

Materials Chemistry Committee Newsletter IOM3

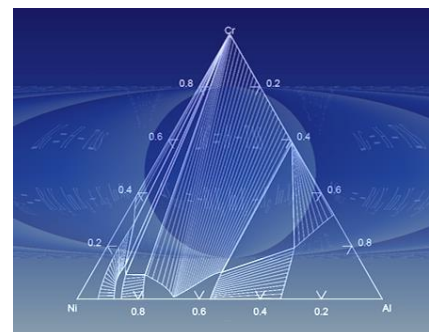
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www.iom3.org/materials-chemistry-committee

The Materials Chemistry Committee (MCC) is one of the 22 technical divisions and societies, groups and associations of Institute of Materials, Minerals and Mining (IOM3). Our aim is to provide UK industry and research organisations with consultancy and access to reliable up-to-date fundamental scientific information of phase equilibria and the thermodynamic properties of all classes of functional engineering materials, which plays a vital role in underpinning many spheres of materials science & technology.

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@MatChemComm

Chairman's chat

Welcome to the latest edition of the Newsletter from the *Materials Chemistry Committee* of the *IOM3*. First of all, I should apologise for us having missed the Spring edition this year, but the committee has been very busy organising this year's Hume-Rothery Seminar and also AToMS2019; conference reports appear below. We're already looking towards next year when we will be holding AToMS2020 at the University of Cambridge. We're very excited to be holding our conference alongside the summer meeting of the *Molten Salts and Ionic Liquids Discussion Group* of the *Royal Society of Chemistry*, and I'm sure that there will be plenty of interesting discussions taking place between the two groups during the coffee breaks and in the bar....

It's becoming a regular theme in our Newsletters sadly, where we report on the loss of friends and colleagues from our community. Both Greg Doughty and Günter Effenberg were well known to members of the MCC and will be sorely missed by friends and colleagues alike. Brief obituaries are given below.

As always, if you would prefer not to receive our Newsletters and wish to be removed from the mailing list, please drop a line to matsiom3chem@gmail.com with the subject line 'UNSUBSCRIBE NEWSLETTER'. Of course, we hope that you don't..... And if you feel that there's something that's not covered in the Newsletter, or if you have an item of news or an article you'd like to share with the community, let us know. We'd be pleased to hear from you.

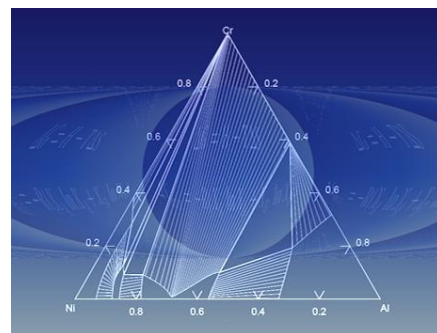
So, until next time, 'Be seeing you'

Andy

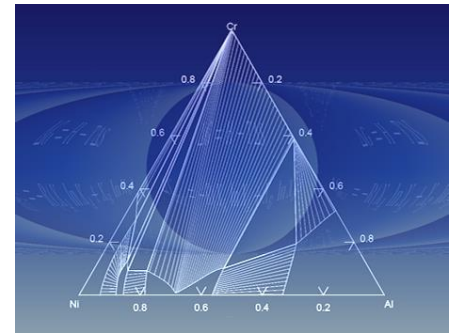
Obituaries

Greg Doughty – An appreciation

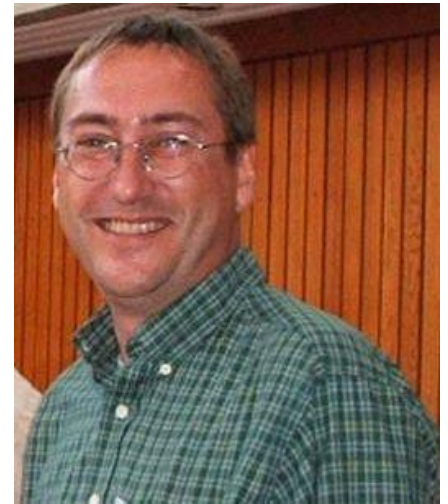
Greg Doughty made several major contributions to many areas of materials technology, not only in the UK but elsewhere in the world and, possibly in the future, even in outer space. He led a very interesting and extremely varied life which started in Truro, Cornwall in 1963 and progressed to the University of Leeds in Yorkshire, where he graduated in Materials Science and Engineering, followed by Ph.D in the same discipline and then to many places around the world. First, in Nova Scotia, where he worked on ceramic sensors



