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.

Chairman’s chat

Welcome to this, the 3rd Newsletter of the Materials Chemistry Committee of the IOM3; I hope that you will find it of interest. Our aim is to keep you informed of developments within the Materials Chemistry Committee and in Materials Chemistry as a whole. The Newsletter is just one of a number of new initiatives that we are undertaking in order to enable us to communicate with our community more effectively. We have the Materials Chemistry Committee website of course, which is where you will have found this Newsletter. We are populating that with useful resources for those with an interest in the Phase Diagrams and Thermodynamics of Materials. We already have a LinkedIn group (Chemical
Thermodynamics of Materials), and if you have not already done so, I invite you to join. We also plan to have a Twitter feed in the near future too. Of course, we have our first research meeting to look forward to, 'AToMS2018', details of which you will find at the end of this Newsletter. I do hope to see you there. In addition, we hope to repeat our successful Hume-Rothery seminar in 2019 too...details in the next edition of the Newsletter.

Feel free to pass on this Newsletter to your colleagues, and why not ask them to subscribe by contacting us using the email address above? The Newsletter is still evolving and I would expect that the content will increase over time. I want you to see this as your Newsletter, so please feel free to let us know what you think about it, what we should include, what we shouldn’t.

If you have any suggestions or comments regarding Newsletter content, please let us know by emailing to matsiom3chem@gmail.com. We want you as the reader to feel that it is your Newsletter as well as ours and should be shaped to represent our interests.

Be seeing you,

Andy Watson, Chair MCC

Member profile

Dr David Parfitt joined the committee in October 2017. He is currently a senior lecturer at Coventry University in the Faculty of Engineering, Environment and Computing. Before joining Coventry, he worked for the Materials, Chemistry and Corrosion Department at Rolls-Royce and prior to that he was a postdoctoral research associate at Imperial College London.

Dave has a wide range of research interests in energy materials, particularly the chemistry of lithium-ion batteries and solid-oxide fuel cells, but also in long term irradiation effects on nuclear components including fuels, cladding and steel pressure vessels. Most of his work focuses on using atomic scale simulations to predict the performance of these materials especially where we can use these simulations to better understand experimental data.

As well as his research, Dave also teaches a wide range of undergraduate and postgraduate courses on materials and...
manufacturing engineering in Coventry and is always interested to hear about applications of materials chemistry that can be used in these courses.

**News**

**Committee News**

The *Materials Chemistry Committee* has a new member. We are pleased to welcome Steve Pagden, who joined us at the end of 2017. Steve works at Heraeus Electro-Nite in Chesterfield and has a special interest in the manufacture of sensors for use in molten iron and steel making. Steve, along with Stuart Mucklejohn (Ceravision Ltd) and Duncan Putman (Rolls Royce Plc), bring a much-needed experience and appreciation of the Industrial environment to the committee.

We are pleased to announce that one of our members, Mudith Karunaratne, has recently taken the post of Senior Lecturer in the Department of Materials Engineering at the Sri Lanka Institute of Information Technology. Mudith worked for many years at Loughborough University before returning to his native Sri Lanka in the summer of 2017. As a very active member of the MCC in the past, we are pleased that he wishes to continue his association with us, even if from a distance.

We would also like to congratulate Michael J. Rushton in his new position at Bangor University. Michael has been a valued member of the MCC for several years whilst at Imperial College. We wish him well in his new post.

