

Technical Committee Meeting Minutes
Thursday, 14 March 2019
International Centre Headquarters
9:30 a.m. – 12:30 p.m.
Conference Room A
Mark Rodriguez, Chairman

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 2018 Minutes Mark Rodriguez

Motion 1: Rodriguez moved to approve the 2018 Technical Committee meeting minutes.
Seconded by Delgado.
Unanimous – Motion passed.

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

A. Eastern Pacific Rim	Takashi Ida
B. European Community	Matteo Leoni
C. India	T.N. Guru Row
D. Indian Ocean Rim	Vanessa Peterson
E. Newly Independent States	Evgeny Antipov
F. North America	Mark Rodriguez
G. People's Republic of China	Xiaolong Chen
H. Latin America Region	Miguel Delgado
I. United Kingdom & Ireland	Steve Hillier

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 ICDD consider offering PDF® users the option of choosing the standard cell (Crystal Data or Parthe') that best suits the needs of the user.

Notes:

- (1) Parthe' is now used as a standard cell by LPF, ICSD, and many experimenters
- (2) The nearly completed Metals and Alloys PSCI-IV review and the current PSCI-V review are adding Wyckoff sequences to the database that reflect the Parthe' setting.
- (3) This motion (if implemented after the requested consideration) will require significant programming effort at the ICDD and should be considered in that light.

Wallace moved, Dann seconded – **Motion passed unanimously.**

3) Micro and Meso	Cyrus Crowder
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Motion 3: The Micro and Meso Subcommittee recommends to the Board of Directors that ICDD follow the guidelines specified in the paper by Batten, et al. for giving the IUPAC names for MOFs, and if not available, use the name prescribed by the author and/or the chemical name.

Crowder moved, Peterson seconded - **Motion passed unanimously.**

4) Minerals

Andy Roberts

Motion 4: The Mineral Subcommittee recommends to the Technical Committee the following: within the Mineral Name field, Schaller modifiers should be replaced by the term “-bearing”. For example, “Fluorapatite, strontian” would now become “Fluorapatite, Sr-bearing”.

Minerals with two or more Schaller modifiers would have the pertinent elemental symbols separated by commas; e.g. “Barite, calcian, strontian” thus becomes “Barite, Ca-,Sr-bearing”. The Mineral Task group has agreed to this terminology, but this is not IUPAC approved. The IUPAC recommendation (as proposed by Peter Bayliss) is to use the term “-rich”. We believe that the English word “rich” implies the wrong connotation, and would prefer “bearing” instead.

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 – No motions

Alina Bruma

2) Non-Ambient Diffraction – No motions

Bryan Wheaton

3) Synchrotron & Neutron Scattering Methods

Robert Papoular

Motion 5: The Synchrotron and Neutron Scattering Methods Subcommittee recommends to the Technical Committee that a task group be assembled to meet in the fall to discuss the issue of TOF (time of flight) data, and how it can be properly incorporated in the PDF database.

Papoular moved, Lind-Kovacs seconded - **Motion passed unanimously.**

4) X-ray Diffraction Methods

Chris Gilmore

Motion 6: The X-ray Methods Subcommittee recommends to the Technical Committee that clustering techniques be incorporated into the database as a matter of priority. A task group should be set up to this end.

Gilmore moved, Wallace seconded - **Motion passed unanimously.**

5) X-ray Fluorescence

Mark Rodriguez

Motion 7: The XRF Subcommittee recommends to the Technical Committee that ICDD implement combined XRD-XRF validation analysis in the 2021 product based on the RIR method.

Rodriguez moved, Taylor seconded - **Motion passed unanimously.**

C. ICDD Activities

1) Education

Carlo Segre

Motion 8: The Education Subcommittee recommends to the Technical Committee to request ICDD Staff to initiate and conduct a survey of crystallography and diffraction education among the membership. Carlo Segre will lead the task group to help develop the survey. Earle Ryba will help Carlo Segre.

Segre moved, Kaduk seconded - **Motion passed unanimously.**

2) PDF Editorial Staff

Soorya Kabekkodu

Motion 9: The PDF Editorial Subcommittee recommends to the Technical Committee that a subfile for Solar Materials to be created.

Definition: Solar materials (SOL) are a class of semiconductors with bandgaps of 0.50 - 4.96 eV, which can absorb solar irradiation (wavelength of 250 nm- 2500 nm).

Subfile reviewer Dr. Lan.

Kabekkodu moved, Faber seconded - **Motion passed unanimously.**

7. New Business

Mark Rodriguez

8. Adjournment

ICDD Spring Meetings, Newtown Square, PA, 14 March 2019

Reports of Regional Co-chair, Eastern Pacific Rim (Japan, Korea & Philippines)

Takashi IDA, Japan

井田 隆 (日本)

Advanced Ceramics Research Center,

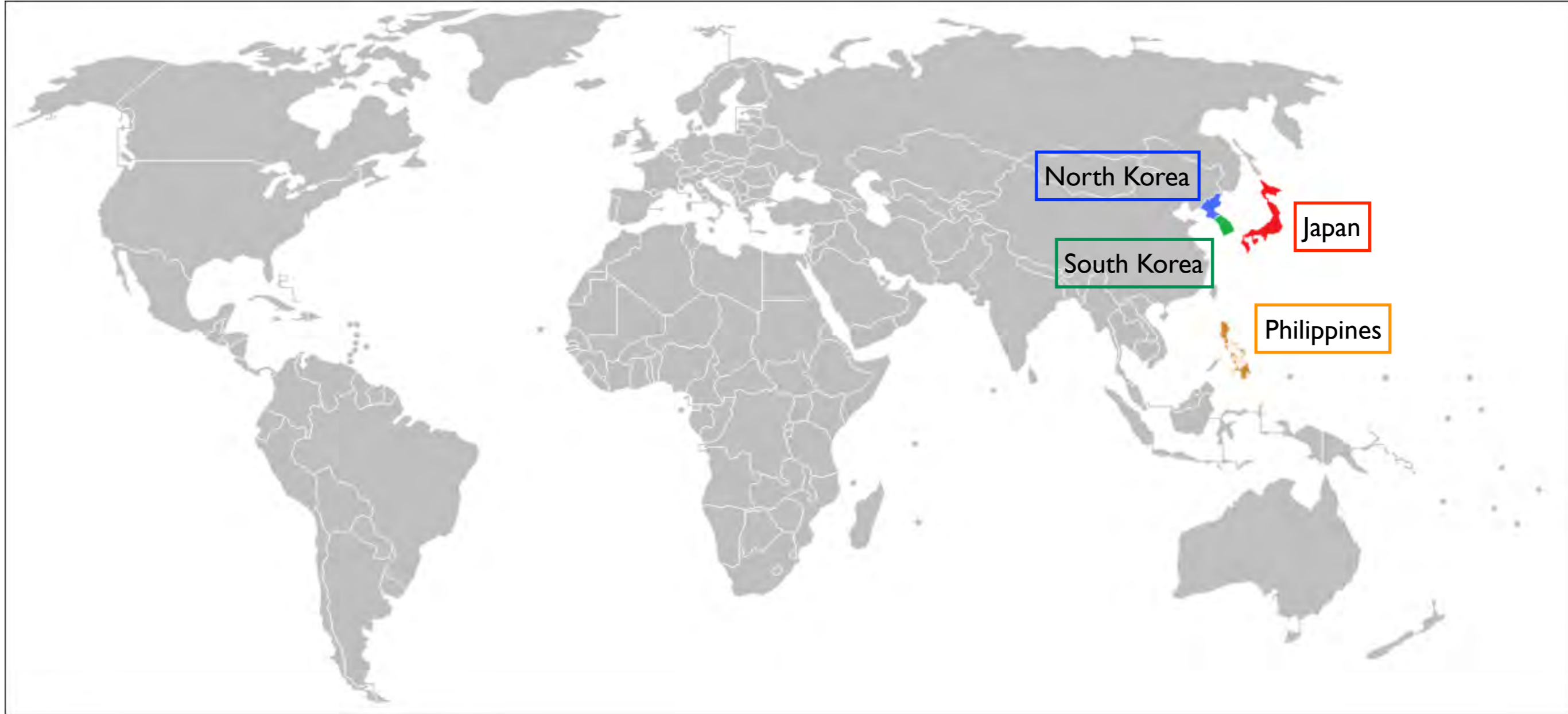
Nagoya Institute of Technology, Japan

Aichi Synchrotron Radiation Center, Japan



AichiSR

Eastern Pacific Rim



Democratic People's Republic of Korea

North Korea

South Korea

Republic of Korea

Japan

Philippines

Republic of the Philippines

Contents

Scientific Meetings in Japan & other countries

2018 (2 meetings)

