IUPAC

Interdivisional Sub-Committee on Materials Chemistry

Informal Meeting on 14th August 2006 in Seattle

Room 105, Department of Chemistry, University of Washington

DRAFT MINUTES

Present: J. Corish (Chairman), A.V. Chadwick (Secretary), L.V. Interrante, A.R. West, G. Rosenblatt, J. Garcia-Martinez, M. Leskela, C. Campbell (Local host).

1. Welcome

The Chairman welcomed the members of the Sub-Committee to the meeting and thanked Charlie Campbell from the Chemistry Department for acting as the local host and providing facilities for the meeting.

2. Minutes of the last meeting

The minutes of the last meeting of this Sub-Committee at Beijing were tabled and discussed. It was not clear how many members of the group had received electronic copies of the minutes, therefore they should be re-circulated.
[Action: Secretary to e-mail minutes of the Beijing minutes out to members]
The matters arising from the Beijing minutes mainly concerned progress on projects and will be covered elsewhere in the agenda for the meeting.

3. Reports of progress on projects

a. Defining Materials Chemistry

This is an accepted and funded project led by Peter Day (Chemistry, Oxford, UK) as the Task Group leader.
Professor Day had initiated a meeting in London earlier this year organised by the Royal Society of Chemistry and there was a report from this meeting (Annex 1). Unfortunately Professor Day could not attend the present meeting because of travel difficulties associated with increased security. The meeting appreciated the report but were unclear about what the next stage of the project would be and noted that the Task Group had not yet formally met. Tony West is the monitor for this project. The Chairman suggested that it would be useful for the Task Group to meet with members of this Sub-Committee with a view to bring the project to completion because the outcome of the project was so fundamental to the work of the Sub-committee. Tony West thought that the project still had sufficient funds to finance such a meeting possibly at the next

General Assembly (The project was funded $8k, and most of this was still available for such a meeting). The Sub-Committee endorsed the proposed meeting.
[Action: Tony West to contact Peter Day to discuss plans for the completion of the project]

b. Project to Produce a Glossary of Terms Used in Materials Chemistry: Nano-related Terminology

This is a proposed project from Sanjay Mathur. There had been considerable discussion of this proposal at Beijing. There were concerns that the cost was initially too high and the project did not have sufficient focus. At Beijing it was left to Sanjay to follow up with a revised proposal. This has not yet been completed although some progress had been made and the Sub-Committee was sympathetic to the difficulties in producing a proposal on this subject. It was noted that some good starting points for the nomenclature; the book by Ozin and the Vocabulary PAS 71:2005 produced by British Standards. Tony West suggested a workshop on the topic could be held in conjunction with GA at Turin. It was clear that Sanjay would need help in preparing the proposal. After much discussion the following procedure was proposed to forward this project.

Step 1: The Chairman to ask Sanjay Mathur if he would be willing (with assistance from other members of the Sub-Committee) to run a workshop in Turin and still wishes to run the project that might be defined there. The aim of the workshop would be to assess the scope and viability of the project.
[Action: The Chairman to contact Sanjay Mathur to discuss plans for the project]

Step 2: Tony West and Javier Garcia-Martinez to assist Sanjay Mathur by (i) distilling information from the available glossaries of nanomaterials terminology (see above) and (ii) compiling a list key people who could eventually form a Task Group for the project. Potential Task Group members within IUPAC could be identified from the Blue Book.
[Action: Tony West and Javier Garcia-Martinez to distil glossaries and find potential members and convey the information to Sanjay Mathur]

Step 3: Tony West will publicise this plan to have the workshop at the Bureau Meeting in Madrid. This will inform IUPAC and the other Division Presidents of the plan and will help identify other people within IUPAC who could be on the Task Group.
[Action: Tony West to publicise plans at the Bureau Meeting]

Step 4: (Added after the meeting). Since the above steps involve several people it seems appropriate for the Secretary to monitor progress on the steps.
[Action: The Secretary to monitor the steps]

c. Experiments in Materials Chemistry

Dr. Bosova, who was asked to coordinate the project, feels the project should be dropped as the task force has disintegrated. In addition she has no students to test the

experiments. Gerd Rosenblatt gave the history of the project describing it as still being of potentially great value to the community if it could be completed in the future.. However, in the present circumstances it does look as though this project should be terminated. This will be reported at tomorrow's meeting of the Division Committee.

