- To provide focus and direction into specific technological areas
- To hold trans Russia conferences
- To participate as co-organizers of the conferences abroad

**II General Activities of the members of the National Committee of Thermal Analysis and Calorimetry in 2020**

1. 13th Symposium on „Thermodynamics and Materials Science" with international participation. 15-19 June, 2020, Novosibirsk. (Canceled due to COVID-19)
2. XVI International Conference on Thermal Analysis and Calorimetry in Russia, 5-10 July 2020, Moscow, Russia. The conference covers following topics: Experimental investigation of thermodynamic properties of inorganic and organic materials, methods/standards/databases of thermal analysis and calorimetry, phase equilibria and phase transformation, Calphad method, ab initio calculations. (Canceled due to COVID-19). Plenary session was carried

out on-line. Recordings are available on https://rtac2020.chem.msu.ru/ and youtube.

3. **III. Upcoming events.**

The workshop on Data and Computation for Materials Science and Innovation within XXIII Data Analytics and Management in Data Intensive Domains conference 26.10.2021-29.10.2021 (Combined off-line and on-line participation)

XXIII International Conference on Chemical Thermodynamics in Russia (RCCT) was postponed from 23-28th of August 2021 to 2022 and will be combined with International Conference on Thermal Analysis and Calorimetry in Russia (RTAC).

| System | Ex PD | Ex TD | CA | TD Md | AS | Comment | Contact person | Country |
|---|---|---|---|---|---|---|---|---|
| SiO2 | | | F | F | | NUST MISIS, Hampton Thermodynamics | I Bajenova, AV Khvan, A Kondratiev, A T Dinsdale, | Russia, UK |
| GeO2 | | | F | F | | NUST MISIS, JIHT RAS, Hampton Thermodynamics | I Bajenova, A T Dinsdale, A V Khvan, N Aristova | Russia, UK,France |
| Ge (to be published in 2021) | | | F | F | | | A V Khvan, IA Uspenskaya, A.Ivanov, N.M. Konstantinova, AT Dinsdale | Russia, UK |
| Sn | | x | F | F | F | NUST MISIS, MSU, Hampton Thermodynamics | A V Khvan, TBabkina, IA Uspenskaya, ASuzdikova, M Belov, N Drujinina, A T Dinsdale. | Russia, UK |
| In(to be published in 2021) | | x | F | x | | NUST MISIS, MSU, Hampton Thermodynamics | A V Khvan, IA Uspenskaya, AT Dinsdale | Russia, UK |
| Si (to be published in 2021) | | | F | F | | NUST MISIS, MSU, Hampton Thermodynamics | A V Khvan, IA Uspenskaya, A.Ivanov, N.M. Konstantinova, AT Dinsdale | Russia, UK |
| Pb-Sn(to be published in 2021) | | | x | x | | NUST MISIS, Hampton Thermodynamics, Thermo-Calc AB | AV Khvan, AT Dinsdale, Q Chen. | Russia, Sweden,UK |
| Si-Ge(to be published in 2021) | | | F | F | | NUST MISIS, MSU, Hampton | IA Bajenova, A V Khvan, | Russia, UK |

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|---|---|---|---|---|---|---|---|---|
| | | | | | | Thermodynamics | IA Uspenskaya, Dinsdale AT | |
| Fe-Co-La | F | | F | | | NUST MISIS | I Fartushna, AV Khvan, | Russia |
| Fe-Ni-La | F | | F | | | NUST MISIS, Universtiy of Vienna | I Fartushna, AV Khvan, K Richter | Russia Austria |
| Fe-Co-Sm | F | | F | | | NUST MISIS | I Fartushna, AV Khvan, | Russia |
| Cr-Co-Mn | x | | x | | | NUST MISIS | I Fartushna, AV Khvan, | Russia |
| W-Ta-Cr | x | | x | | | NUST MISIS | I Fartushna, AV Khvan, S Kuzovchikov | Russia |
| Ta-Be | x | | x | | | NUST MISIS | I Fartushna, AV Khvan, S Kuzovchikov | Russia |
| Fe-Al-Sn | x | | x | | | NUST MISIS | I Fartushna, AV Khvan, | Russia |
| HfO2 (crystal,amorphous) | | x | | | | NUST MISIS | IA Bajenova, AV Khvan | Russia |
| Ln2Hf2O7, Ln = La, Nd, Sm, Eu,Er | | x | | | | NUST MISIS, IGIC RAS | IA Bajenova, MS Derevyanko, K.S Gavrichev AV Khvan | Russia |
| CaO-Al2O3-MgO | | x | | | | NUST MISIS, SiMAP | AV Khvan, A Pisch | Russia, France |
| CeO2 | | | x | | x | JIHT RAS | NM Aristova | Russia |
| ZrC, HfC, TaC | | | F | | F | JIHT RAS | NM Aristova, AI Savvatimskiy, SV Onufriev | Russia |
| $RBaCo_2O_{6-\delta}$ (R – Y, Pr, Nd, Gd) | | F | | | | UrFU, University of Caen | AYu Zuev, DS Tsvetkov, VA Cherepanov, A Maignon | Russia, France |
| $BaZr_{1-x}Pr_xO_{3-\delta}$ (x=0-1) | | F | | | | UrFU | AYu Zuev, DS Tsvetkov, VV Sereda, DA Malyshkin, IL Ivanov | Russia |
| $BaCa_{(1+y)/3}Nb_{(2-y)/3}O_{3-\delta}$ (y = 0, | | F | | | | UrFU | AYu Zuev, DS Tsvetkov, | Russia |