combining interesting science with practical applications. In 1991 he returned to the University of Leeds where he worked in the Wolfson Advanced Ceramics Unit solving industrial problems before moving 100 yards to undertake research on methods of adding sodium to molten metals, in particular, molten aluminium in the Department of Mining and Mineral Engineering. This was a project which involved interacting with scientists and engineers from all over Europe at which Greg excelled. The research group transferred to the Department of Materials Science and Metallurgy, University of Cambridge in 1996 where the work was successfully concluded.



In 1997, he joined Welding Alloys Ltd where he was in charge of product development which entailed creating a cored wire feeder in Baotou in the autonomous Chinese region of Inner Mongolia which must have been an interesting and demanding experience. After he and the team there had officially agreed the floor plan of the new facility, the team manager changed it secretly so that its geometry would fit in better with the Chinese lucky numbers. Greg of course somehow accommodated the new constraint and still completed the plant successfully. Apart from missing out on the relevance of lucky numbers for the future success of a plant, Greg was highly regarded there, because the staff working there had only ever heard of one university from abroad and that happened to be Cambridge!



Returning to the UK, for a quieter life, he joined British Titanium plc, a start-up company from the University of Cambridge, developing the FFC Cambridge Process for the extraction of titanium which entailed building furnaces that worked at the 10 kg scale. At this time, NASA was very interested in extracting oxygen from rocks on the moon and British Titanium plc won a contract to apply the FFC Cambridge Process to develop concepts for extra-terrestrial operation. As well as the scientific problems, the administration was a nightmare as NASA was not used to dealing with companies with only three staff. Greg dealt with this situation admirably as well as developing reactors that could function on the moon with engineers from NASA, University of Florida, Kennedy Space Center, Timet Inc., the US titanium company. At the end of the first year, NASA's view was that the project had exceeded expectations and had performed outstandingly well, all due to the efforts of Greg. Even today, the European Space Agency is still interested in the technology and it is featured in science fiction book, Artemis by Andy Weir which is about to be turned into a film by Twenty Century Fox so soon you will

be able to see Greg's work at your local cinema!! He also worked with Norsk Hydro developing the FFC Cambridge technology.

Greg was then employed for two small companies, Transition International Ltd, a ferrotitanium producer and Inertius Ltd developing inert anodes with the Light Metals Research Centre, Auckland University, New Zealand.

His last position was at Metalysis Ltd which he joined in 2010 and where he had a very major impact on the development of the FFC Cambridge Process for titanium and tantalum powders and alloys that are not readily made by any other process. He played a very significant part in the success of the company and rose to the position of Principal Scientist before retiring.

Greg was an active member of the scientific community being engaged with the Royal Society of Chemistry and the Materials Chemistry Committee of the Institute of Materials, Minerals & Mining. He was a longstanding member of the RSC's Molten Salts Discussion Group and served as secretary 2015 – 2017.

Greg was an ambitious hobby diver in his younger years and possessed the full diving gear. He liked outdoor activities in general and was always extremely fit and even, in February 2018, when he was visiting Oman he went out hiking in the nearby mountains that he so loved.