2019 (2 meetings)

New Database released in Japan in 2018

AtomWork-Adv

Meetings in 2018 (1/2 - 1/2)

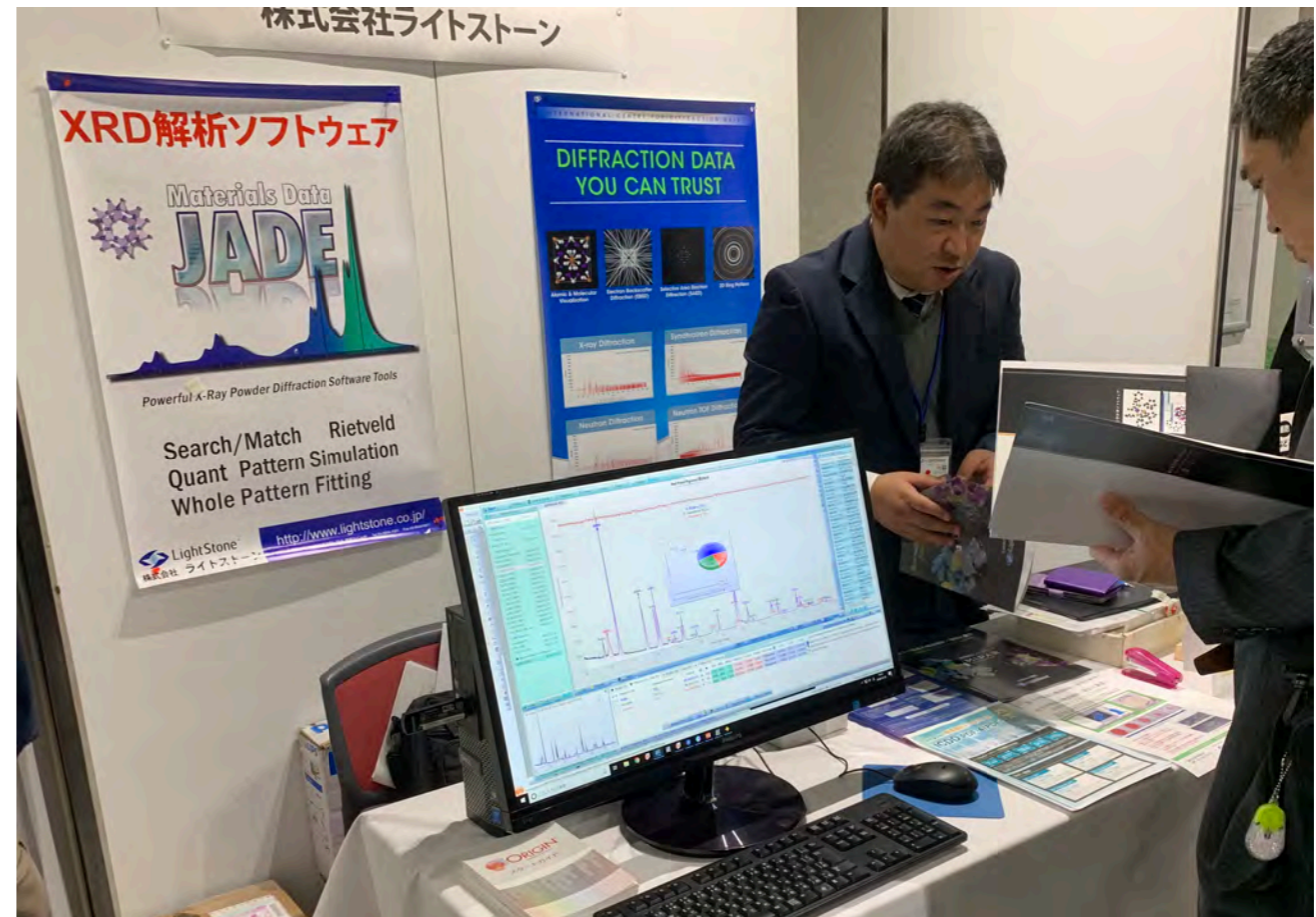
I. Annual Meeting 2018 of Japanese Crystallographic Association

Nov. 10–11, 2018, Tokyo, Japan

<http://analytsci.org/crsj2018/index.html>

Annually held in Japan.

Exposition booth of
LightStone Corp.
(distributor of
ICDD products)



Meetings in 2018 (1/2 - 1/2)

I. Annual Meeting 2018 of Japanese Crystallographic Association

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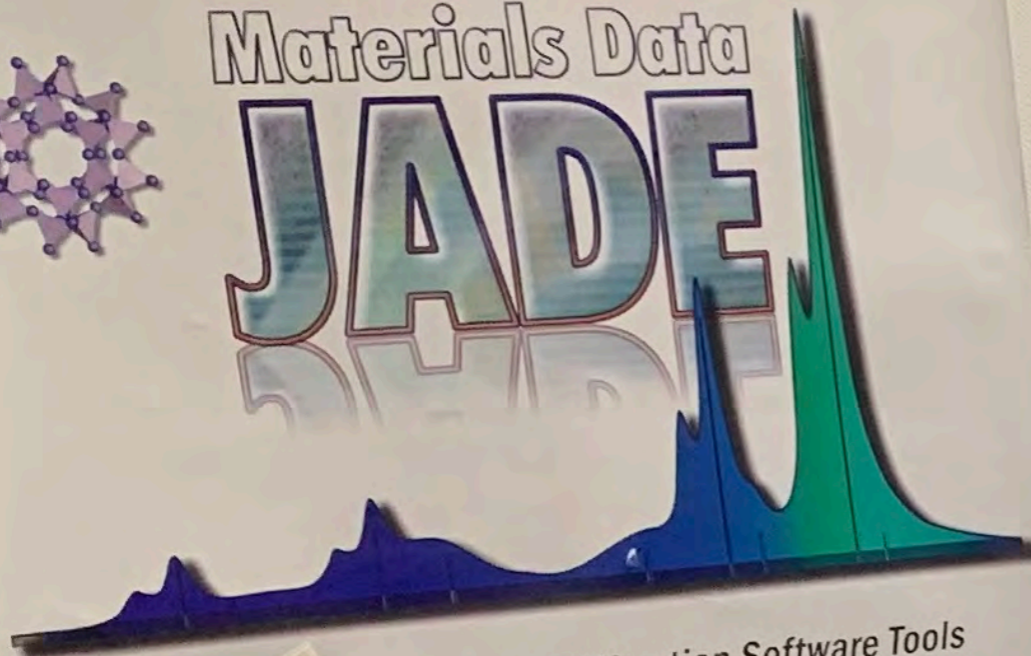


XRD解析ソフトウェア



Materials Data

JADE



Powerful X-Ray Powder Diffraction Software Tools

Search/Match Rietveld
Quant Pattern Simulation
Whole Pattern Fitting

Light Stone
株式会社 ライトストーン

<http://www.lightstone.co.jp/>

INTERNATIONAL CENTRE FOR DIFFRACTION DATA

DIFFRACTION DATA YOU CAN TRUST

Atomic & Molecular Visualization Electron Backscatter Diffraction (EBSD) Selective Area Electron Diffraction (SAED) 2D Ring Pattern

X-ray Diffraction Synchrotron Diffraction
Neutron Diffraction Neutron TOF Diffraction



Meetings in 2018 (1/2 - 1/2)

I. Annual Meeting 2018 of Japanese Crystallographic Association

Nov. 10–11, 2018, Tokyo, Japan

<http://analytsci.org/crsj2018/index.html>

Mr. Hajime Kawamura

We like to recommend & provide High-Quality, Reliable Data to Japanese Customers

Exposition booth of LightStone Corp. (distributor of ICDD products)



Meeting in New Zealand in 2018 (2/2)

2. Asian Crystallographic Association Meeting (AsCA2018)

Dec. 2–5, 2018, Auckland, New Zealand (Indian Ocean Rim)

<http://asca2018.org>

2 times / 3 years held
in Asia.