4. HTMC-XII Vienna

All information on this meeting is on the Web. It is IUPAC sponsored. There will be approximately 150 attendees, similar to the previous meeting in Japan. A presentation from IUPAC is normally given at this meeting; however there does not appear to be an attendee who is an IUPAC member. It could be possible that Hilpert or Chatillon are attending and he could give the presentation.
[Action: Gerd Rosneblatt to contact Hilpert and Chatillon to ascertain his attendance at the conference]

4. HTMC-XIII (2009)

The venue selection committee, chaired by Hilpert, considered five to six good applications to hold meeting. Within the established schedule it was time to hold the meeting in the US and it will be organised by Alexander Navrotsky at Davis.

5. WAM III (Workshops on Advanced Materials)

This was held in Stellenbosch, South Africa in September 2005. A full report, written by Piet Styne and the Chairman, is available on the Web and was published in Chemistry International. The Chairman attended the workshop and reported that it was a very successful meeting with wide representation of students from African countries. Sanjay Mathur had organised a mini-symposium jointly funded by National Research Foundation (South Africa) and the Deutsche Forschungsgemeinschaft (Germany) in conjunction with the meeting. All of the presentations at this symposium were given by research students.

6. WAM IV

An offer had been received from Thailand to host this meeting, to be organised by Joydeep Dutta at Asian Institute of Technology in Klong Luang Pathumthani. Sanjay Mathur will be involved in assisting the organisers. This application was reviewed and was considered to be an excellent and well thought out proposal and should be endorsed.
[Action: Chairman to contact the organisers and provide assistance in seeking IUPAC funding for the meeting]

7. New Projects

7.1. Terminology for conducting, electroactive and field-responsive polymers

This is a proposal submitted from Division IV, coordinated by Prof Ober. Gerd Rosenblatt said that it was good and needs to proceed, but we (the Sub-Committee)

have no budget. But the Sub-Committee could give it support as being a good project. However, there is no inorganic chemistry in the project, hence the Division might not agree to fund it. Gerd Rosenblatt suggested we give it the backing of this Sub-Committee, such that The Chairman could write to the Secretariat strongly endorsing the proposal. The Sub-Committee was happy with this course of action.

7.2 Nomenclature for mesoporous materials

Javier Garcia-Martinez felt that there is confusion in nomenclature. It is a much focused area and is part of the nanomaterials area. A lot of work done by IUPAC in the area of porous materials nomenclature (as early as 1985) but area is now getting confused with the new materials and nanotechnology. Thus there is room for a focused project. To pursue this it the interest of other Divisions should be assessed. Tony West will consult Division Heads at the Bureau meeting in Madrid.
[Action: Tony West to consult at Bureau meeting]

8. Future of Sub-Committee

The Chairman pointed out that this Sub-Committee was formed in Brisbane and it was time to review the status. Several members commented that materials chemistry is a growing area, but where does it fit into the current structures of IUPAC? There is no funding, so how does the Sub-Committee continue? There have not been a lot of projects in the materials chemistry area and no outstanding successes despite the fact that Materials Chemistry had formed significant parts of recent IUPAC Congress Programmes and will feature again in Turin. Gerd Rosenblatt said it would be hard to start a Division for Materials Chemistry; a strong case could not be made and Inorganic Division itself is not currently one of the stronger divisions. Tony West pointed to the experience of the Royal Society of Chemistry in setting up its very successful Materials Forum suggested that it was necessary to move carefully and slowly in building up successful structures that could effectively assist this subject. The future of the Sub-Committee will be raised at the Division II meeting to seek a wider view.