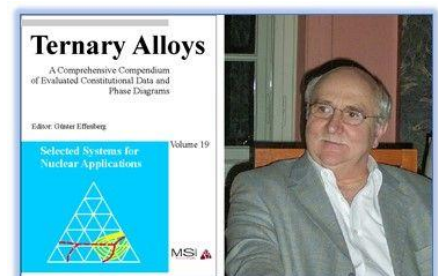
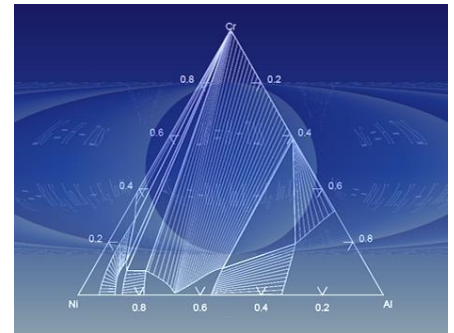
As well as contributing his considerable skills in science and technology, he was a great pleasure to work with as he was always calm, patient, honest, and extremely polite with an amazing ability to engage with people, irrespective of their position in life or nationality. He is considerable loss to the scientific community but his exceptional legacy will continue to endure into the future.

Derek Fray, March 2019

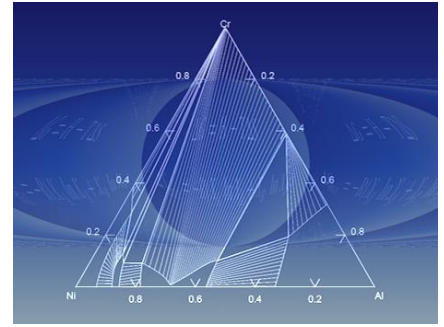
Remembering Günter Effenberg

It is with great sadness that we learned of the death of Guenter Effenberg, who was a great friend of many of the MCC for many years. Below is a tribute to him by his successor at Materials Services International, Svitlana Iljenko.

For nearly 35 years, Günter Effenberg and his Team of experts from around the world (the MSIT® <http://www.msiport.com/msit/msit/>) have been responsible for the publication of almost 60 books on



phase diagrams and the electronic platform MSI Eureka <https://search.msi-eureka.com/search>, which has become one of the outstanding information resources on materials constitution in the world. The success of the MSIT is really due to one man, without whom none of this great work would have been possible. Günter has almost single-handedly promoted and kept alive the field of phase constitution study (in particular in Europe) through the compilation, editorship and publication of phase diagram compendia.



The beginning of his tremendous life's work was the publication of the phase diagram compendium 'Ternary Alloys'. Recently, still jointly with Günter, MSI started preparing Volume 19 in this series, "Selected Systems for Nuclear Applications". We will complete the volume without Günter and will dedicate it to his memory, to honor his life's work, his passion for phase diagrams and for books - the roots of his life-long activity.

We all at MSI and MSIT are fortunate to have worked closely with Günter for many years and to be counted among his friends.

His visions will live on in the effort put forth by his Team.

Born in Hausen, Bavaria on 10.09.1945, Dr. Günter Effenberg was a physicist - engaged in Materials Science - since his thesis was undertaken at the RWTH Aachen / University of Sheffield.

Subsequently he served in a number of positions,

- At the RWTH Aachen
- As scientific advisor to the Joint Research Center of the European Union, Petten, Netherlands.
- At the Max-Planck-Institute for Metals Research, Stuttgart
- As chairman of APDIC (He is one of the founding members of APDIC, The Alloy Phase Diagram International Commission)
- As chairman of the European Awards Committee of ASM International
- As CEO of MSI - Materials Science International Services GmbH - from 1989 until 2019.

In 2012 he has been awarded the Hume-Rothery prize by the IOM3, London.

In 2014 he has received an Honorary Doctor Degree from the Frantsevich Institute for Problems of Materials Science (FIPMS) of the National Academy of Science of Ukraine.