Jade shop in
Security (Tax Free) Area
of Auckland Intl' Airport



Meeting in New Zealand in 2018 (2/2)

2. Asian Crystallographic Association Meeting (AsCA2018)

Dec. 2–5, 2018, Auckland, New Zealand (Indian Ocean Rim)

<http://asca2018.org>

2 times / 3 years held
in Asia.

Many Chinese were in
jade (翡翠) shop in

Security (Tax Free) Area
of Auckland Intl' Airport



China (Han)

**Jade dragon
(BC2C-0C)**



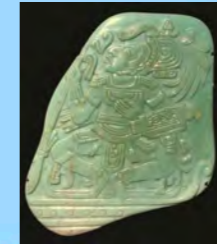
Japan

India



**Dagger with Jade hilt
(17C-18C)**

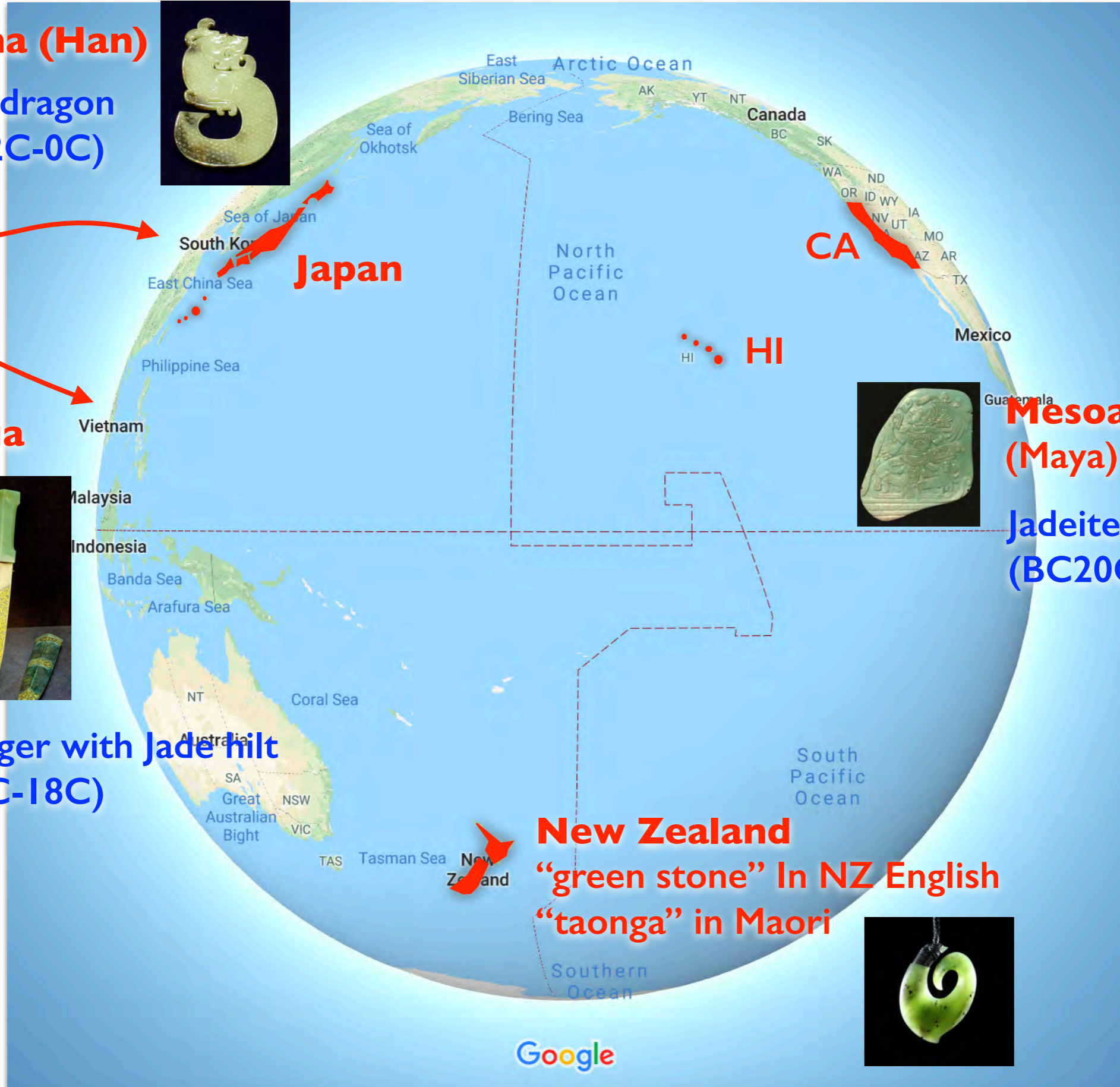
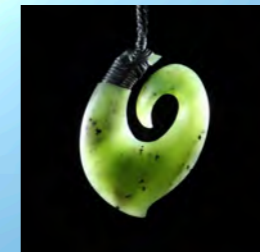
**Mesoamerica
(Maya)**



**Jadeite pectoral
(BC20C-16C)**

New Zealand

**“green stone” In NZ English
“taonga” in Maori**



Google

China (Han)

