$MSI\,/\,MSIT^{\circledR}$ activities in the year 2022

APDIC Report, June 2023

Including the activities of MSIT®, Materials Science International Team

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MSIT® Community Activities



7th MSIT N Winter School on Materials Chemistry

The 7^{th} MSIT Winter School on Materials Chemistry was held at the Castle Ringberg on 12 - 17 March 2023 in parallel with the 37^{th} MSIT Annual Workshop.

Organised by:

MSI, Materials Science International GmbH, Germany/ Dr. Svitlana Iljenko Hampton Thermodynamics Ltd., United Kingdom/ Dr. Andrew Watson Max-Planck-Institut für Eisenforschung GmbH, Germany/ Dr. Frank Stein, Dr. Martin Palm

The aim of the MSIT Winter School is to provide first-class tuition in a selection of subjects closely associated with the study of phase equilibria in Materials Science. Each module involves lectures, demonstrations and problems classes. The lectures are given mainly by members of the MSIT who are world experts in their respective fields. The <u>Programme</u> of the 7th MSIT Winter School has included the following courses spreading over 36 hours in total:

The format of the Winter School, which combines theory and practice of the evaluation of phase equilibria and thermodynamics, leading to the thermodynamic modelling of a real binary system has proved to be extremely popular. The MSIT Winter School became established as the premier event for the training of postgraduate students and more mature researchers in the basic principles and the applications of phase equilibria and thermodynamics.

And we are pleased to say that the MSIT Winter School will return in 2024. Again, to the Castle of Ringberg. Registration is open https://www.msiport.com/msit-school/next-msit-school/



International Seminar on the Evaluation of Heterogeneous Multicomponent Equilibria

The Annual Meeting of the MSIT members has taken place in parallel with the 7th MSIT Winter School. The Group Work on **Critical Evaluation** of constitutional data at the MSIT Workshop works in the following way: small groups of 3-5 scientists write together critical evaluation of data on phase diagrams of a particular system. The literature for evaluation and working infrastructure are provided by MSI. In the group work there is always a knowledge transfer from the senior scientists experienced in the evaluation work to the younger scientists. The Guidelines for Critical Evaluation you can see here.

2nd MSIT A AFRICA Workshop

International Seminar on the Evaluation of Heterogeneous Multicomponent Equilibria

Organised by: MSI, Materials Science International Services GmbH & African Research University Alliance -Centre of Excellence in Materials, Energy and Nanotechnology **Hosted by:** University of Witwatersrand (Prof. L. Cornish) & University of Ghana (Dr. D. Dodoo-Arhin)

The 2^{nd} MSIT-Africa Meeting was held on 29 May -2 June 2023 in Accra, Ghana. 30 participants have been working in 6 groups on **Critical Evaluation** of constitutional data of binary & ternary refractory materials systems with the great outcome of upcoming publications.

Successful start of the new series of educational events



The 1st MSIT Advanced School lasted for two full days. This was a deep dive into the topic of diffusion in materials. With the very high level of the lectures our lecturers revealed many "secrets" from their own experiences which led to lively discussions with the participants. Particularly well received was the practical training session given by John Ågren on the DICTRA module of the Thermocalc software. But the highlight of the School was the session "ask the experts", where participants were encouraged to share their diffusion related problems and experiences and receive suggestions from the lecturers and other participants.

ANNOUNCEMENT: UPCOMING MSIT EVENTS



Rare-Earth Materials Magnet Technology





22 - 23 November 2023, Stuttgart, Germany

Scope

The seminar will be focused on permanent magnets and the supply of the raw materials. We will start with fundamentals of the RE elements and magnetism, the principals of RE permanent magnets chemistry, thermodynamics, and constitution, same as measurement techniques. Showing the processes from mine to magnet and recycling is the approach to close the circle for sustainability and environmental protection of Earth. Applications and the future of global markets will be shown, as well as new opportunities of global sourcing.