Dr. Svitlana Iljenko

MSI, Materials Science International Services, GmbH

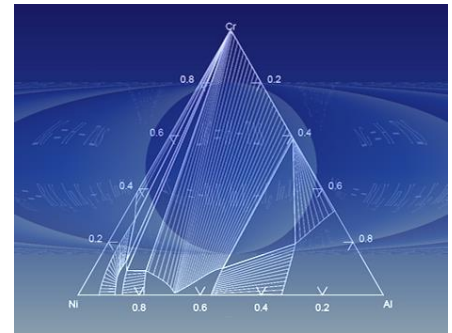
Stuttgart

Germany

Member profile

Dr. Kathy Christofidou joined the committee in August 2018. In September 2019, she joined the Department of Materials Science and Engineering at The University of Sheffield as a Lecturer in Metallurgy. Prior to this role, she held roles at the University Cambridge, as part of the Rolls-Royce University Technology Centre, and the University of Manchester, where she also worked in close collaboration with the Henry Royce Institute for Advanced Materials. She holds a PhD in Metallurgy from the University of Cambridge and MEng in Aerospace Materials Engineering from Imperial College London.

Her research focuses on multiple facets of high temperature physical metallurgy, alloy design and manufacturing. As part of her collaboration with Rolls-Royce plc, she has developed new polycrystalline Ni-based superalloys for turbine disc applications, as well as exploring strategies for the design of high temperature materials amenable to laser-based additive layer manufacturing. CALPHAD and thermodynamic-based approaches form a critical part of the alloy development and microstructure design methodologies she utilizes. In addition, a major area of her research interests is that of high entropy alloys and the possibilities that these materials offer for expanding our understanding of physical metallurgy beyond a single base element, the associated thermodynamic principles governing this behavior and how these may be used to further improve predictions.



News

Committee News

First of all, many congratulations to Duncan Gregory (University of Glasgow) on receiving the 2019 Kroll medal and prize. A relative newcomer to the committee, the award was presented at one of our committee meetings at IOM3 HQ.

Congratulations are also extended to Kathy Christofidou who has recently taken a lectureship in the Department of Materials Science and Engineering at the University of Sheffield. Following a brief stint at the University of Manchester, she decided to come over to the eastern side of the Pennines. The committee now boasts three members from Sheffield.

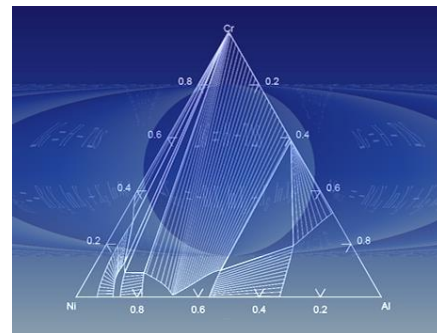
New members

The Materials Chemistry Committee continues to grow with the arrival of 5 new members since the summer of 2018. Richard Longbottom, recruited at AToMS2018 works at British Steel in Scunthorpe and is a useful addition to our group from Industry, something that we are very keen to foster. Two new members join us from the University of Manchester; Ed Pickering and Pratheek Shanthraj. Ed is an experimentalist - something of a rarity these days and Pratheek's interests lie in Phase Field and coupled chemo-thermo-mechanics. The most recent additions to the fold are Lewis Owen from the Department of Materials Science and Metallurgy at the University of Cambridge, and Simon Middleburgh from Bangor University.

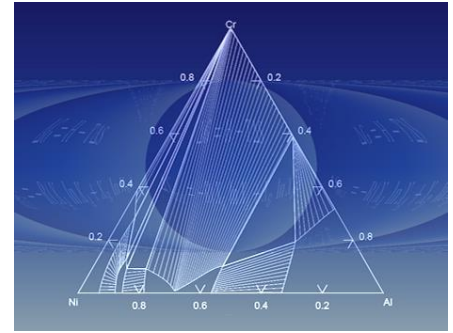
That brings our number of active members up to 21, from both Industry and academia, covering all types of different materials and aspects of materials chemistry.

Hume-Rothery Seminar 2019

The second Hume-Rothery seminar was held on the 12th and 13th of February, again at the Riverside Centre in Derby. As before, we are indebted to the staff of the Centre for making us welcome, and I'm sure that there will be more visits in the future. As the first seminar was such a success we decided to keep the format for the second meeting, inviting SGTE to run day two.



