



**IUPAC**

International Union of Pure and Applied Chemistry

## Inorganic Chemistry Division (II) Newsletter 2009 (b)

**Editors Note:** The 2009 Glasgow General Assembly has passed and it's already getting towards the end of 2009 so that means it's time for another Division II newsletter. Due to my earlier than planned move to the Presidency of Div II (see below) in 2010, this may well be my last newsletter as editor and I am now looking for a volunteer to take over for 2010. If you are interested please let me know. Many thanks to those who have provided photos and news items for the newsletter – it's your input that helps make the newsletter what it is. In the mean time if you have an item or images about any of the Division members or associated activities, please forward these to me, preferable via email. ([r.loss@curtin.edu.au](mailto:r.loss@curtin.edu.au)). All the best, from Bob Loss.

### Division II People (2010-11)

**President:** Loss, Robert D., **Vice President:** Reedijk, Jan, **Secretary:** Interrante, Leonard V.

**Past President:** Tatsumi, K.

**Titular members:** Ding, Tiping, Holden, Norman E., Garcia-Martinez, J., Pavel, K., Sakai, K, Mathur, S.

**Associate members:** Basova, Tamara V., Coplen, Ty, Drabik, Milan, Liu, Leskelä, M., Ling-Kang, Öhrström, L. R.

**National representatives:** Bologna Alles, A., Chadwick, A. V., Chandrasekhar, V., Gonfiantini, R., Dasgupta, T., Yoon, K., Goh Lai-Yoong, Kilic, A., Hossain Tarafder, T.

### Division II Subcommittees and Commissions

Subcommittee on Isotopic Abundance Measurements

Subcommittee on Characterization of Carbonaceous Materials and New Carbons

Interdivisional Subcommittee on Materials Chemistry

Commission on Isotopic Abundance and Atomic Weights

### Election/Membership news

Congratulations to current Division II President, Professor Kaz Tatsumi, on his election to the Presidency of IUPAC during the recent General Assembly. Together with former President Prof Sean Corish, as current IUPAC Treasurer, we can now say that Div II has excellent representation at the highest levels of IUPAC! Kaz also becomes Div II Past President.



*From left, Incoming VP Reedijk, TM Suh, incoming IUPAC President and Naomi Tatsumi*

The Div II President vacancy created by the incoming IUPAC President Tatsumi has been filled by the editor, which in turn has created a vacancy for Div II Vice-presidency.

Following a recent election, Division II Titular Members elected Professor Jan Reedijk as Division II Vice President and President Elect of Division II for the term 2010 - 2013. Jan already has a long involvement with IUPAC and I'm, sure you will agree that Jan will continue to serve us, and IUPAC well.

Ty Coplen has also agreed to fill the remaining vacancy as Associate Member for a 2 year.

### Meetings and conferences

#### **International Symposium on Novel Materials and Their Synthesis (NMS-V)**

18-22 October, 2009, Fudan University, Shanghai, China; (<http://www.nms-iupac.org/>)

#### **High Temperature Materials Chemistry Conference (HTMC-13),**

14-18 September 2009, Davis, California, USA.

#### **Division II off year meeting.**

13 – 14 October 2010, Kyushu University, Fukuoka, Japan.

## IUPAC 46th General Assembly and Congress, "Chemistry Bridging Innovation Among the Americas and the World"

August 2011, San Juan, Puerto Rico

### Report on IUPAC-sponsored Conference on Solid State Chemistry (SSC 2008) and notice of SSC2010. Bratislava, Slovakia

The eighth conference in the series since 1986, was held over 6–11 July 2008 and focused on a range of solid-state and materials chemistry.

The invited lectures, together with a number of influential papers are published in the special issue of *PAC* - Vol. 81, No. 8 (2009) with each covering a key conference topic, including the lecture by Prof. P. Day on the Defining materials chemistry (cf. also the IUPAC Technical Report, doi: 10.1351/PAC-REP-09-03-02). This publication should become an excellent base for discussions and future developments in the field.

Over 200 participants from 29 countries representing Europe, Asia, the Americas, and Africa attended the conference and presented 18 invited talks, 73 lectures, and 146 posters.

The conference continues to provide a friendly atmosphere for the exchange of new results and ideas among groups active in different areas of solid state and materials chemistry.