Organised by:

MSI. Materials Science International Services GmbH, Germany and ppm materials GmbH, Kirchheim/Teck, Germany

> Chairman: Dr. Bernd Grieb

Topics:

- Raw Materials and Resources
- **REE Processing**
- Magnet Materials Basics
- Alloying
- Magnet Production
- Mechanical Processing
- Magnetization
- Soft Magnetics for Permanent Magnetics
- Recycling
- Applications
- Market
- Geopolitical Aspects
- Current Global Activities

https://www.msiport.com/msit-school/msit-advanced-school/



MSIT Winter School on Materials Chemistry

The Programme includes

- Principles of Chemical Thermodynamics
- Phase Diagrams and Phase Equilibria (basic and advanced level), incl. practical
- · Experimental Determination of Phase Diagrams, incl. practical session analysis of
- · Crystallography, incl. practical session
- Experimental Methods in Thermodynamics, incl. practical session analysis of data
- Critical Evaluation of Constitutional Data
- Application of DFT in the Context of Phase Diagram Modelling
- Computational Materials Thermodynamics & Calphad Method, incl. practical session Thermodynamic Modelling of Phase Equilibria

21 - 26 January 2024, Castle Ringberg Germany

Organised by

MSI, Materials Science International Services GmbH, Germany Hampton Thermodynamics, UK Max-Planck-Institut für Eisenforschung GmbH, Germany

https://www.msiport.com/msit-school/next-msit-winter-school/

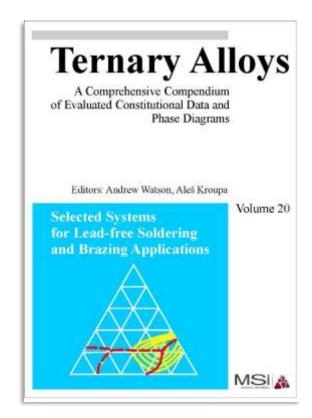


International Seminar on the Evaluation of Heterogeneous Multicomponent Equilibria

Organised by: MSI, Materials Science International Services GmbH & African Research University Alliance -Centre of Excellence in Materials, Energy and Nanotechnology **Hosted by:** University of Witwatersrand (Prof. L. Cornish) & University of Ghana (Dr. D. Dodoo-Arhin)

The 3rd MSIT-Africa Meeting will take place on 14 – 18 August 2023 again in Accra, Ghana. In the focus of the Group Work on Critical Evaluation of constitutional data will be binary & ternary refractory materials systems.

The volume 21 of Ternary Alloys has been published



The Volume 21 of the book series *Ternary Alloys- A Comprehensive Compendium of Evaluated Constitutional Data and Phase Diagrams*

"Selected Al-Fe-X Ternary Systems for Industrial Applications" is published in November 2022.

ISBN 978-3-932120-51-0;

Editors: Frank Stein and Martin Palm;

Authors: MSIT[®];

596 pages.

Table of content

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70565 Stuttgart (Germany), 2022

Fe—Al-based materials are an economic alternative to Cr-Ni steels and Ni-based superalloys for structural applications. They are also the basis of corrosion- and wear-resistant coatings and magnetic materials, e.g. Heusler alloys. In addition, they are applied in catalysis and hydrogen generation and storage, and in many systems quasicrystalline phases form, which exhibit remarkable properties. Fe—Al-based materials have been

of interest for structural applications for more than a century. Materials based on intermetallic phases can offer a high ratio of strength in relation to their density. Therefore, specifically the Al-containing intermetallics with Ni, Ti, and Fe are of interest in the view of energy saving aspects. Knowledge of Fe–Al–X systems plays also an important role in the development of various coatings.

The current compendium critically evaluates and summarizes all the available knowledge on phase equilibria, phase transformations, crystallographic details of the phases and their known properties and applications of 22 Fe–Al–X ternary systems and the Fe-Al binary system, which are important for industrial applications.

The system reports are arranged in the alphabetical order and have a standard format, allowing easy access to the required data. The following information is provided: liquidus projections, isothermal and vertical sections, quasibinary sections, reaction schemes, invariant equilibria, crystallographic data, thermodynamic data and materials properties, accompanied by short descriptive texts and extensive references.