| Compound | C1 | C2 | C3 | C4 | C5 | Institution | Authors | Country |
|---|---|---|---|---|---|---|---|---|
| 0.18 and 0.5) | | | | | | | VV Sereda, DA Malyshkin, IL Ivanov | |
| $CsPbX_3$ (X – Cl, Br, I) | | F | | | | UrFU | AYu Zuev, DS Tsvetkov, VV Sereda, DA Malyshkin, IL Ivanov, MO Mazurin | Russia |
| $APb(X_{1-y}M_y)_3$ (A – $CH_3NH_3$, Cs; X,M – Cl, Br, I) | X | X | | | | UrFU | AYu Zuev, DS Tsvetkov, VV Sereda, DA Malyshkin, IL Ivanov, MO Mazurin | Russia |
| $A2BX4$ (A – amino acid, CH3NH3; B – Pb, 3d-element; X – Cl, Br, I) | X | X | | | | UrFU | AYu Zuev, DS Tsvetkov, VV Sereda, DA Malyshkin, IL Ivanov, MO Mazurin | Russia |
| MgO | | | x | x | | MSU | A.Perevozshikov, N.A.Kovalenko, I.A.Uspenskaya | Russia |
| CaO-Al2O3-TiO2 | | | x | | | MSU, SiMAP | A.S.Arkhipin, I.A. Uspenskaya, A.V. Khvan, A.Pisch | Russia, France |
| Mo | | | x | x | | MSU | A.Perevozshikov, N.A.Kovalenko, I.A.Uspenskaya | Russia |
| GaAs - InAs | | | x | x | | | A.Ivanov, N.M.Konstantinova, I.A.Uspenskaya | Russia |
| $Pr_2Sn_2O_7$ | | | x | x | | IGIC RAS | K.S. Gavrichev V.N. Guskov P.G. Gagarin | Russia |

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|---|---|---|---|---|---|---|---|---|
| | | | | | | | A.V. Khoroshilov<br>A.V. Tyurin | |
| HoVO$_4$ | | x | x | | | IGIC RAS | O.N. Kondrat'eva<br>G.E. Nikiforova<br>K.S. Gavrichev<br>A.V. Tyurin | Russia |
| TmTaO$_4$ | | x | x | | | IGIC RAS, IM&M RAS | K.S. Gavrichev<br>V.N. Guskov<br>A.V. Guskov<br>P.G. Gagarin<br>A.V. Khoroshilov<br>A.V. Tyurin | Russia |
| DyTaO$_4$ | | x | x | | | IGIC RAS, IM&M RAS | K.S. Gavrichev<br>V.N. Guskov<br>A.V. Guskov<br>P.G. Gagarin<br>A.V. Khoroshilov<br>A.V. Tyurin | Russia |
| NdNbO$_4$ | | x | x | | | IGIC RAS | G.E. Nikiforova<br>K.S. Gavrichev<br>A.V. Tyrin<br>A.V. Khoroshilov | Russia |
| HoTaO$_4$, TbTaO$_4$ | | x | x | | | IGIC RAS, IM&M RAS | K.S. Gavrichev<br>V.N. Guskov<br>A.V. Guskov<br>P.G. Gagarin<br>A.V. Khoroshilov<br>A.V. Tyurin | Russia |
| EuTaO$_4$ | | | | | | IGIC RAS, IM&M RAS | K.S. Gavrichev | Russia |