**Jade dragon
(BC2C-0C)**



Japan

**Jade
(BC30C)**



India



**Dagger with Jade hilt
(17C-18C)**

CA

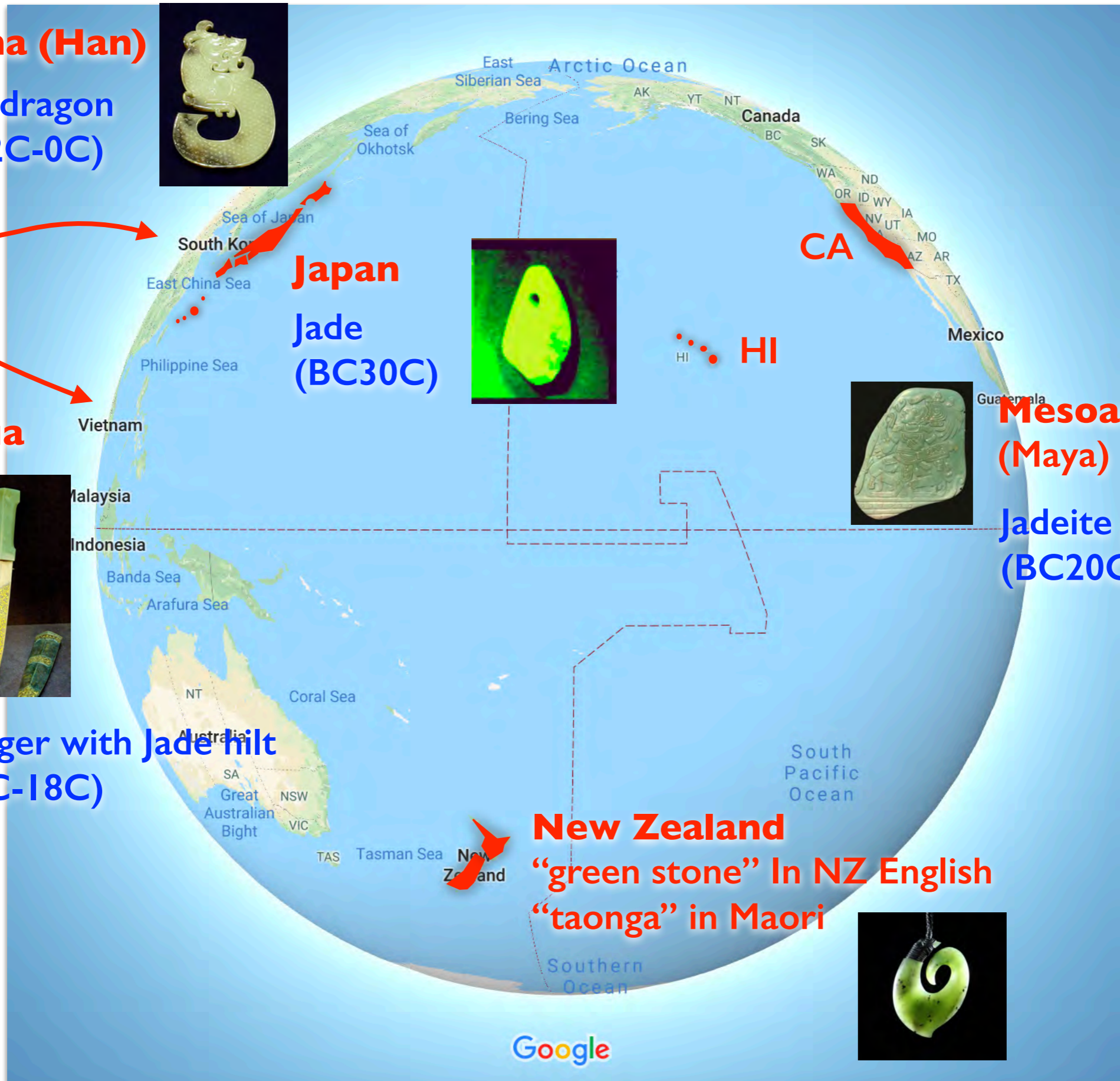
**Mesoamerica
(Maya)**

**Jadeite pectoral
(BC20C-16C)**



New Zealand

**“green stone” In NZ English
“taonga” in Maori**



Meetings 2019-2021 (1/2 - 2/2)

1. Japanese Geoscience Union Meeting 2019 (JpGU2019)

May 26–30, 2019, Makuhari, Japan

http://www.jpгу.org/meeting_e2019/

(7,968 attendees for JpGU2018)

2. PACRIM13 (2019)

The 13th Pacific Rim Conference on Ceramic and Glass
Technology

Oct. 27–31, 2019, Okinawa, Japan

<http://www.ceramic.or.jp/pacrim13/>

(1,200 attendees for PACRIM12 (2017))

Okinawa is called “Hawaii of Japan”





New Database Released in Japan

	AtomWork- Adv	AtomWork	PDF-4+ 2019
Organization	NIMS	NIMS/MPDS	ICDD
Release	May, 2018	Jul. 2010	
X-ray diffraction	550,557	~82,000	412,083
Atomic position	303,855	~82,000	311,125
Phase Diagram	42,406	~15,000	0
Environment	Web browser	Web browser	Windows
Initial Price	1,500 US\$	Free	8,860 US\$
Renewal Price / year	1,500 US\$	-	1,960 US\$
Downloadable items / year	5,000	0	0

INDIA

States and Union Territories



Workshop on PXRD in Pharmaceutical and Materials Industry

June 26, 2018

Organizer: Prof. T. N. Guru Row, IISc, Bangalore

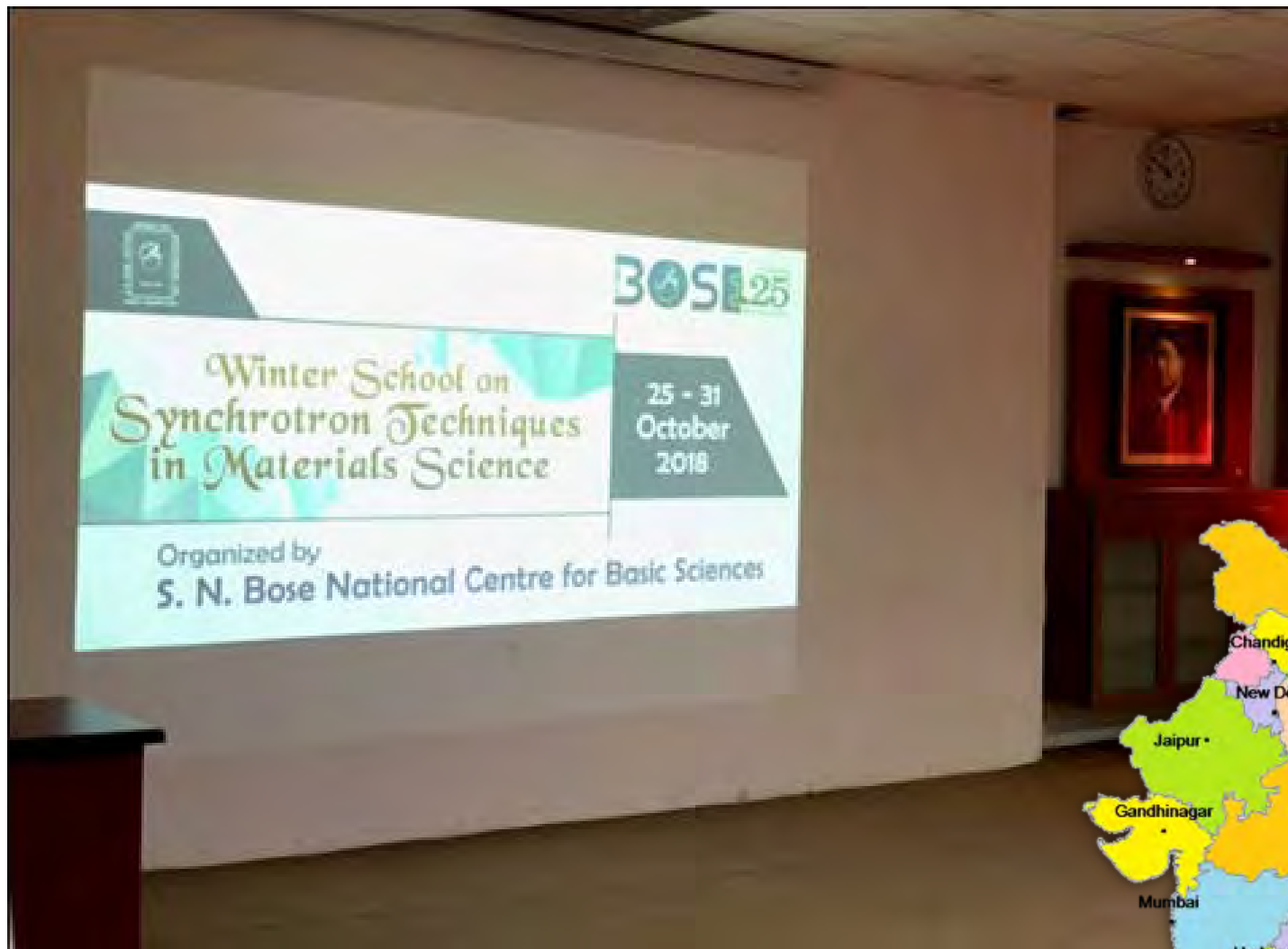
Co-organizer: Prof. B. Padmanabhan, NIMHANS, Bangalore



Characterization of pharmaceutical and functional materials is a prerequisite in modern industry. The workshop is intended to familiarise users of X-ray diffraction techniques for characterization of pharmaceutical and materials. The talks cover the basics of diffraction, techniques and methodologies, examples of applications in industry followed by a hands on training on the use of X'pert highscore plus package. In addition, a webinar on the use and dissemination of diffraction data contained in PDF4+ will be conducted by experts from the headquarters of ICDD in Philadelphia, USA.

**Dr. Tom Blanton conducted the webinar
interactive session from 5:00 to 7:30PM**





- ❖ The Winter School on Synchrotron Techniques in Materials Science was organized to commemorate **125th Birth Anniversary of Prof. S. N. Bose.**
- ❖ Full one day was dedicated for applications of PXRD technique.

Number participants > 80



1. Prof. Nalini G. Sundaram- Basis of powder crystallography and Theory of Rietveld refinement method.
2. Dr. Diptikanta swain- Hands of training to use PDF-4⁺ data base(Phase identification, use of **ICDD** data base), Profile refinement and Rietveld method.
3. Prof. A. Sundaresan- Magnetic and nuclear structures from Neutron powder diffraction.
4. Prof. Chandrabhas Narayan- Powder diffraction at high pressure.