The 9th Conference on Solid State Chemistry will be held in mid-September 2010 in Prague, Czech Republic. A Web page containing an online "expression of interest" form is already active < [www.ssc2010.cz](http://www.ssc2010.cz) >. As in previous years, the aim of the meeting is to have an interdisciplinary discussion with "contact points" in chemical materials and their integrated description. Yet the organizers got 100 preliminary registrations from the entire world.

We look forward to meeting the solid-state and materials chemistry community again at this conference.

**Milan Drábik**, [Milan.Drabik@savba.sk](mailto:Milan.Drabik@savba.sk)

SSC 2008 Conference Editor

**Tomáš Grygar**, [grygar@iic.cas.cz](mailto:grygar@iic.cas.cz)

SSC 2010 Conference Scientific Secretary

### 2009 CIAAW and SIAM Meetings and workshops

The International Commission on Isotopic Abundances and Atomic Weights (CIAAW) and its major working subcommittees met in Vienna over the period 23 – 30 July 2009 to evaluate isotopic data and atomic weights for the 2007 – 2009 period.

The Meetings were held at the impressive Vienna International Centre IAEA facilities hosted by CIAAW titular member Manfred Groening, and CIAAW would like to thank Manfred for arranging such a user-friendly facility and smooth program.



IAEA CIAAW Meeting Venue

A major outcome of these meetings and workshops was the recommendation that a number of naturally variable Atomic Weights be represented as a range rather than a value with an associated uncertainty. A new evaluated Table of Isotopic Compositions of the elements (TICE) was also determined and is currently being prepared for publication.



Over the weekend CIAAW participants were able to enjoy a visit to the Wachau district of Austria.



180° panorama taken by the editor with incoming CIAAW Titular members Zhu (left) and Hirata (right).

### Division II 45GA meeting – Glasgow Scotland

Division II met at the Scottish Exhibition and Conference Centre (SECC) on the 31<sup>st</sup> July and 1<sup>st</sup> of August during the 45<sup>th</sup> IUPAC General Assembly.





*SECC – IUPAC GA 2009 Venue*

An interesting outcome for me was the enthusiasm and involvement of the Young Observers (YO) present at this meeting, with several YO presenting excellent presentations and ideas for the upcoming International Year of Chemistry



*Project Coordinator Ty Coplen keeping Division II informed of the progress despite the “ever growing” list of projects.*



*Div II Glasgow meeting attendees – minus the editor!*



*Div II members networking during a fire alarm evacuation during the 45th GA meeting*

## Project News

### **New Division II Projects**

2009-012-2-200 Task Group Leader, Prof Lars Öhrström:

**Coordination polymers and metal organic frameworks: terminology and nomenclature guidelines,**

2009-023-1-200. Task Group Leader, Dr Michael Wieser,

**Evaluation of Radiogenic Abundance Variations in Selected Elements**

The purpose of this project is to evaluate isotopic abundance variations in selected elements, including Re, Os, Rb, Sr, K, Nd, Sm, Hf, Lu, and Ar in a range of materials, based on peer-reviewed measurements, to create graphical plots of these data, and to provide CIAAW with information to update the Table of Standard Atomic Weights.

Recent developments in inorganic mass spectrometry enable isotope ratio measurement of radiogenic elements at unprecedented precision. A steadily growing body of measurements shows radiogenic isotope abundance variations for elements such as Re, Os, Rb, Sr, K, Nd, Sm, Hf, Lu, and Ar. This raises the question of how far current IUPAC recommendations for the standard atomic weights of these elements and their respective uncertainties incorporate any natural variations in isotope abundances.

Recommendations will be incorporated into those generated by the Subcommittee on Isotope Abundance Measurements (SIAM) and they will be sent to CIAAW for approval. Approved changes will be incorporated into the next CIAAW Table of Isotopic Composition of the Elements (TICE) and Table of Standard Atomic Weights (TSAW).

### Project Reports

**Calibration of organic and inorganic oxygen-bearing isotopic reference materials.** Project number 2005-022-1-200

The isotopic abundance of oxygen in natural terrestrial materials varies by more than 5 percent owing to differences in physiochemical and biological processes. Thus, measurement of oxygen isotopic composition can provide information about sources and processes in atmospheric sciences, biology, environmental studies, forensic science, geology, hydrology, and oceanography.

