

Technical Committee Meeting Minutes
Thursday, 16 March 2017
International Centre Headquarters
9:00 a.m. – 12:30 p.m.
Conference Room A
Mark Rodriguez, Chairman

Regional Co-Chair presentations are on record at ICDD HQ. Please contact Linda Shertz, shertz@icdd.com, should you wish to see a copy.

1. Call to Order and Opening Remarks Mark Rodriguez
2. Roll Call and Attendance
3. Additions and/or Deletions to the Agenda Mark Rodriguez
4. Approval of the 2016 Minutes Mark Rodriguez

Motion 1: Wallace moved to approve the 2016 Technical Committee Meeting Minutes.
Seconded by Faber.

Motion passed unanimously.

5. Reports/Presentations of Technical Regional Co-Chairs and International Guests

- | | |
|---|-----------------------|
| A. Eastern Pacific Rim | Takashi Ida |
| B. European Community | Matteo Leoni |
| C. South America | Miguel Delgado |
| D. India | T.N. Guru Row |
| E. Indian Ocean Rim (not in attendance) | Vanessa Peterson |
| F. Newly Independent States (not in attendance) | Evgeny Antipov |
| G. North America | Terry Maguire, protem |
| H. People's Republic of China | Xiaolong Chen |
| I. United Kingdom & Ireland | David Rendle |

Fawcett thanked the Delgados' for the SARX workshop and meeting. Also, the workshop held at EPDIC in Bari, Italy had the largest attendance ever. Leoni attended the 1st PanAfrican conference. Fawcett thanked the Regional Co-chairs for their work for the past year.

Leoni stated that IUCr is pushing for Africa to become part of the IUCr. We need to push for the core of Africa to become involved.

There was a workshop of 40 people held at AXAA 2017, in Melbourne.

6. Subcommittee Reports and Motions
A. Materials

- 1) Ceramics – No motions Winnie Wong-Ng
- 2) Metals and Alloys Pete Wallace

Motion 2: The Metals and Alloys Subcommittee recommends to the Technical Committee that a **PDF Phase Diagram Capability** be made available to PDF users.

Supplemental Information

We are proposing a phase diagram capability for the PDF that would be (a) valuable to materials scientists and (b) would help in marketing. The proposal relies on the *empirical formula* in the database. The user selects the elements of interest, and clicks on *Phase Diagram*. The output includes *all phases* in the phase diagram, including pure elements. When polymorphism is encountered, the polymorphs are sorted in Pearson symbol code order. This proposal includes higher-order phase diagrams, too.

For a binary phase diagram such as Pb-Pu, the listing begins at one side of the phase diagram and proceeds to the other side:

- Pb (three polymorphs)
- Pb₃ Pu (Cu₃ Au, cP4, 221)
- Pb₂ Pu (Hf Ga₂, tI24, 141)
- Pb₅ Pu₄ (*, hP*, 182)
- Pb₄ Pu₅ (Ti₅ Ga₄, hP18, 193)

- Pb₃ Pu₅ (W₅ Si₃, tI₃₂, 140)
- Pb Pu₃ (Cu₃ Au, cP₄, 221)
- Pu (six polymorphs)

Wallace moved; Roberts seconded. **Motion passed unanimously.**

3) Micro and Meso

Sue Quick, protem

Motion 3: The Micro and Meso Subcommittee recommends to the Technical Committee to modify the Mission Statement to:

The Micro and Meso Subcommittee will identify systems in which ordered pores, channels, and/or cages on the nano, meso, or microscale are important in the diffraction and the performance of the material; and will identify how the ICDD and PDF can serve the scientific community by providing reference and resource material, by creating or adapting a formalized description of these materials, and contributing to techniques by which these materials can be characterized.

Quick moved; Wallace seconded. **Motion passed unanimously.**

Motion 4: The Micro and Meso Subcommittee recommends to the Technical Committee to allow to publication of MOF patterns although the phases do not have an official name at this time. We propose the entries could have the name “unnamed MOFs” at this time.

Quick moved; Faber seconded. **26 Yes, 0 No, 1 Abstain. Motion passed.**

4) Minerals

Andy Roberts

Motion 5: The Minerals Subcommittee recommends to the Technical Committee that a Clay Minerals Task Group be created to improve the quantity and quality of the clay minerals data within the PDF. This task group will be chaired by Stephen Hillier.

Roberts moved; Wallace seconded. **Motion passed unanimously.**

5) Organic and Pharmaceutical – No Motions

Fred Wireko

6) Polymers – No Motions

Lizhi Liu

B. Characterization Methods and Tools

1) Electron Diffraction

Amy Gindhart

Motion 6: The Electron Diffraction Subcommittee recommends to the Technical Committee that funding (estimated \$10,000) be provided for experts in Electron Diffraction and Powder Diffraction File power-users to come together for these purposes:

- Input from the Electron Diffraction community regarding their needs
- Training of ICDD staff
- Education of this community on the capabilities of the PDF-4.

Meeting to be arranged by ICDD staff by September 2017.

Crowder moved; Blanton seconded. **24 Yes, 0 No, 1 Abstain. Motion passed.**

2) Non-Ambient Diffraction – No motions

Andrew Payzant

3) Synchrotron & Neutron Scattering Methods – No motions

Pamela Whitfield

4) X-ray Diffraction Methods – No motions

Chris Gilmore

5) X-ray Fluorescence – No motions

Mark Rodriguez

C. ICDD Activities

1) Education

Carlo Segre

Motion 7: The Education Subcommittee recommends to the Technical Committee that ICDD Staff effort be assigned to exploring the possible reduction in the duration of workshops and clinics by having lectures prepared and viewed in advance online. Estimates of possible time and cost savings are to be reported to the Education Subcommittee.

Segre moved; Wallace seconded. **Motion passed unanimously.**

Motion 8: The Education Subcommittee requests that ICDD Staff effort be assigned to developing a cost model for the preparation and delivery of online lectures and training. Possible options and costs to be reported to the Education Subcommittee should cover in-house preparation (with staffing costs), contracting to professional for-profit company, and contracting to university with online course experience.

Segre moved; Quick seconded. **Motion passed unanimously.**

Motion 9: The Education Subcommittee requests that ICDD Staff effort be assigned to assessment of need for training videos in support of the PDF 4+ database product. The report to the Education Subcommittee will include projections of benefit to sales of PDF 4+ if possible.

Segre moved; Deschamps seconded. **22 Yes, 0 No, 4 Abstain. Motion passed.**

2) PDF Editorial Staff – No motions

Soorya Kabekkodu

Two chemical subclasses are being introduced: antimicrobials stimulants and depressants.

7. New Business

Mark Rodriguez

8. Adjournment