Order form

Starting with the Volume 19, MSI has changed slightly the concept of the handbook series "Ternary Alloys. A Comprehensive Compendium of Evaluated Constitutional Data and Phase Diagrams". Instead of exploring alphabetically all ternary systems based on one chemical element, like Al-X-Y or Mg-X-Y, the future volumes will be dedicated to particular classes of materials or particular application areas, like volume 19 – "Selected Systems for Nuclear Applications". Selected are ternary systems of importance to industrial alloy development and systems which gained scientific interest in the recent years.



Content as of June 2023 (continuously updated)

Links to Literature: 508,520 citations, on 77,620 materials systems MSIT Binary & Ternary Evaluations: 4630 material systems, evaluated by MSIT 1701 systems, not evaluated by MSIT

Research Results: 4296 summaries, from 2022 include brief original publications

Phase diagrams and graphs: 16,340 Tables: 10,220

Total: 508,520 entries & documents

77,620 systems (from unary till 15-component systems) > 10,000 new entries added since last APDIC Meeting

APDIC Best Paper Award 2022 for a MSIAEUREKA publication:

One of the MSI Eureka publications has been chosen as the BEST PUBLISHED MANUSCRIPT ON ALLOY PHASE DIAGRAM DATA by APDIC for the year 2021!

Distl, B., Walnsch, A., Mellor, R. F.L., Gomell, L., Noori, M., Gedsun, A., Stein, F., "Al-Mo-Ti Ternary Phase Diagram Evaluation", in *MSI Eureka*, Watson, A. (Ed.) by MSI, Materials Science International Services GmbH, Stuttgart, **88**, 10.17143.3.2 (2021), https://doi.org/10.7121/msi-eureka-10.17143.3.2

2022 Publications in MSI Eureka®

System	Publication in the Category "Phase Diagram Evaluation" in MSI Eureka®
Al-B-Fe	Rogl, P., "Al-B-Fe Ternary Phase Diagram Evaluation", in <i>MSI Eureka</i> , Watson, A. (Ed.) by MSI, Materials Science International Services GmbH, Stuttgart, 94 , 10.19495.3.5 (2022), https://doi.org/10.7121/msi-eureka-10.19495.3.5
Al-C-Fe	Ghosh, G., Tymoshenko, O., Bondar, A., Dovbenko, O., "Al-C-Fe Ternary Phase Diagram Evaluation", in <i>MSI Eureka</i> , Watson, A. (Ed.) by MSI, Materials Science International Services GmbH, Stuttgart, 94 , 10.13509.4.5 (2022), https://doi.org/10.7121/msi-eureka-10.13509.4.5
Al-Co-Fe	Kumar, H. K.C., Palm, M., Rank, M., Walnsch, A., Watson;, A., Palm, M., "Al-Co-Fe Ternary Phase Diagram Evaluation", in <i>MSI Eureka</i> , Watson, A. (Ed.) by MSI, Materials Science International Services GmbH, Stuttgart, 94 , 10.15955.4.6 (2022), https://doi.org/10.7121/msi-eureka-10.15955.4.6
Al-Cr-Fe	Korniyenko, K., Dreval, L., "Al-Cr-Fe Ternary Phase Diagram Evaluation", in <i>MSI Eureka</i> , Watson, A. (Ed.) by MSI, Materials Science International Services GmbH, Stuttgart, 94 , 10.14873.4.3 (2022), https://doi.org/10.7121/msi-eureka-10.14873.4.3