9. Presentation

Charlie Campbell gave a short presentation on the research in chemistry at the University of Washington.

10. Conclusion

The Chairman thanked the attendees for their participation and Charlie Campbell again for being a splendid local host.

12. Date of next meeting

The Sub-Committee will meet at the Turin General Assembly.

Alan Chadwick - 23 September 2006

ANNEX 1

IUPAC Inorganic Chemistry Division Committee

Seattle, USA, 15-16 August 2006

Defining Materials Chemistry: IUPAC Project – Prof. Peter Day

Background

In the last 10-15 years materials chemistry has rapidly emerged as a distinct discipline within the broad family of chemical sciences. A significant fraction of all publications in chemistry claim to form part of this new field. Two examples will suffice: Googling 'materials chemistry' results in no fewer than 175M hits, while the number of articles submitted to one of the major journals in the field has increased almost 15-fold in 15 years (Fig. 1). Nevertheless, finding an agreed definition of what constitutes 'materials chemistry' is not easy. Materials chemistry transcends the traditional sub-divisions of chemistry. So can we devise and inclusive but meaningful definition? To date the discipline has developed organically and to a large extent, the common idea of what constitutes materials chemistry is circularly linked to the type of work that those calling themselves materials chemists do.

Faced with these facts IUPAC set up a project to furnish a succinct definition of the subject area covered by materials chemistry and recommend how this new discipline might best be represented within the IUPAC structure. Apart from collecting information from practitioners and from the journals principally devoted to the subject, one of the key tools in the project was a Workshop, kindly organised by the Materials Chemistry Forum of the UK's Royal Society of Chemistry. The MCF brings together representatives, not only of the relevant subject groupings in the RSC but also from contiguous disciplines like physics and materials science, all of which contributed, in addition to international speakers. The workshop aimed to provide a definition and discuss the nature of the discipline. The opinions and ideas collected provide valuable feedback to the publishing and funding communities, as well as the IUPAC project. The brief comments that follow draw heavily on that discussion. I am grateful to Dr Rachel Brazil of the RSC for her notes.

What is a Material?

In defining materials chemistry, it becomes clear that one of the most difficult tasks would be defining what constitutes a material in contrast to just a chemical. This would be the key to defining materials chemistry. The dictionary defines a material as 'a physical substance which things can be made from'. To devise a more technical definition many felt that the idea of functionality or application needed to be considered. A material is something that has properties which give is a particular useful application, either structural, as with a building material, or functional, as with materials used to make devices (electronic, optical or magnetic). A material is generally though of as a solid or highly viscous phase where interactions between the entities forming the aggregate play a large role, rather than a liquid or gas.

Another key concept is that of ‘emergent properties’ Materials are assemblages of sub-units. The properties of a material emerge from the way these sub-units are put together. Whilst a single molecule will have properties related to its chemical structure which remains constant, the properties of a material are dependent on how its subunits are assembled. In fact, properties can arise from structural defects and materials made of the same chemical sub-units can have different properties. This relationship between structure and property could be used to define a material and differentiate it from a chemical. An example of a material would be a nanotube, whose properties will vary depending on its structure. This can be compared to a molecule of benzoic acid, which is a chemical whose properties are related only to its chemical make-up.

The work of a materials chemist

To develop ideas about the sub-discipline it is useful to look at some of the processes and priorities of researchers in the discipline.

- *application as motivation*

  Much materials chemistry is motivated towards discovery and development of materials that may be exploited for desired applications. Whilst this is an essential motivating factor, there does also need to be some scope for purely studying the structure and properties of materials. Chemists will generate new materials before their potential applications may have been conceived. The discipline must include the ability to synthesise, study and assess new materials.