| | | | | | | Authors | Country |
|---|---|---|---|---|---|---|---|
| | | | | | | V.N. Guskov<br>A.V. Guskov<br>P.G. Gagarin<br>A.V. Khoroshilov<br>A.V. Tyurin | |
| $RE_2FeTaO_7$ (RE=Y, Sm, Gd) | | x | x | | | A.V. Egorysheva<br>K.S. Gavrichev<br>A.V. Tyurin<br>N.N. Efimov | Russia |
| $Eu_2FeTaO_7$ | | x | x | | IGIC RAS | A.V. Egorysheva<br>K.S. Gavrichev<br>A.V. Tyurin<br>O.G. Ellert | Russia |
| $Sm_2ScTaO_7$ | | x | x | | IGIC RAS | A.V. Egorysheva<br>K.S. Gavrichev<br>A.V. Tyurin<br>O.G. Ellert | Russia |
| $Na_3REE(PO_4)_2$, $Na_3REE(VO_4)_2$ (REE=Gd, Y) | | x | x | | IGIC RAS | M.A. Ryumin<br>K.S. Gavrichev<br>I.S. Pikulin<br>A.V. Khoroshilov | Russia |
| $AuSb_2$ | | x | x | | IGIC RAS, Dubna University | A.V. Tyurin<br>N.A. Polotnyanko<br>D.A. Chareev | Russia |
| $Tb_2O_3 \cdot 2ZrO_2$ | | x | x | | IGIC RAS | P.G. Gagarin<br>V.N. Guskov,<br>K.S. Gavrichev<br>A.V. Tyurin<br>A.V. Khoroshilov | Russia |

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|---|---|---|---|---|---|---|---|---|
| nano-$EuPO_4$ | | x | x | | | IGIC RAS, | K.I. Pechkoskaya<br>K.S. Gavrichev<br>G.E. Nikiforova | Russia |
| nano- $MgFe_{1.2}Ga_{0.8}O_4$ | | x | x | | | IGIC RAS, SPbSU | O.N. Kondrat'eva<br>G.E. Nikiforova<br>M.N. Smirnova<br>E.V. Shevchenko | Russia |
| $WO_3$ | | x | x | | | IGIC RAS, Jiangsu University | B.-Yu. Han<br>A.V. Khoroshilov<br>A.V. Tyurin<br>A.E. Baranchikov<br>M.I. Razumov<br>O.S. Ivanova;<br>K.S. Gavrichev<br>V.K. Ivanov | Russia,<br>China |
| $PtS_2$ | | x | x | | | IGIC RAS, Dubna University | A.V. Tyurin<br>N.A. Polotnyanko<br>D.A. Chareev | Russia |
| $HoPO_4$ | | x | x | | | IGIC RAS, IGeochem. & Analyt. Chem. RAS | A.V. Tyurin,<br>M.A. Ryumin,<br>A.V. Khoroshilov,<br>V.M. Gurevich.<br>K.S. Gavrichev | Russia |
| $YbTaO_4$ | | x | x | | | IGIC RAS | K.S. Gavrichev<br>V.N. Guskov<br>A.V. Guskov<br>P.G. Gagarin<br>A.V. Khoroshilov | Russia |

| | | | | | | Institution | Authors | Country |
|---|---|---|---|---|---|---|---|---|
| | | | | | | | A.V. Tyurin | |
| $RE_2Hf_2O_7$ (RE=Nd-Lu) (to be published in 2021) | | x | x | | | IGIC RAS | K.S. Gavrichev V.N. Guskov A.V. Guskov P.G. Gagarin A.V. Khoroshilov A.V. Tyurin | Russia |
| $LaLnZr_2O_7$ (Ln= Sm, Gd, Dy) | | | | | | IGIC RAS | P.G. Gagarin V/N/ Guskov K.S. Gavrichev A.V. Tyurin A.V. Khoroshilov | Russia |
| $Y(VO_4)_{1-x}(PO_4)_x$ | | | | | | IGIC RAS, Moscow State Textile University | A.P. Kritskaya, O.N. Kondrat'eva, G.E. Nikiforova, M.A. Ryumin, K.I. Bryukhanova, B.A. Kolozhvari | Russia |
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Ex.PD = Experimental phase diagram study

Ex.TD = Experimental study of thermodynamic data

CA    = Critical Assessment of literature

TD Md. = Thermodynamic Modeling, CALPHAD-type

AS    = Atomistic Simulations / First Principles

Comment = notes on application etc., free text

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F = finished in **2020**

X = work in progress