System	Publication in the Category "Diagrams as Published" in MSI Eureka
Cu-Ti-Zr	Velikanova, T., Turchanin, M., Agraval, P., "Cu-Ti-Zr Ternary Phase Diagram Evaluation", in <i>MSI Eureka</i> , Watson, A. (Ed.) by MSI, Materials Science International Services GmbH, Stuttgart, 92 , 10.19042.2.2 (2022), http://www.msi-eureka.com/full-html/10.19042.2.2/Cu-Ti-Zr Ternary Phase Diagram Evaluation
Cu-Sn-Ti	Klotz, U. E., "Cu-Sn-Ti Ternary Phase Diagram Evaluation", in <i>MSI Eureka</i> , Watson, A. (Ed.) by MSI, Materials Science International Services GmbH, Stuttgart, 92 , 10.19550.2.7 (2022), https://doi.org/10.7121/msi-eureka-10.19550.2.7
Cu-Ni-Sn	Ghosh, G., Zhao, J., "Cu-Ni-Sn Ternary Phase Diagram Evaluation", in <i>MSI Eureka</i> , Watson, A. (Ed.) by MSI, Materials Science International Services GmbH, Stuttgart, 91 , 10.11399.3.1 (2022), httml/10.11399.3.1/Cu-Ni-Sn Ternary Phase Diagram Evaluation
Cu-In-Sn	Velikanova, T., Turchanin, M., Fabrichnaya, O., Huang, D., Wang, Y., Xu, L., Xia, D., "Cu-In-Sn Ternary Phase Diagram Evaluation", in <i>MSI Eureka</i> , Watson, A. (Ed.) by MSI, Materials Science International Services GmbH, Stuttgart, 91 , 10.21071.2.0 (2022), http://www.msi-eureka.com/full-html/10.21071.2.0/Cu-In-Sn Ternary Phase Diagram Evaluation
Cr-Ni-Si	Ghosh, G., Zobac, O., Kroupa, A., "Cr-Ni-Si Ternary Phase Diagram Evaluation", in <i>MSI Eureka</i> , Watson, A. (Ed.) by MSI, Materials Science International Services GmbH, Stuttgart, 91 , 10.11188.2.1 (2022), httml/10.11188.2.1/Cr-Ni-Si Ternary Phase Diagram Evaluation
B-Fe-La	Kolchugina, N., Dobatkina, T., Dormidontov, N., Bakulina, A., "B-Fe-La Ternary Phase Diagram Evaluation", in <i>MSI Eureka</i> , Watson, A. (Ed.) by MSI, Materials Science International Services GmbH, Stuttgart, 92 , 10.13561.1.9 (2022), https://doi.org/10.7121/msi-eureka-10.13561.1.9
B-Cr-Ni	Bondar, A., Tymoshenko, O., "B-Cr-Ni Ternary Phase Diagram Evaluation", in <i>MSI Eureka</i> , Watson, A. (Ed.) by MSI, Materials Science International Services GmbH, Stuttgart, 91 , 10.19695.2.1 (2022), httml/10.19695.2.1/B-Cr-Ni_Ternary_Phase_Diagram_Evaluation
Al-O-Ti	Ilatovskaia, M., Kahrobaee, Z., Omar, N., Palm, M., Schmitt, L., Yang, Y., Dreval, L., "Al-O-Ti Ternary Phase Diagram Evaluation", in <i>MSI Eureka</i> , Watson, A. (Ed.) by MSI, Materials Science International Services GmbH, Stuttgart, 92 , 10.15250.2.9 (2022), https://doi.org/10.7121/msi-eureka-10.15250.2.9
Al-Fe-W	Stein, F., "Al-Fe-W Ternary Phase Diagram Evaluation", in <i>MSI Eureka</i> , Watson, A. (Ed.) by MSI, Materials Science International Services GmbH, Stuttgart, 94 , 10.19029.2.7 (2022), https://doi.org/10.7121/msi-eureka-10.19029.2.7
Al-Fe-Mo	Wang, J., Peng, J., Wang, C., "Al-Fe-Mo Ternary Phase Diagram Evaluation", in <i>MSI Eureka</i> , Watson, A. (Ed.) by MSI, Materials Science International Services GmbH, Stuttgart, 94 , 10.17959.3.7 (2022), https://doi.org/10.7121/msi-eureka-10.17959.3.7
Al-Fe-Hf	Stein, F., "Al-Fe-Hf Ternary Phase Diagram Evaluation", in <i>MSI Eureka</i> , Watson, A. (Ed.) by MSI, Materials Science International Services GmbH, Stuttgart, 94 , 10.15704.2.7 (2022), https://doi.org/10.7121/msi-eureka-10.15704.2.7