Report of Kolkata Meeting

Speakers



Prof. Nalini G. Sundaram
Poornaprajna Institute of Scientific
Research, Bangalore, India



Dr. Diptikanta Swain
SSCU, Indian Institute of Science
Bangalore, India

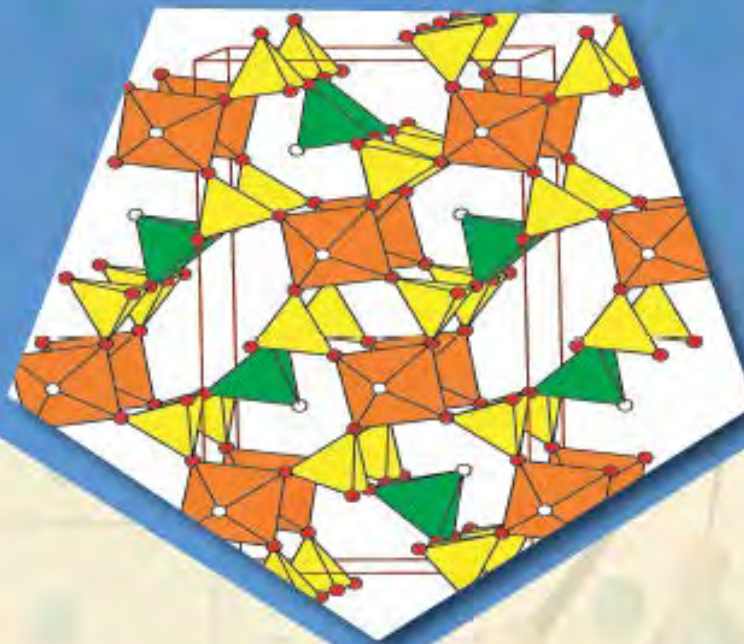


Prof. A. Sundaresan
CPMU, JNCASR, Bangalore



Prof. Chandrabhas Narayan
CPMU, JNCASR, Bangalore

5th Conference of Bangladesh Crystallographic Association



Programme & Abstracts

25-26 January 2019

Venue

*A F Mujibur Rahman Ganit Bhaban
University of Dhaka, Dhaka, Bangladesh*



International Union of Crystallography



Bangladesh Crystallographic Association

ICDD CONFIDENTIAL INFORMATION

Workshop on X-ray Powder Diffraction and Data Analysis

The 5th conference of Bangladesh Crystallographic Association (BCA) will be held on 25-26 January 2019 at the University of Dhaka (for detail please visit BCA website www.bd-ca.org). BCA has decided to organize a post conference **one-day workshop on X-ray Powder Diffraction and Data Analysis** for young student, faculty and scientist. Interested participants may register for the workshop. **A maximum of 50 participants** can be accommodated in the workshop.

Date of the workshop: **27 January 2019**

Venue: Centre for Advanced Research in Sciences (CARS)

University of Dhaka, Dhaka 1000

Last date of registration: **31 December 2018**

Registration fee of the workshop:

Student: BD Taka **500/-**

Faculty/scientist: BD Taka **1000/-**

Contact Person

Dr. Rumana A. Jahan

Principal Scientist

Centre for Advanced Research in Sciences (CARS)

University of Dhaka, Dhaka 1000

Mobile: 01827171949

e-mail: rumana.jahan@du.ac.bd

ICDD CONFIDENTIAL INFORMATION

Problems in structure determination from PXRD

Basic phase problem → Common to all crystallographic structure analyses: Single crystal XRD or PXRD

Reflection overlap problem → Specific to PXRD data

Single approach has emerged as the optimal one !!!

Choice depends upon the nature and quality of PXRD data.



Hydrophobic interactions

- Aggregation of nonpolar moieties in an aqueous media
- In the realm of noncovalent interactions, they are abundant in nature next only to hydrogen bonding
- key role in various processes like enzyme-substrate/ drug-receptor binding, formation of micelles and lipid bilayer in cell walls and stabilizes the conformation of proteins in their native folding states.
- **In the context of material science applications:** water repelling surfaces, microporous silica membranes for gas separation, and clathrate hydrates for gas storage.
- A common notion is that **water molecules** play an exclusive role in mediating hydrophobic interactions between non-polar molecules.

Electrospray ionization mass spectrometry (ESI-MS), showed HIs between protein-hydrophobic ligand complexes are preserved even in the gas phase

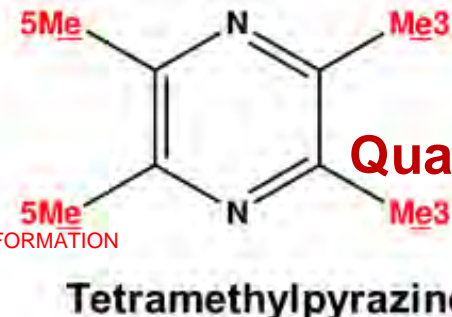
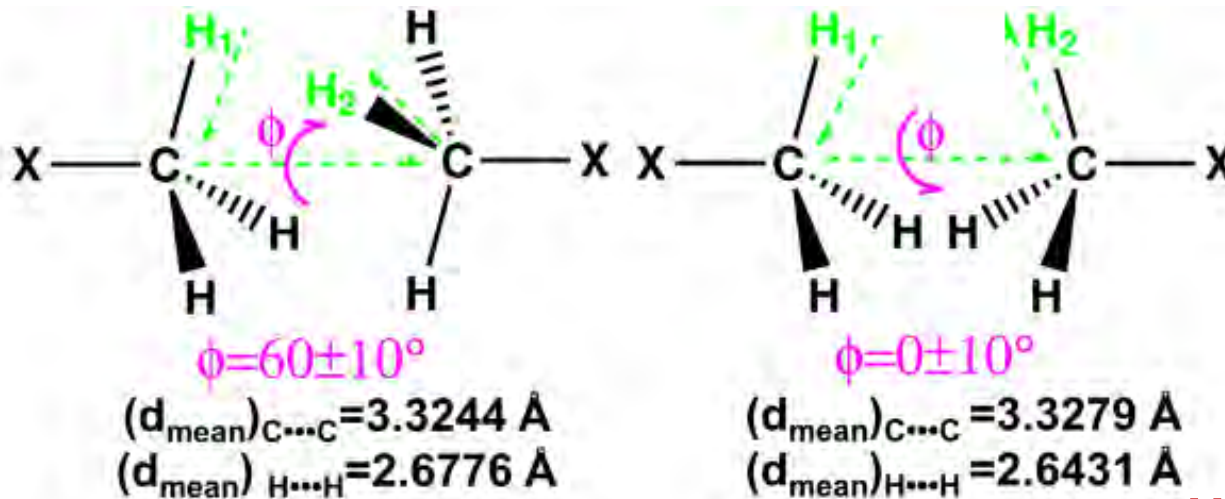
Surface force measurements on hydrophobic surfaces in aqueous electrolyte solutions revealed hydrophobic interactions are of long range order compared to typical van der Waals interactions

Atomic force microscopy (AFM) studies show that the strength of interactions between non-polar surfaces under the influence of proximally immobilized cations such as ammonium and guanidinium ions

Close Encounters of the same kind: Electronic nature of attractive $\text{CH}_3\cdots\text{CH}_3$ Hydrophobic Interactions in the solid-state

Cambridge Structural Database (CSD) with $\text{C}\cdots\text{C}$ separation distance less or equal to the sum of van der Waal radii for C atoms (3.4 Å), 3038 crystal structures (without disorder) containing $\text{Me}\cdots\text{Me}$ motifs. 1840 have 'face to face (3:3)' staggered conformation 69 hits are 'face to face (3:3)' eclipsed.