**APDIC News**

The 6th APDIC World Round-robin Seminar on ‘Phase Diagrams as a Tool for Efficient Materials Design’ was held at Schloss Ringberg in the beautiful Bavarian Alps, from the 11th-14th of February ([http://www.msiport.com/msit-school/next-msit-school-wrs/](http://www.msiport.com/msit-school/next-msit-school-wrs/)). This formed the 2nd MSIT Winter School on Materials Chemistry, a new initiative by MSI in Germany to train young Materials Scientists (and not so young) all aspects of Phase Equilibria and associated subjects. The seminar was organised by Günter Effenberg of MSI, Prof Hans-Jürgen Seifert of KIT, Germany and Andy Watson from the MCC (and Coventry University), comprising three days of lectures given by experts in their respective fields covering topics such as Classical Thermodynamics, Crystallography, the construction and
understanding of Phase Diagrams, Computational Thermodynamics and Experimental Techniques. A Significant part of the meeting was devoted to the application of phase diagrams and Computational Thermodynamics, and Dr. Claire Utton of the MCC (and the University of Sheffield) gave an invited talk on ‘New Materials for Aero Engines.’ Other contributors came from The University of Witwatersrand (South Africa), GTT Technologies, MPI Dusseldorf and T.U. Clausthal (Germany), The University of Vienna (Austria) and IIT Madras India. The seminar was designed in such a way that it was assumed that students had little prior knowledge of the subject. Following the seminar, students were invited to join the Annual Workshop on Heterogeneous Multicomponent Equilibria, which was running in parallel to the seminar, for the remainder of the week. The APDIC WRRS generally runs biennially, but the MSIT Winter School should be back at Ringberg in early 2019.
**MSDG News**

Molten Salts Discussion Group Summer Meeting, 24 to 26 July 2018, Cambridge

The MSDG Summer Meeting, to be held in Downing College, will feature the inaugural Fray Lecture when Professor Derek Fray FRS will deliver an overview of his recent research and outline some suggestions for the next generation of scientists and engineers to tackle. The Fray Lecture will be held annually and will complement the Inman Lecture which now forms an integral part of the MSDG Christmas Meeting. Professor Tom Welton from Imperial College will be after dinner speaker. Details of abstract submission and registration are available from the MSDG website (www.msdg.uk).

**Obituaries**

David Godfrey Pettifor : 9 March 1945 - 16 October 2017

David Pettifor was one of the pioneers in the use of DFT ab initio calculations to calculate the thermodynamic properties of elements and compounds in various crystal structures. As a result he was involved in CALPHAD at its outset where he saw clearly how his interests overlapped directly with those of us who were trying to describe the variation of thermodynamic properties of different phases with composition and temperature. His insights into the apparent contradiction between theoretical values and our CALPHAD values for the “lattice stabilities” – the difference in Gibbs energies between two phases of an element – proved invaluable. His early work concerned the systematic change in crystal structures of non-magnetic transition metals along the second and third long rows of the Periodic Table.

David was a great communicator, one of those people who could make a complex subject seem very simple when you talked to him. In a sense this showed his ability, to identify the key nature of a problem and present the solution in a simple, easy to understand way. The best example of this is in terms of “structure maps” for which he probably best known. These are diagrams which clearly identify which combination of elements form particular crystal structures and have been a great bonus for material scientists trying to design alloys.
David spent most of his career at Imperial College, London or as the Isaac Wolfson Professor in the Department of Materials in the University of Oxford where he was instrumental in the establishment of a materials modelling laboratory to model the properties of materials across length and time scales. His outstanding scientific work was recognised through the award of a CBE in the Queen’s Birthday Honours in 2005 and other prestigious awards including the Hume-Rothery Prize of the Institute of Materials in 1990.

His untimely death towards the end of last year from multiple myeloma represents a great loss to the materials community in UK and internationally.

Hans Leo Lukas

It is with great sadness that we inform you that Leo Lukas passed away on the 22nd of October this year. Leo is probably most well-known for his software for the optimisation of thermodynamic parameters in the assessment of phase diagrams. His pioneering work in the 1970s led to BINGSS and TERGSS; computer programs for the optimisation of binary and ternary systems. Many people in the Calphad community performed their first optimisations using Leo's software, and for them, the programs will be the gold standard against which all other software for Computational Thermodynamics will be compared. But it was because of the generous nature of the man that he made his software freely available to those who wished to use it. Moreover, he was more than happy to make changes or additions to the code on the suggestion of anyone that used it.
Leo was a member of the MSIT at the very start of the programme, way back in 1986, attending the first Ringberg meeting, and he made a significant contribution to the development of the MSIT standards for critical intellectual evaluation of constitutional data, and of course, a regular contributor to the Ternary Alloys series. As a member of the MSIT Board, Leo was always very helpful in solving scientific disputes between authors and reviewers, which was of great help to the editorial office. Leo was a 'gentle giant' of a man. Very softly spoken but with a razor-sharp mind. He would ponder a problem or a question quietly for quite a few moments, before giving the perfect solution.