Critical to advances in these sciences is that measurements in laboratories globally be

comparable. That is, measurement of the same homogeneous sample by any laboratory worldwide should yield the same isotopic composition within analytical uncertainty. Internationally distributed isotopic reference materials enable laboratories to achieve this aim.

To assess measurement data from an international calibration of organic and inorganic isotopic reference materials, IUPAC funded project 2005-022-1-200, titled "Calibration of organic and inorganic oxygen-bearing isotopic reference materials." These solid reference materials needed to be calibrated to an international water scale; thus, a means to introduce 0.5 mg samples into the analysis system with minimal evaporative loss was needed.

This proved challenging and at an IUPAC sponsored meeting in Pisa in 2007, a replacement for the conventional method to seal liquid water in silver capsules prior to introduction into a high temperature conversion system was sought. It was decided to seal water in a metal tube using a pinch and seal technique, such as is used for sealing copper tubing in vacuum systems (making a cold weld during the pinching process). The complete assembly is shown below.



*Semi-automated squeeze and cut system*

The water-filled metal tubing is advanced identical distances with a stepping motor under computer control. A torque wrench enables the operator to seal each end of the metal tubes containing water of specified isotopic composition. The final product (metal tubes each containing 0.5 mg water) is shown below.



*Seven metal tubes filled with H<sub>2</sub>O*

## **Reconstitution of the Interdivisional Subcommittee on Materials Chemistry**

*Item Provided By Prof Len Interrante, Div II Secretary*

This Subcommittee was established by Division II after the demise of "Commission 2.4" on High Temperature Materials in the wake of the reorganization of IUPAC in 2000. Several Commission 2.4 Projects were continued after that, with the participation and support of Division I (Physical Chemistry). Later Projects on polymeric materials, originating in Division IV (Polymer), were cosponsored by Division II and became part of the scope of this Subcommittee. For much of this time, Division II member John Corish served as its Chairman, until his election as Treasurer of IUPAC, whereupon Tony West assumed this role.

During this period, the Subcommittee meetings were attended primarily by Division II members, and one or two members of Divisions I and IV became occasional participants, when meetings were held as part of the biennial GAs. The relative infrequency of these biennial meetings (during off-years, the Subcommittee continued to meet without participation of other Divisions) and the predominance of Division II members at all of the meetings, insured that this Subcommittee would remain largely 'inorganic' in scope and Project focus, with the "Interdivisional" aspect remaining essentially unrealized in practice.

Throughout much of this time, it was recognized that the true scope and importance of the growing field of 'materials chemistry' was not being adequately addressed by this Subcommittee and, in 2005, a Project entitled "What is Materials Chemistry" was begun, with Prof. Peter Day as the Project Leader. The goals of this Project were:

*"to 'assemble, collate and disseminate information about the scope of the newly-emerging discipline of materials chemistry, leading to an authoritative definition of the subject within the family of chemical sciences' and further, as a corollary, 'to recommend to IUPAC how this new discipline might best be represented within the IUPAC structure'."*

This Project is now completed with two publications [Chemistry International, May-June 2009, pp. 4-8; Pure Appl. Chem., 81(9), 1707-1717(2009)] and a proposed definition of materials chemistry resulting:

***Materials chemistry comprises the application of chemistry to the design, synthesis, characterisation, processing, understanding and utilisation of materials, particularly those with useful, or potentially useful, physical properties.***

Moreover, it was concluded that:

*“materials chemistry impacts on, and requires input from, many of the traditional Divisions of chemical science (physical, organic, inorganic, macromolecular etc) as defined by IUPAC. It can also be argued that its ubiquity and importance both for science and industry merit a more prominent status in the IUPAC structure.*

*At present the interests of the subject are overseen by the Subcommittee on Materials Chemistry, which is formally placed under the Inorganic Chemistry Division. We argue that this arrangement no longer responds adequately to the size and reach of the materials chemistry community, which encompasses a broad range of materials and disciplines. Indeed, although the Subcommittee on Materials Chemistry was intended from the outset to function as an interdisciplinary committee, with members from Divisions other than Division II, it has proven difficult under the current structure to attract to its meetings (especially off-year meetings) a sufficiently broad representation from other Divisions.*