Co-Mn	"Co-Mn Phase Diagrams as Published", in <i>MSI Eureka</i> , Watson, A. (Ed.) by MSI, Materials Science International Services GmbH, Stuttgart, 91 , 30.12889.2.7 (2022), http://www.msi-eureka.com/full-html/30.12889.2.7/Co-Mn_Phase_Diagrams_as_Published
B-La	"B-La Phase Diagrams as Published", in <i>MSI Eureka</i> , Watson, A. (Ed.) by MSI, Materials Science International Services GmbH, Stuttgart, 92 , 30.14328.2.1 (2022), http://www.msi-eureka.com/full-html/30.14328.2.1/B-La_Phase_Diagrams_as_Published
Fe-La	"Fe-La Phase Diagrams as Published", in <i>MSI Eureka</i> , Watson, A. (Ed.) by MSI, Materials Science International Services GmbH, Stuttgart, 92 , 30.19641.1.0 (2022), http://www.msi-eureka.com/full-html/30.19641.1.0/Fe-La Phase Diagrams as Published
Cr-Si	"Cr-Si Phase Diagrams as Published", in <i>MSI Eureka</i> , Watson, A. (Ed.) by MSI, Materials Science International Services GmbH, Stuttgart, 94 , 30.19503.2.9 (2022), http://www.msi-eureka.com/full-html/30.19503.2.9/Cr-Si_Phase_Diagrams_as_Published
Cr-Ni	"Cr-Ni Phase Diagrams as Published", in <i>MSI Eureka</i> , Watson, A. (Ed.) by MSI, Materials Science International Services GmbH, Stuttgart, 94 , 30.12109.2.5 (2022), http://www.msi-eureka.com/full-html/30.12109.2.5/Cr-Ni_Phase_Diagrams_as_Published
B-Cr	"B-Cr Phase Diagrams as Published", in <i>MSI Eureka</i> , Watson, A. (Ed.) by MSI, Materials Science International Services GmbH, Stuttgart, 94 , 30.12220.2.9 (2022), http://www.msi-eureka.com/full-html/30.12220.2.9/B-Cr_Phase_Diagrams_as_Published
Hf-Pd	"Hf-Pd Phase Diagrams as Published", in <i>MSI Eureka</i> , Watson, A. (Ed.) by MSI, Materials Science International Services GmbH, Stuttgart, 96 , 30.29563.2.7 (2022), http://www.msi-eureka.com/full-html/30.29563.2.7/Hf-Pd Phase Diagrams as Published
Fe-Hf	"Fe-Hf Phase Diagrams as Published", in <i>MSI Eureka</i> , Watson, A. (Ed.) by MSI, Materials Science International Services GmbH, Stuttgart, 94 , 30.25405.2.9 (2022), http://www.msi-eureka.com/full-html/30.25405.2.9/Fe-Hf_Phase_Diagrams_as_Published
Sb-Sn	"Sb-Sn Phase Diagrams as Published", in <i>MSI Eureka</i> , Watson, A. (Ed.) by MSI, Materials Science International Services GmbH, Stuttgart, 94 , 30.22555.2.2 (2022), http://www.msi-eureka.com/full-html/30.22555.2.2/Sb-Sn_Phase_Diagrams_as_Published



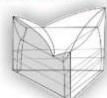
DATA ⇒ INFORMATION ⇒ KNOWLEDGE

Comprehensive platform for materials constitution data

Phase configurations &

Phase transformations with changing temperature, pressure, composition

- phase diagram information
- thermodynamics & kinetics
- crystal structure data
- morphology
- materials properties
- ideal resource of validated input data for Calphad & ab-initio simulations



Inorganic Materials:

Alloys (metals, steels, bronzes, magnets, implants, electronic materials,...& more) Non-metals (ceramics, sensors, semiconductors,... & more)

Composites (cermets, ceramic matrix composites, metal matrix composites & more)

Unary, binary, ternary & multicomponent systems, up to 15 components

Relevant for:

Engineering

Materials Science

Crystallography

Thermodynamics

Crystal growth

Materials design

Alloy development

Chemistry

Physics

Industrial engineering across multiple industries

"Phase diagrams are the beginning of wisdom -not the end of it."