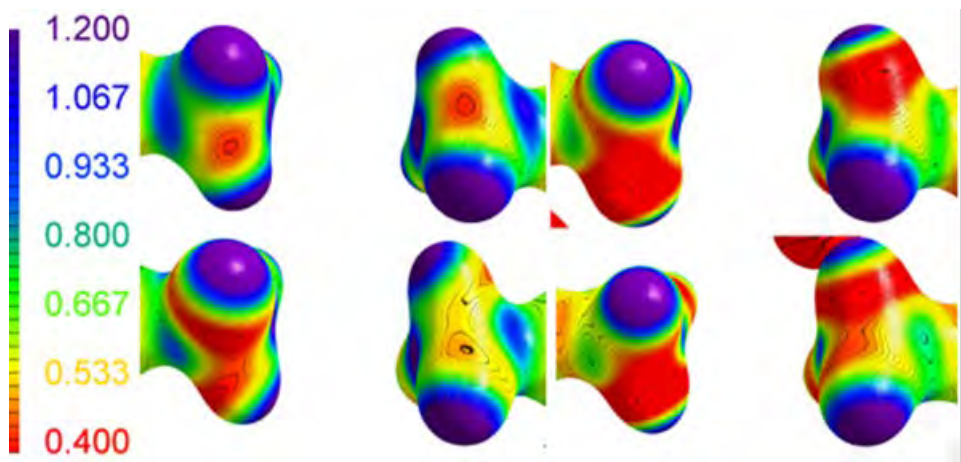
Sounak Sarkar



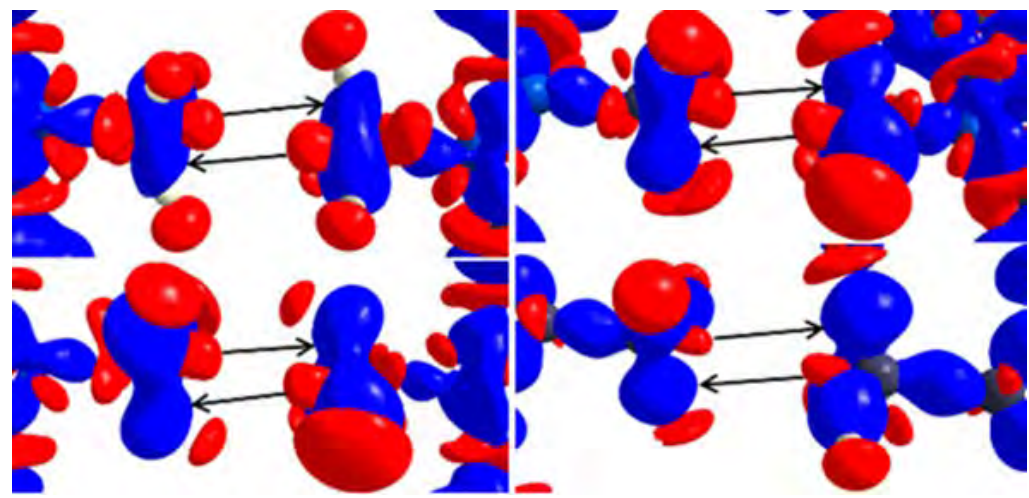
High resolution
Charge density analysis

Quantum Crystallography

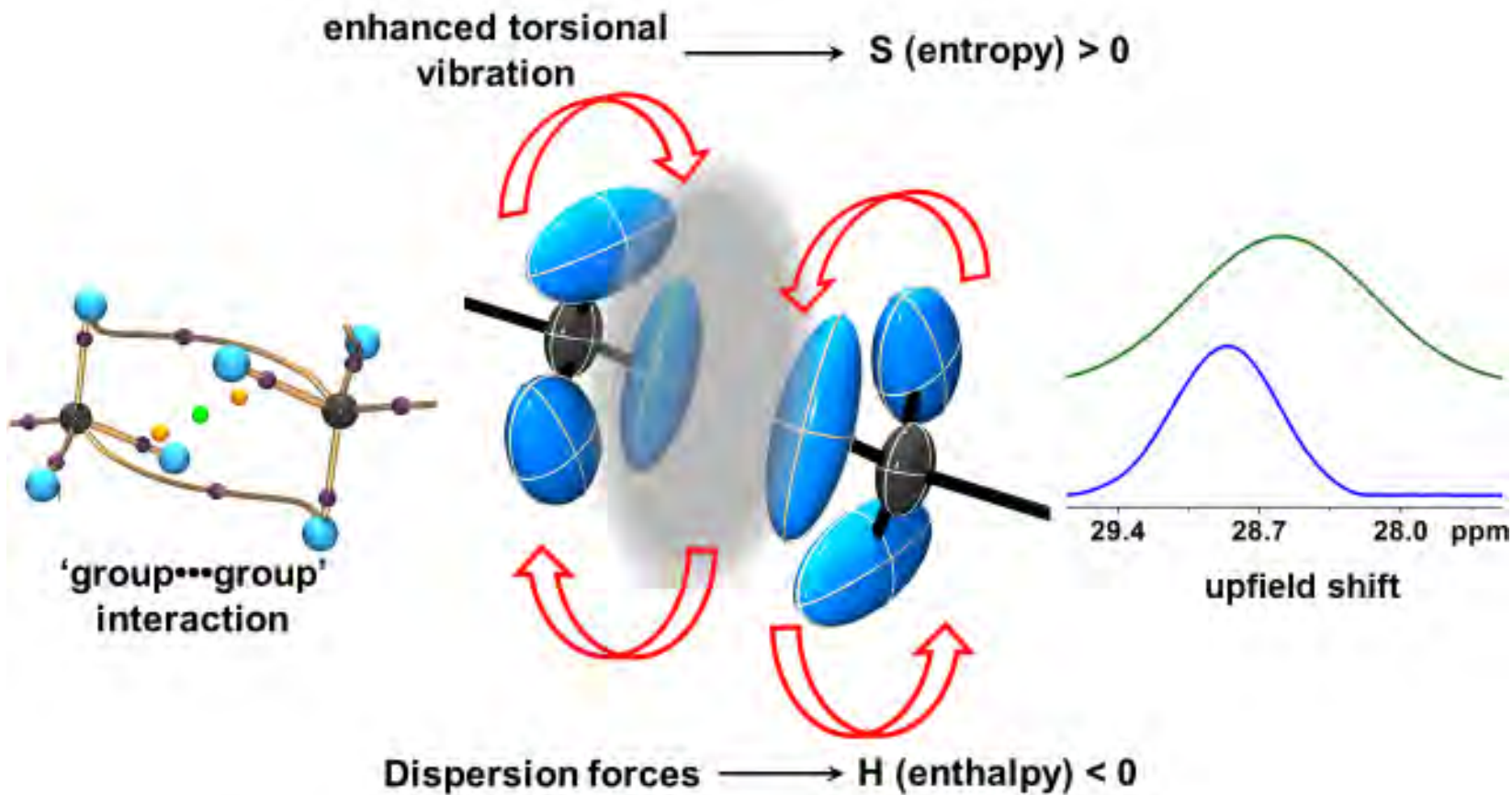
Quantum Crystallography techniques based on high resolution X-ray data , charge density analysis and quantum chemical calculations



ESP maps



3D Deformation maps



Me...Me hydrophobic interactions in molecular crystals are found to be weak but stabilizing in nature, their stability arises mainly from dispersion and an entropy contribution associated with the methyl rotational oscillations.

Me...Me HIs are quite distinct from the homohalogen interactions such as Cl...Cl or Br...Br in their electronic nature and more importantly in the significant role of rotational entropy in their stabilization .

A systematic upfield shift found consistently in the C13-ssNMR spectra of these crystalline complexes are characteristic of these Me...Me contacts, and these signatures may serve as means to identify hydrophobic interactions in the solid-state.



UNIVERSITY OF
WOLLONGONG



ICDD Regional Co-Chair: Indian Ocean Rim

Prof. Vanessa K. Peterson
Australian Centre for Neutron Scattering
& University of Wollongong
vanessa.peterson@ansto.gov.au

Science. Ingenuity. Sustainability.