*The Project WG suggests that IUPAC address the present deficiency by establishing a cross-divisional Committee that would work with all the current IUPAC Divisions to develop and co-sponsor new projects, in the area of chemical education, nomenclature, terminology, health and safety, etc., that will increase the recognition of the current and future importance of this field to the international chemistry community.”*

As an initial response to this call for a change in the status of materials chemistry within IUPAC, the members present at our meeting in Glasgow decided to reconstitute the Interdivisional Subcommittee on Materials Chemistry in a manner that would make it truly “Interdivisional” in scope and function. Len Interrante agreed to take on this task as interim chairman of this Subcommittee.

Based on initial discussions with members of Divisions I and IV, two members of each Division were designated to serve as initial members of the reconstituted Subcommittee and a meeting was scheduled for October 17, 2009 at Cornell Univ. in Ithaca, NY to discuss the future of the Subcommittee, and of materials chemistry, within IUPAC and to come up with ideas for some proposed Projects that would recognize the truly interdisciplinary nature of this field.

## HotPaper

*Item submitted by Professor Myunghyun Paik Su, Seoul National University and Div II TM*

Professor Suh’s article on “Highly Selective CO<sub>2</sub> Capture in Flexible 3D Coordination Polymer Networks”, in *Angewandte Chemie* (doi: 10.1002/anie.200902836) has been selected as newsworthy and deemed a “HotPaper”.

### **Opening the Door for CO<sub>2</sub>**

#### **Flexible, three-dimensional lattice binds carbon dioxide selectively and efficiently**

Not too long ago, factory smokestacks that produced nothing but carbon dioxide and water vapor were considered exemplary. Now CO<sub>2</sub> has become notorious as a greenhouse gas, and the danger of climate change has become one of the most pressing environmental problems of our time.

How can we slow the increasing release of CO<sub>2</sub>?

Efficient methods for the separation of this greenhouse gas from industrial exhaust are being sought. Korean researchers have now developed a porous material that can bind and store CO<sub>2</sub> efficiently and highly selectively. As Myunghyun Paik Su and Hye-Sun Choi report in the journal *Angewandte Chemie*, the lattice-like network contains flexible “columns” that can open the pores of the three-dimensional lattice for CO<sub>2</sub>.

Many porous materials are able to absorb CO<sub>2</sub> and other gas molecules. However, the selective, room-temperature extraction of CO<sub>2</sub> at atmospheric pressure from industrial exhaust containing other gases such as nitrogen, methane, and water, remains a major technical challenge.

The research team has now developed porous, three-dimensional networks of coordination polymers. The building blocks used are various nickel complexes and organic molecules. These assemble into two-dimensional lattice-like planes that grow into stacks held together by “columns”. The special trick in this case is that the columns are not rigid, but very flexible. The corresponding cavities in the structure are thus of variable size and can accommodate themselves to the guest molecules that enter.

The symmetric molecule carbon dioxide has a permanent electrical quadrupole moment that can be described as two electrical dipoles sitting back-to-back. This quadrupole interacts with the three-dimensional lattice, and this effect causes the columns to open the “gates”, allowing the gas to enter the cavities. In contrast, nitrogen, hydrogen and methane have much smaller quadrupole moment. The pores thus remain closed to them. The exclusion of nitrogen, which makes up a large proportion of air, is essential for any potential CO<sub>2</sub>



capture. In addition, the new nickel-containing materials are stable at temperatures up to 300 °C and are air and water stable—also an important requirement for eventual industrial application.

If the surrounding pressure is reduced, the stored CO<sub>2</sub> is released. This type of material is thus suited for processes in which carbon dioxide must be cyclically stored and then released through a change in pressure.

## Interesting Research

### Phase change materials for new non-volatile memories

*Item submitted by Professor Markku Leskelä, Univ of Helsinki and Div II TM*

Phase change memory (PCM) materials are already employed in optical data storage and recently they have gained a lot of interest also as promising candidate for future electronic storage applications in non-volatile memory devices known as phase-change random-access memory (PCRAM).