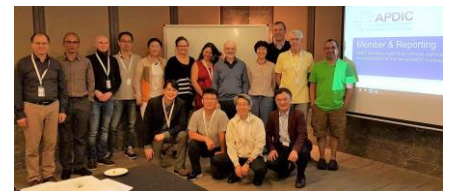
The philosophy behind the seminar is quite different from that of a research conference. The seminar is more a teaching and demonstration event where people can come to learn about phase equilibria and thermodynamics, from the very basics to how the latest powerful software for computational thermodynamics can address a number of industrial problems in material design, processing and application. Day 1 was split into morning and afternoon sessions with presentations given by MCC members and also invited from industry. The morning session dealt with basic concepts and techniques relating to phase diagrams and thermodynamics - experimental techniques, calculation of phase equilibria and use of density function theory. The afternoon session was more application based - Lighting infrastructure and materials, solidification, solid state manufacture of high-entropy alloys, and the MCC gratefully acknowledges the contributions from Allan Howard of WSP and Mike Ellis from Metalysis. For the first time, Day 1 also included a virtual lecture live from Bangalore, India from the 2018 Hume-Rothery Award winner Prof. Tom Jacob of the Indian Institute of Science in Bangalore, India, which was received well by the attendees. The program for Day 2 was run by SGTE and focused on demonstrative presentations from three of the main thermodynamic modelling software providers; Thermo-Calc Software, MTDATA (Hampton Thermodynamics) and FactSage-Simusage (GTT Technologies).



As with the inaugural Hume-Rothery Seminar in 2017, the seminar was attended from representatives from both academia and industry, with a large fraction of attendees being early career researchers (PhD students, Postdocs and junior researchers). The large proportion of early career representation at the seminar further highlights the need for a holistic approach to training researchers on the use of thermodynamics, thermodynamic modelling tools as well as the necessary experimental processes required for the development of databases.

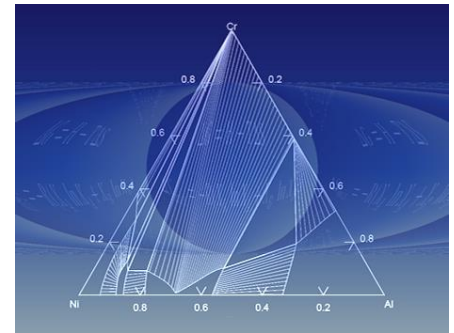
APDIC News

The 2019 APDIC meeting was held immediately following Calphad XLVIII, which was held in Singapore in June. Three new representatives joined APDIC at this meeting. *Dr. Silvana Sommadossi* of the Universidad Nacional de Comahue representing Argentina, *Prof Malin Selleby* of KTH Stockholm representing Sweden, and *Prof Hari Kumar* representing IIT, Madras, India. In addition, the APDIC best paper award was presented at the Calphad dinner, the



recipients being P. Sauerschnig, A. Grytsiv, J. Vrestal, V.V. Romaka, B. Smetana, G. Giester, E. Bauer and P. Rogl for their paper on *The constitution and thermodynamic modelling of the system Zr-Ni-Sn*, which appeared in the Journal of Alloys and Compounds. Details are given on the APDIC website <http://www.apdic.info/>

The next APDIC meeting will take place following Calphad XLIX, which will take place in Sweden next year.



MSDG News

MSDG re-named MSILDG

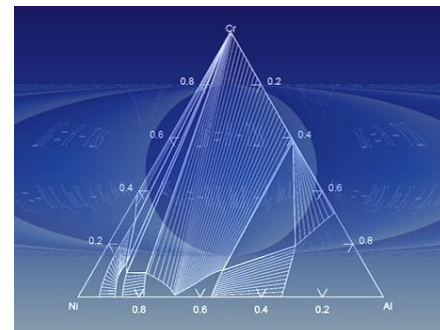
Following approval from the Royal Society of Chemistry, the Molten Salts Discussion Group (MSDG) has become the Molten Salts & Ionic Liquids Discussion Group (MSILDG). The first meeting of the newly named group was held at Churchill College, Cambridge, in August. The event opened with the 2nd Fray Lecture presented by Donald Sadoway (MIT) who gave a fascinating and wide ranging insight into the way materials chemistry has, and will continue to, address the demand for electricity, particularly the need to improve ways to store electrical energy. The first evening's social event was kindly sponsored by GLABAT to celebrate the 20th anniversary of the publication of the patent describing the FFC Cambridge Process. After a full second day of contributed papers and posters, the banquet was followed by Duncan Bruce's (University of York) overview of ionic liquids chemistry. The third day saw the inaugural MSILDG lecture delivered by Tom Welton (Imperial College) who gave a detailed account of the solvation properties of ionic liquids. The meeting concluded with a discussion, led by George Chen (University of Nottingham, Ningbo), on the history and future for the FFC Cambridge Process. Churchill College proved to be an excellent venue for this short conference with modern facilities and accommodation supported by friendly and cooperative staff.