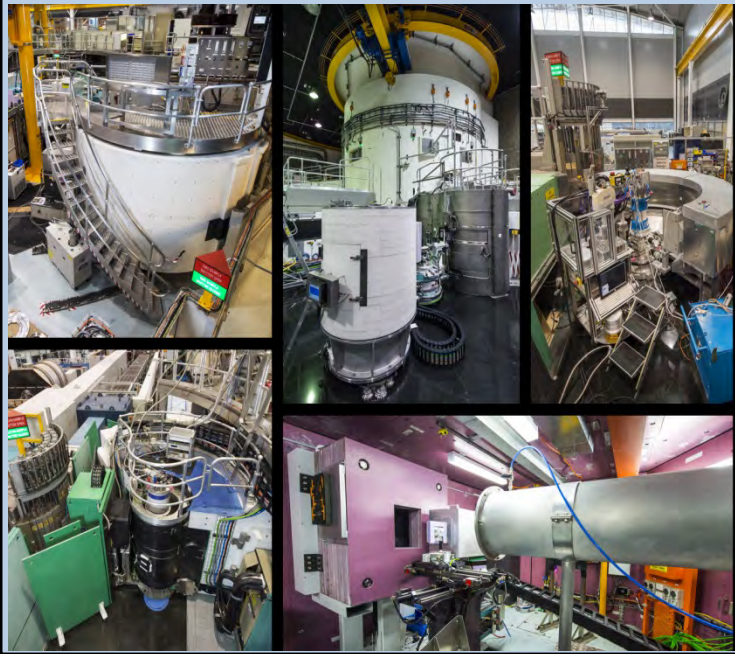


Australian Centre for Neutron Scattering

UNIVERSITY OF
WOLLONGONG



INSTITUTE FOR
SUPERCONDUCTING AND
ELECTRONIC MATERIALS



Collaborative Research Project: Functional Materials for Energy Systems & Devices

Battery materials

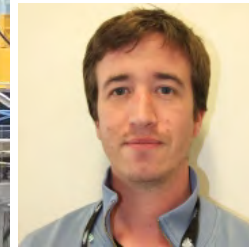
- Dr Christophe Didier (current – 2020)
- Dr Wei Kong Pang (2013-16: U of Wollongong)
- Dr Neeraj Sharma (2009-12: UNSW)



Coordination framework materials

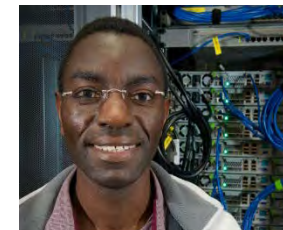
- Dr Josie Auckett (2015-18: Durham)
- Dr Hubert Chevreau (2012-15: Soleil)
- Dr Sam Duyker (2011-14: USyd)

SCIENCE AND
INDUSTRY
ENDOWMENT
FUND



Computational methods

- Dr Elvis Shoko (2010-13: Wits Uni, South Africa)



Indian Ocean Rim

“Down Under”



Region Overview

Membership:

- Good active membership (10 members in Australia – 11 last year).
- What about New Zealand? Singapore?
- Engage biological community in Australia – protein crystallography

Ludo Frevel Scholarships:

- Awardee: Alexios Vicatos, University of Cape Town, Cape Town, South Africa “Supramolecular Derivatisation of Pharmaceutically Relevant Compounds via Co-Crystallization and Cyclodextrin Inclusion Complexation” (another in Australia in 2017).
- Applications (note ICDD activity in Ghana recently)
 - Australia 4
 - Malaysia 1
 - South Africa 8
 - Nigeria 4
 - Zimbabwe 1

Grant-in-Aid:

- None in region in Cycle I or II 2019.
- Future: Opportunity in the region – promote to members

Past Activities: March - July 2018

No physical exhibits from ICDD in region in 2018

- Focus on Microscopy Singapore, 25th March 2018



Past Activities: August 2018

1st meeting:
Colombo 2016

SUNWAY UNIVERSITY
A CLASS ABOVE
DU 025 (B)

2ND SOUTHEAST ASIAN CONFERENCE ON CRYSTAL ENGINEERING (SEACCE-2)

6-8 August 2018 | Sunway University, Malaysia

[Find out more](#)

POSTER PRIZES TO BE WON!

Diamond Sponsors:

Other Sponsors:

XXII MEETING OF THE INTERNATIONAL MINERALOGICAL ASSOCIATION
13-17 AUGUST 2018 | MELBOURNE



- International Mineralogical Association 22nd meeting
- Melbourne, Australia (August 2018)

Past Activities: September 2018



- 9th interdisciplinary workshops: South African Crystallographic Society (SACrS) & IUCr's Structural Chemistry Commission (Indaba 9): "Modelling of Structure and Properties"



- Kruger National Park, South Africa

Past Activities: October 2018

Neutrons and Food 5



Venue

Novotel Darling Harbour
100 Murray Street
Pyrmont NSW 2009

Sydney, Australia



Past Activities: November 2018

Combined Australian Materials Societies



CAMS 2018
Advancing Materials and Manufacturing

The 6th conference of the Combined Australian Materials Societies;
incorporating Materials Australia and the Australian Ceramic Society.

Materials
Australia

November 27-29
University of
Wollongong
NSW AUSTRALIA



Past Activities: November 2018



NEUTRON SCATTERING SYMPOSIUM 2018

NOVEMBER 19 - 21 | SYDNEY - AUSTRALIA



10TH AONSA 2018 NEUTRON SCHOOL

11 -16 NOVEMBER 2018 ANSTO, SYDNEY AUSTRALIA



ICDD CONFIDENTIAL INFORMATION

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Past Activities: December 2018

- Asian Crystallographic Association (AsCA) & 32st Conference of the Society for Crystallographers in Australia and New Zealand (CRYSTAL 32)
- 6th International Conference on Metal-Organic Frameworks and Open Framework Compounds (MOF2018)
- Auckland, New Zealand

AsCA 2018  **CRYSTAL 32**
December 2-5 2018 | Auckland, New Zealand

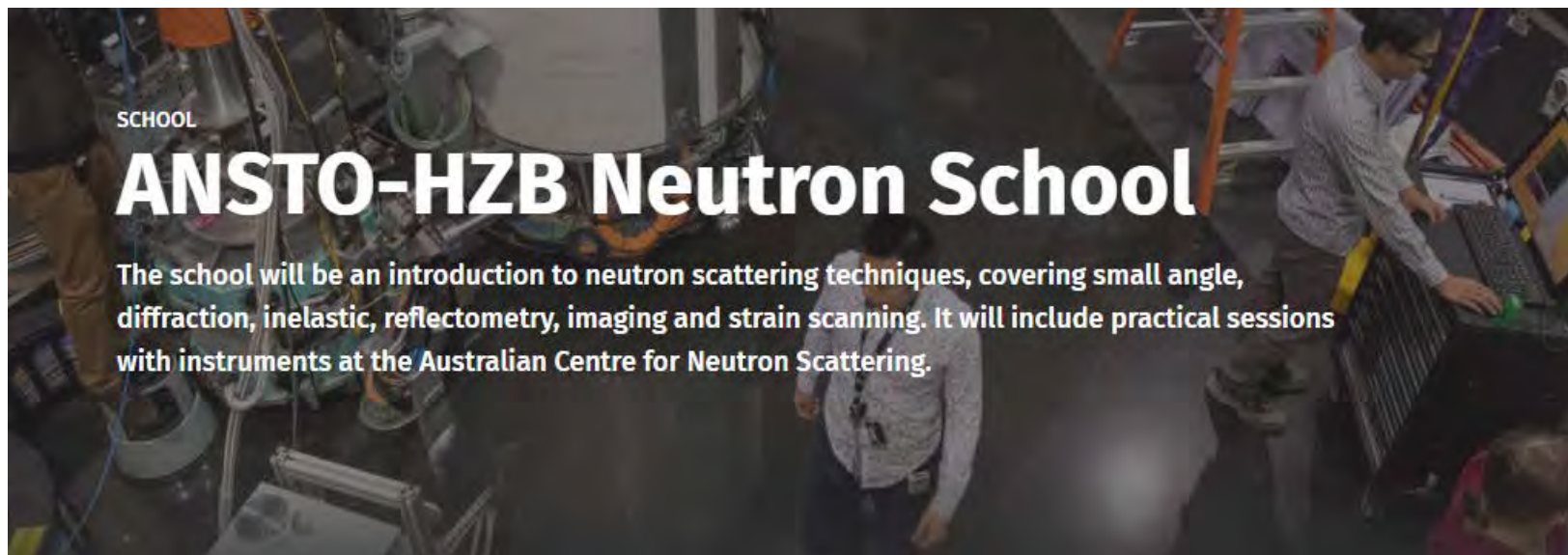


MOF2018
6th International Conference
ON METAL-ORGANIC FRAMEWORKS
& OPEN FRAMEWORK COMPOUNDS

DECEMBER 9-13, 2018
AUCKLAND, NEW ZEALAND

- Conference committee

Upcoming Activities: June 2019



Australian Centre for Neutron Scattering

Upcoming Activities: September 2019



The Mineralogical Society
of Western Australia Inc.