-Sir William Hume-Rothery

MSI JURINA includes



MSIT Documents: full-text factual database on materials constitution Includes the following data categories: "Binary & Ternaty Evaluations", "Diagrams as Published", "Research Results", p-T-x Diagrams"

- · 4,630 critical evaluations of binary & ternary systems
- 4,296 extended extracts from literature "Reserach Results"
- · 16,340 phase diagrams and graphs
- · 10,220 tables, like Crystal Structures, Invariant Reactions, Thermodynamic Properties, Physical Properties, etc.

and continuously updated



Materials World Library "Links to Literature" bibliographic database focused on materials constitution

all materials systems are cross-linked with relevant publications, allows delivery of relevant search results only

benefit from the Materials Ontology approach and find similar materials with one click

- . 508,520 bibliographic entries on all inorganic materials ever published, related to
- 77,620 material systems
- coverage better than in large bibliogrpahic databases on the web
- · and continuously updated



www.msi-eureka.com/search





Find material properties by combining search criteria: elements + keywords

MSI Eureka is a one-stop platform that offers everything related to materials constitution: from exhaustive bibliography to high-quality evaluated phase diagrams.

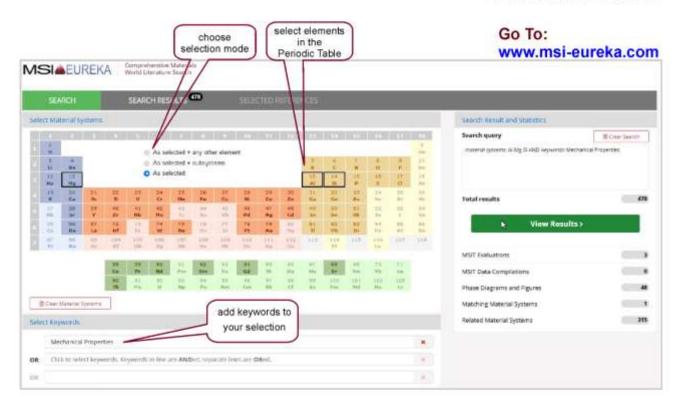
The new search interface brings together journal articles with material systems and many other sources of information, including conference proceedings, books, theses, case studies, reference handbooks and databases.

77,620 systems with 508,520* bibliographic citations link material systems and all thier publications, for each individual system!

The bibliographic database "Links to Literature" covers all relevant publications from 1830 up to the present, providing a valuable and constatntly growing information source.

The NEW search interface is <u>integral part of MSI Eureka</u> and free of charge for subscribers.

* as of Jan. 2023, continuously updated



Advantages of Literature Search in MSI Eureka



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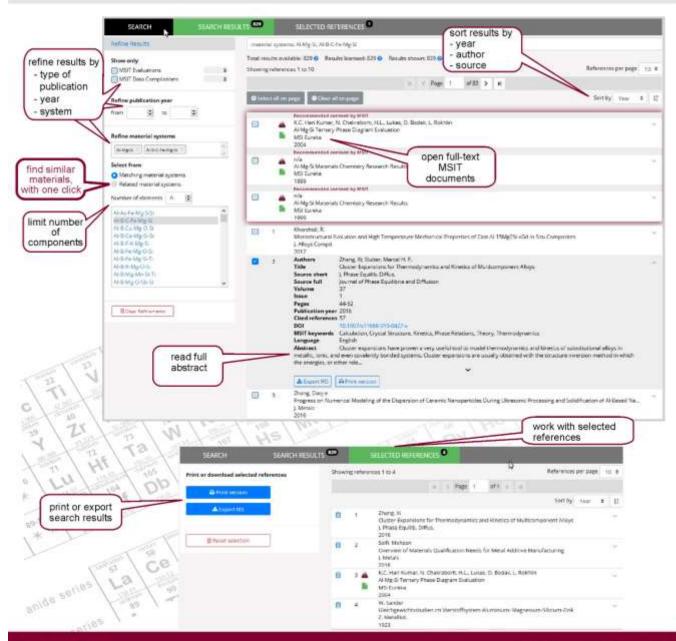
Find data, evaluated, validated and peer-reviewed by MSIT experts. Accessible and optimized for both desktop and mobile devices.

MSIT EVALUATIONS provide critical intellectual evaluations of all data on constitutional properties, phase equilibria, thermodynamic and crystallographic data. Critical evaluation means: where contradictory information is published, data and conclusions are compared and assessed, broken down into firm facts and re-interpreted in the light of all present knowledge.