AToMS 2019

The 2nd Annual Thermodynamics of Materials Symposium (AToMS 2019) was held on the 4th July at University of Birmingham. The aim of the meeting was to showcase research on thermodynamics and phase equilibria in the UK and further afield, and to build a strong network in this area. The meeting was organised by Dr Claire Utton, Dr Hajime Kinoshita and Dr Kathy Christofidou (Uni. Sheffield), Prof. Andy Watson (Uni. Coventry), Dr Howard Stone (Uni. Cambridge) and Dr Nils Warnken (Uni. Birmingham). We welcomed around 40



participants to the meeting. We had the great pleasure of hosting the IOM3 2019 Hume Rothery prize-winner, Dr Suzana Fries as the keynote speaker, who gave the opening talk titled The Grey Matter of Gibbs Energy Sets for Materials. A full list of the presentations and abstracts are available on the MCC IOM3 microsite.



AToMS 2020 will be held at Churchill College, Cambridge on 23rd July. The conference will take place in parallel with the 2020 Summer Research Meeting of the Royal Society of Chemistry Molten Salt and Ionic Liquids discussion group. Further info on this event will be available later in the year.

The sponsors of AToMS 2019 were Thermo-Calc Software, Netzsch and GTT-Technologies.

Awards

Hume-Rothery Prize 2019

Dr. Suzana G. Fries has been awarded the 2019 Hume-Rothery Prize in recognition of distinguished achievements concerned with phase relationships in metallic materials or non metallic materials of metallurgical interest.

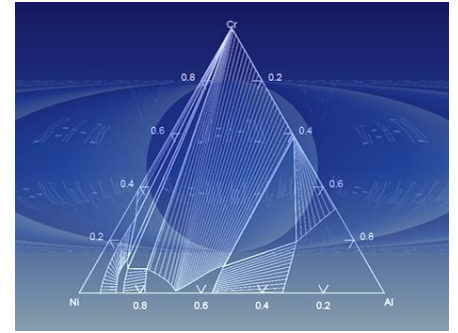
Suzana G. Fries was born in Brasil in 1953. She received her Bachelor in Physics degree in 1975 from the Federal University of Rio Grande do Sul in Porto Alegre, Brazil. Following her Master in Physics degree, she received her Doctor in Science degree in 1985, and by the age of 30, had already become Professor.

Whilst at the Max Planck Institute in Stuttgart, Suzana learned about modelling phase stability to extend the range of her studies, working closely with Hans Leo Lukas (winner of the Hume-Rothery prize in 1993). Together, they wrote the book entitled "Computational Thermodynamics: the Calphad Method" published in 2007 by Cambridge University Press. A special book that collected Dr. Lukas's long experience in the field, combined with Suzana's knowledge on solid state physics, and as third author, Bo Sundman (Hume-Rothery prize winner, 2005), who was then in the Materials Science Department at KTH, Stockholm, and was the main driving force behind Thermo-Calc, arguably the most used software for Computational Thermodynamics today.

One of the most remarkable achievements of Dr. Fries has been to show the importance of crystallography in thermodynamic



modelling. She has also been a pioneer in the use of first-principles calculations for complex phases with many sublattices. Suzana has also been involved in the transfer of thermodynamic data to microstructure simulations using the phase field approach. She was instrumental in showing the importance of bringing more 'physics' into Calphad, to reduce the inherent empirical nature of the technique.