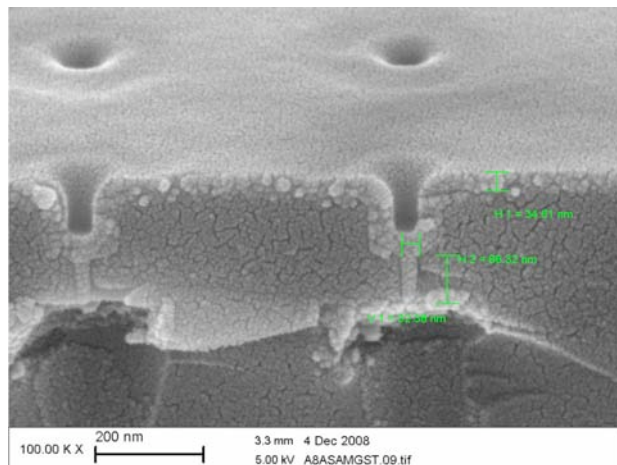
PCMs use different storage mechanism than flash memories since the data is not stored as charge but as a structural difference in the material (amorphous not conducting – crystalline conducting phase). Chalcogenides, especially Ge-Sb-Te (GST) alloys, are considered as very interesting PCRAM materials because of their many advantages: the phase change is very fast (tens of nanoseconds) and reversible, records can be rewritten up to 10<sup>13</sup> times, records can be retained stably for tens of years, it is scalable to 20 nm node, and integration into logic CMOS process flow is possible.

To make high-density memory devices with low power consumption PCRAM must be scaled down to dimensions of a few tens of nanometers and the material has to be deposited as thin conformal films. The conformality requirement means that chemical deposition methods, CVD (Chemical Vapor Deposition) or preferably ALD (Atomic Layer Deposition) has to be used.

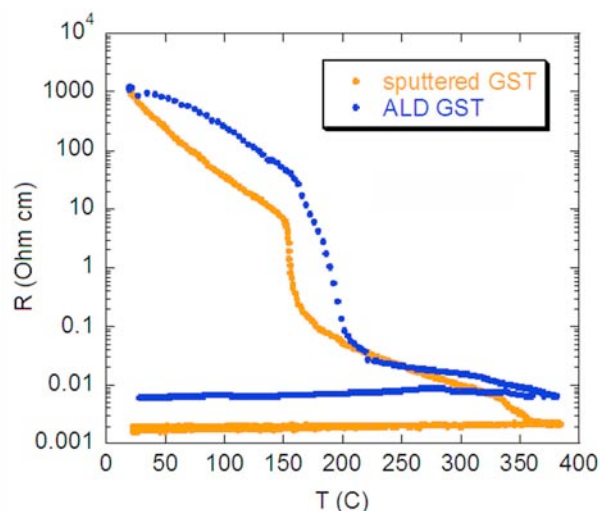
The chemical depositions of GST films have been limited because of the lack of suitable precursors, in particular tellurium precursors. The group at University of Helsinki has made a breakthrough and shown that alkylsilyls of tellurium can be used as tellurium precursors in ALD of GST materials (V. Pore, T. Hatanpää, M. Ritala and M. Leskelä, J. Am. Chem. Soc., 131, 3478 (2009)). (R<sub>3</sub>Si)<sub>2</sub>Te reacts with various metal halides producing metal telluride thin films and Ge<sub>2</sub>Sb<sub>2</sub>Te<sub>5</sub> films were deposited by ALD at 90 °C using (Et<sub>3</sub>Si)<sub>2</sub>Te, SbCl<sub>3</sub> and GeCl<sub>2</sub>·C<sub>4</sub>H<sub>8</sub>O<sub>2</sub> as

precursors. By adjusting the exposure times and cycle ratios GST films with controlled composition could be achieved.

The as-deposited amorphous films crystallize at 130 °C as rock salt structure and at around 250-300 °C the structure changes to hexagonal. Phase change studies of the ALD GST films have shown at least similar behavior as the state-of-the-art sputtered reference films.



Cross-section of a PCRAM cell structure showing the conformality of the ALD GST film.



Resistivity vs. temperature for GST films made by ALD (blue) and sputtering (orange). Low-temperature: amorphous, non-conducting, High-temperature: crystalline, conducting.