MSIT Evaluation Reports discuss and settle up conflicting data and rationalize the choice of the most appropriate data sets. Evaluation Reports are authentic publications, peer reviewed under authorities of MSIT Editorial Board.

Reliable phase diagrams provide scientists and engineers with basic information of crucial importance for fundamental research and for the development and optimization of materials.

Evaluation Reports is an ideal source for computer-aided modeling & simulations, as an input of reliable validated data.



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 - · saving energy, resources and time, leads to efficient research strategies.
 - · multiple search criteria and advanced result refining options.
- Supplement and accelerate genomic approach for materials design and Integrated Computational Materials Engineering

Features

- Covers unary, binary, ternary and ...multi-component materials systems.
- Retrieves only relevant information, unlike other sources - no irrelevant search results!
- Largest number of critically evaluated <u>material systems</u>, over 4,630 - result of the only global Program on Evaluation of ConstitutionI Data - runned by MSIT® since 1984.
- Intuitive & specific search interface via periodic table.
 Extensive search functionalities, by elements, properties, authors, sources, etc.
- Best coverage of literature data on materials constitution, from 1830 - present, over 508,520 entries.
- · Comprehensive and continuously updated.

MSI Eureka is unique by

- Coverage
 - inorganic materials, ALL ever published
- > 77,6200 material systems
- > 508,520 entries / publications
- Unparalleled in depth and breadth at highest quality unlike others, MSIT Evaluation Reports are critically evaluated, and independently peer-reviewed by experts
- Extensive search possibilities highly effective search engine
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 registration to the annual MSIT School s on Materials
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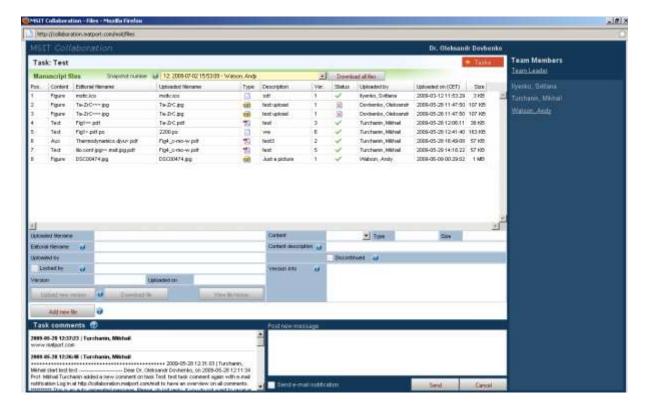


MSI Collaboration Tool

teams with features to track the growth of knowledge whilst working & publishing remotely within their joint projects. The IT system and operational know-how developed for collaborative work and management purposes in numerous MSIT projects, can be provided to the third parties projects. The Collaboration Tool continuously updates the current state of a project and retains all results accessible, also retrospectively. The current state of research in the entire project can be viewed by the project Management as well as by the external coordinators (if required), at any time and can be redefined if necessary. This allows the participants to focus entirely on the scientific work and to jointly produce publications, reports, plan experiments, etc.

It includes the following features:

- a. Purely web-based solution, no special client software required.
- b. Administration of the project-network by "Projects" and Tasks" (Task-e.g. subproject, topic, etc.)
- c. Defining different rights for participants according to missions in the project, e.g. "Task Leader", "Task Members", Reviewers, others.
- d. Allowing participants to develop collaboratively and update documents and research reports in all common formats from distributed locations. Such may be e.g. thermodynamic data files for simulation calculations, publications for journals, reports for the EU, parts of thesis, etc.
- e. Archiving of the collective state of knowledge in the project at the time Z. The tool keeps track of all files, comments and messages and how they belong together. It is the central access point for all co-workers involved in a task.
- f. Other collaboration features (lock files, discontinue, ...)
- g. Documenting **cross-project** collaborations!



MSI Graphics Editor

Phase diagrams for MSI Eureka are drawn by the MSIT authors using new software "MSI Graphics Editor", launched by MSI in 2010. The software is developed and designed for researchers and students to easily draw phase equilibria diagrams for binary and ternary systems, as well as other graphs, e.g. p-T, p-x, etc. A number of useful options and tools have been incorporated in this software based on the 36 year's experience of MSI in editing & publishing phase diagrams.