- *structural or functional*

  Today, the work of most materials chemists is focused on producing functional device materials and the discipline is often seen as being focused on the production of materials with function – electrical, optical or magnetic. The production of structural materials such as alloys, composites and plastics has been seen as the province of materials scientists. Polymer science, whilst carried out by chemists was not always historically strongly connected to other materials chemistry, largely due to the number and strength of journals devoted to macromolecular chemistry alone. However, with the development of the field of conducting polymers, the materials chemistry and polymer science communities are moving closer together. The development of new nanostructured and smart materials is also uniting communities and bringing the science involved in functional and structural materials together. Materials chemistry can encompass both structural and functional materials. Structural properties such as strength or flexibility can be considered as another type of functionality. At the moment chemists are more interested with other types of functionality but this may change in the future.

- *designing and processing materials*

  The concept of ‘design’ was seen as very important in defining the work of materials chemists. Rather than purely investigating properties, the materials chemist tries to manipulate the synthetic process to produce a desired end product. The relationship between method of synthesis and design of the final end product is crucial for a materials chemist.

- *Characterisation and analysis*

  Characterisation techniques are important to the work of all chemists. However, whilst many mainstream chemists are primarily concerned with characterising the chemical or molecular structure, materials chemists are often interested in looking at

higher level structure in addition. Microscopy is an important element of the work of many materials chemists.

The difference between materials science and materials chemistry

In defining materials chemistry, the differences between materials science and materials chemistry were examined. Many materials science departments have appointments in materials chemistry. However the areas of study described as materials chemistry can differ from the materials chemistry practised within chemistry departments. Materials chemistry from the chemistry perspective should be considered a sub-discipline of chemistry.

Materials chemistry does share some common elements with materials science, but often the scale of elements studied differ, with materials chemistry being concerned with a molecular understanding of materials, whilst materials scientists are looking at a larger scale. Materials chemistry can be concerned with properties up to the micron scale though.

It must be recognised that there is a big overlap and many materials scientists will be working to the same end as many materials chemists.

Another element that may differentiate materials chemistry from materials science is the interdisciplinary nature of the work. Materials chemistry may require an understanding of the principles of both chemistry and materials science and sometimes physics and biology.

A working definition of materials chemistry

Some definitions suggested at the workshop:

Materials chemistry is the chemistry of the design, synthesis and characterisation of assemblies of molecules whose properties arise from interactions between them.

Materials chemistry is the understanding, synthesis, processing and exploitation of compounds or substances in their assembled form.

Materials chemistry is the synthesis, processing, characterisation, understanding and exploitation of compounds that have useful or potentially useful properties and applications.

What is *not* materials chemistry?

It may be agreed that simply synthesising a new chemical substance in nano- or macroscopic form is not materials chemistry but just chemical synthesis. For it to be considered materials chemistry there needs to be an element of application, function or novel design. Work on novel materials that may show potential applications must be included as materials chemistry since chemists may generate new types of materials with previously unknown properties leading to unimagined applications.

Research in (non-materials) chemistry is focused on adding to our understanding of the science of chemistry itself, of how matter is composed, interacts and how fundamental properties arise.

Inevitably there are areas of contention when trying to define the sub-discipline materials chemistry. Would catalysis be considered part of the field? Homogeneous catalysis would certainly not fit the definition above, but would heterogeneous catalysis? The synthesis of novel catalyst materials does certainly fit the parameters by which materials chemistry has been described.

There are other areas that could be debated, in which the chemical synthesis is of a precursor to the material itself. Examples are CVD precursors, new liquid crystal molecules (synthetic chemistry or materials chemistry?) or the ball milling of ceramics (materials science or materials chemistry?).

Materials Chemistry in IUPAC

It is abundantly clear that materials chemistry impacts on, and requires input from, many of the traditional sub-groups of chemical science (physical, organic, inorganic, macromolecular etc). At present the interests of the subject are overseen by a Materials Chemistry Working Group that is formally a sub-committee of the Inorganic Chemistry Division Committee. It could be argued that this arrangement no longer responds adequately to the size and reach of the materials chemistry community. IUPAC should address this deficiency. One model to study is that of the 'Special Interest Group' in the RSC structure, of which the Materials Chemistry Forum is one example.

22 July 2006