The result of Suzana's influence is a community of experimentalists, materials scientists and physicists that now share a common language that has been able to unleash the true predictive nature of Computational Thermodynamics for the design of new materials and process control. She has published extensively (more than 120 publications in peer-reviewed journals) and is a regular attendee of the annual Calphad conference and Thermodynamics of Alloys, and also at other more application-based meetings such as those concerning Superalloys. She has given around 40 invited lectures and in the region of 60 conference presentations.

Suzana is never still. She works with scientists all over the world. She is in demand as a teacher and as an invited lecturer. It could be said that there is no one in the Calphad community that does not know Suzana or her work. For her lifelong dedication to Computational Thermodynamics, This prize comes as a recognition for her impact on the field and the debt of gratitude that she is owed by the entire Calphad community.

Acknowledgement

Photograph of Late Dr. Gregory Doughty was kindly supplied by Professor George Chen, University of Nottingham.

Conference announcements

1. 34th Annual MSIT meeting and 4th MSIT Winter School on Materials Chemistry - Schloss Ringberg, Germany, 16-21/2/20
<http://www.msiport.com/msit/msit/next-msit-meeting/>
2020 sees the 34th annual 'Ringberg Meeting' of the MSIT, the global team of Materials Scientists responsible for compendia such as Ternary Alloys' and the 'Phase Equilibria of Ternary Alloys' published for Landolt-Börnstein. In addition, running in parallel to the evaluation work will be the 4th Winter School on Materials Chemistry. The aim of the Winter School is to teach the 'students' how to evaluate experimental information with a view to carrying out a Calphad Optimisation of a binary alloy system. The School was very popular

last year, so much so that the accommodation at the Castle was fully booked some of the participants had to 'decamp' to hotels in town.

2. Calphad (XLIX) May 24-29, 2020, Tallberg in Dalarna, Sweden
<https://calphad-conference.org/calphad-2020-home>

The Calphad conferences go from strength to strength, visiting Sweden for the first time since 2002.

3. AToMS2020 - July 23rd 2020 - Churchill College, University of Cambridge. In parallel with the summer meeting of the Molten Salts and Ionic Liquids Discussion Group of the Royal Society of Chemistry (22-23 July 2020).

Our very own AToMS meeting, for the first time being held in parallel with another in order to allow discussions between both groups.

4. Moscow, 5-19 July 2020 - XVI INTERNATIONAL CONFERENCE ON THERMAL ANALYSIS and CALORIMETRY in RUSSIA (RTAC-2020)

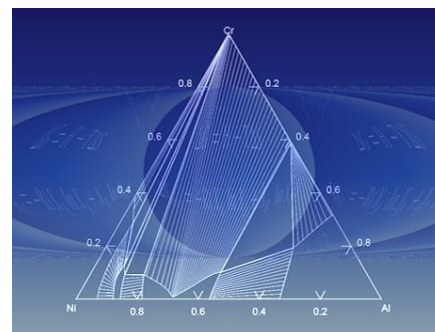
5. 17th Discussion Meeting on the Thermodynamics of Alloys (TOFA 2020), 28 September – 2 October 2020 • Bad Staffelstein, Germany.
<https://www.tofa2020.de/>

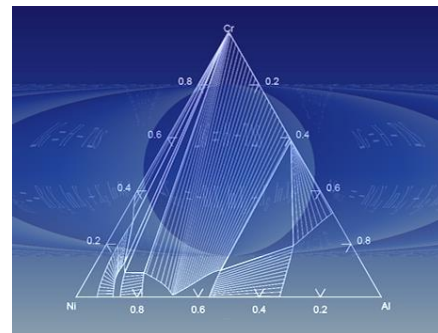
The biennial TOFA conference.

6. TMS2020 - Hume-Rothery Symposium: Thermodynamics, Phase Equilibria and Kinetics for Materials Design and Engineering, honoring Ursula Kattner (current APDIC chair) with the TMS Hume-Rothery prize.

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