Leo came from that generation that was active in the 'Golden Years' of in the 70s and 80s. When collaboration was 'King' and people exchanged ideas and computer software all for the advancement of science. Sadly, with the advent marketing departments and sales targets those days are gone, and there are not many of the 'Golden Generation' left; and we owe them all so much. Leo will be missed by the whole 'Phase Diagram and Thermodynamics' community, but not more than those that worked with him, especially his many students.

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Conference Announcements

1st Annual Thermodynamics of Materials Symposium (AToMS2018)

Call for Abstracts

We are pleased to announce we are now calling for abstracts for the 1st Annual Thermodynamics of Materials Symposium (AToMS2018) at the University of Sheffield on the 26th June 2018. This one day meeting will bring together people working in the areas of phase equilibria and thermodynamics and associated fields. The aims of the meeting are to discuss current research (both experimental and computational) and to develop a UK network of scholars and practitioners with an interest in phase equilibria and thermodynamics.
Oral and poster contributions from participants are invited. Topics include, but are not limited to:

- Experimental phase equilibria, thermodynamics and kinetics
- Thermodynamic and diffusion modelling
- Ab-initio (first-principles) calculations
- CALPHAD assessments and database development
- Applications of phase equilibria and thermodynamics in materials science, chemistry and geology

Closing date for abstract submission has been extended to the 13th April 2018.

Full details on registration and abstract submission can be found on the IOM3 conference website.

https://www.iom3online.org/atoms2018

This conference is jointly organised by the IOM3 Materials Chemistry Committee and the University of Sheffield and sponsored by CALPHAD Inc, Thermo-Calc Software and Netzsch.

Organising committee:

Dr Claire Utton, University of Sheffield (Chair)

Dr Hajime Kinoshita, University of Sheffield

Prof. Andy Watson, University of Coventry

Dr Nils Warnken, University of Birmingham

Dr Howard Stone, University of Cambridge
Call for abstracts – submit by 13th April 2018

**AToMS 2018**

Annual Thermodynamics of Materials Symposium 2018

At ‘The Edge’, The University of Sheffield, 26 June 2018

An annual one day meeting for UK materials community working in phase equilibria and thermodynamics to discuss the state-of-the-art research, develop networks and initiate new collaboration. The meeting is organised by the Materials Chemistry Committee of IOM3.

Abstracts are invited for oral and poster contributions on:

- Experimental phase equilibria, thermodynamics and kinetics
- Ab initio (first principles) calculations
- CaLphad assessments and database development
- Applications of phase equilibria and thermodynamics in Materials Science, Chemistry and Geology

Abstract deadline 13th April 2018

Bursaries available for Students.

Contact: Dr Claire Utton
c.utton@sheffield.ac.uk
+44 (0)114 215 7099

To register or submit an abstract go to: [https://www.iom3online.org/atoms2018](https://www.iom3online.org/atoms2018)

“Underpinning Phase Equilibria is crucial to successful materials design, processing, and application. It is key to understanding materials behaviour”

Prof. Andy Watson, Chair, IOM3 Materials Chemistry Committee
38th Cement and Concrete Science Conference

First announcement and call for abstracts
The Institute of Materials Minerals and Mining annual cement and concrete science meeting will be held this year at Coventry University, in the Faculty of Engineering, Environment and Computing building.

Abstracts are invited for presentations and posters to be received by Monday 2 April 2018 by email to: 38ccs@coventry.ac.uk

Date and timing:
Monday 10 and Tuesday 11 September 2018

Venue:
EEC Building, Coventry University

More details:
Further details of the event will be announced on the conference web page: www.coventry.ac.uk/38ccs
Further to the article in the September edition, the program for the 16th International Symposium on the Science & Technology of lighting (LS16) is nearly complete. In the opening lecture on Sunday 17 June Ian Tutt will present his talk describing the history and development of lighthouses. A list of the plenary and invited speakers is posted on the symposium website (www.ls16.org) together with the topics covered and details of registration and social events. The deadline for the submission of abstracts is 08 May and the closing date for the discounted registration rates in 10 May.