TRAPS IN MINERALOGY PSEUDOMORPHS, LOOK-ALIKES, FAKES AND SYNTHETICS

42nd Joint Mineralogical Societies of Australasia Seminar

31 August – 1 September 2019 • Perth, Western Australia

Other activities and field trips will take place before and after the seminar.

INTERNATIONAL CONFERENCE ON
MATERIALS SCIENCE
AND ENGINEERING 2019



Event Date: September 16-18, 2019



Event Location: Pullman Melbourne Albert Park, Australia

Upcoming Activities: December 2019



- Chunhua Xu, ICDD Office, China

NIS Co-Chair report (2018 – 2019)

3rd Baikal Materials Science Forum 9-15 July 2018



**III Байкальский материаловедческий форум,
9-15 июля 2018 г. (г. Улан-Удэ и оз. Байкал, с. Горячинск)**

Sponsored by the ICDD

263 participants from 20 cities in Russia (Chernogolovka, Irkutsk, Krasnoyarsk, Magnitogorsk, Moscow, Novosibirsk, Perm, Saint Petersburg, Skolkovo, Sterlitamak, Syktyvkar, Tomsk, Troitsk, Tumen, Voronezh, Ufa, Ulan-Ude, Vladivostok, Yakutsk, Yekaterinburg, Zelenograd),

and from Canada, Germany, Mongolia, France, Sweden, and Switzerland

The ICCD booth was exhibited

3rd Baikal Materials Science Forum



Conference participants at the lake Baikal (left) and the winners of the best presentations of young scientists and students (right)

ICDD booth



Dmitry Sklovsky, Evgeny Antipov and Elena Khaikina (conference organizer) at the ICDD booth during the conference

IX Crystal Chemistry conference – June 4-8 2018, Suzdal



218 participants from Russia

Plans for 2019/2020

XIX INTERNATIONAL MEETING ON CRYSTAL CHEMISTRY, X-RAY DIFFRACTION AND SPECTROSCOPY OF MINERALS 2-5 JULY 2019, APATYTY



Dedicated to the memory
of Academician E.S. Fedorov (1853 - 1919)



Sponsored by the ICDD,
ICDD booth

Report of the Technical Regional Co-Chair – North America –

**March 2019
Mark Rodriguez**

2018 XRF Clinic



24-28 April • 14 Attendees

Fundamentals
5 – 9 June
26 attendees

2018 XRD Clinics



26



18

2018 Rietveld Refinement and Indexing Workshop

Basic & Advanced

25 – 27 Sept • Registrations: 17





67th Annual Denver X-ray Conference

57 Exhibits Sold • 44 Companies
417 Attendees + Exhibit staff



North American Meetings: 2018-19

Key Exhibits, Educational Events, Student Support

Materials Research Society

Phoenix, AZ • 2 - 6 April 2018

EXHIBIT + STUDENT SUPPORT

ACA Summer Course in Chemical Crystallography

Univ. Notre Dame, IN • 10 – 18 June 2018

DEMO DATABASES

Gordon Research Seminar

Sunday River, ME • 23 – 24 June 2018

STUDENT SUPPORT

New York University X-ray Workshop

New York, NY • 27 - 28 June 2018

STUDENT SUPPORT



MRS Spring – Phoenix
Exhibit &
Students Supported by ICDD

North American Meetings: 2018-19 *(continued)*

Microscopy & Microanalysis

Baltimore, MD • 5 – 9 August 2018

EXHIBIT

Denver X-ray Conference

Westminster, CO • 6-10 August 2018

EXHIBIT, USERS' MEETING, DEMO DATABASES

Materials Science & Technology

Columbus, OH • 14 – 18 October 2018

EXHIBIT

Geological Society of America

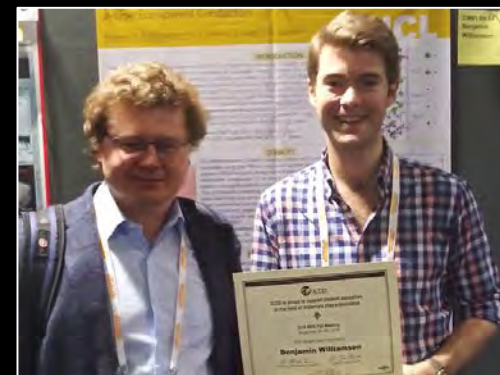
Indianapolis, IN • 4 - 7 November 2018

EXHIBIT

Materials Research Society

Boston, MA • 25 - 30 November 2018

EXHIBIT + STUDENT SUPPORT



MRS Fall – Boston
Students Supported by ICDD

Regional Report from China

Xiaolong Chen

Beijing National Laboratory for Condensed Matter Physics
And Institute of Physics, Chinese Academy of Sciences

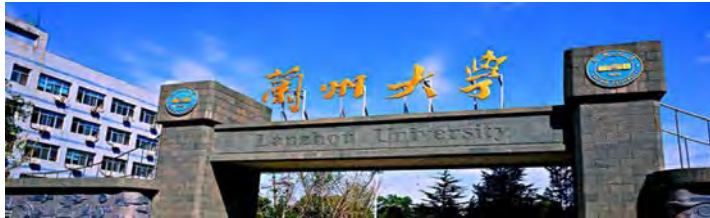
ICDD CONFIDENTIAL INFORMATION
March 14, 2019 ICDD Headquarters

2018 Events

13th National conference on x-ray diffraction and ICDD workshop

Place: Lanzhou City

Time: 28. July-01. August 2018



中国地图



审图号：GS(2016)2881号
国家测绘地理信息局 监制

Attendee:

ICDD CONFIDENTIAL INFORMATION

~380 Page 66 of 108

2018 Events

13th National conference on x-ray diffraction and ICDD workshop

第十三届全国X-射线衍射学术大会暨国际衍射数据中心(ICDD)研讨会
13th National Conference on X-ray Diffraction and ICDD Workshop

2018.7.30 兰州



ICDD CONFIDENTIAL INFORMATION

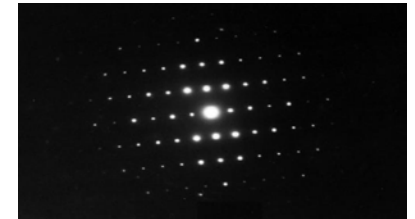
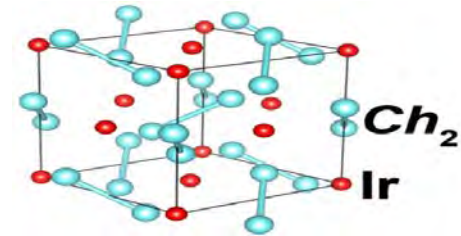
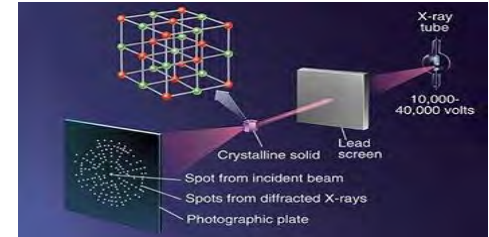
Page 67 of 108

13th National conference on x-ray diffraction and ICDD workshop

Topics

- X-ray diffraction technology
- Structural analysis
- New materials
- Film and interface
- Small angle scattering
- Texture and stress
- Neutron and electron diffractions
- **Industrial applications**

...

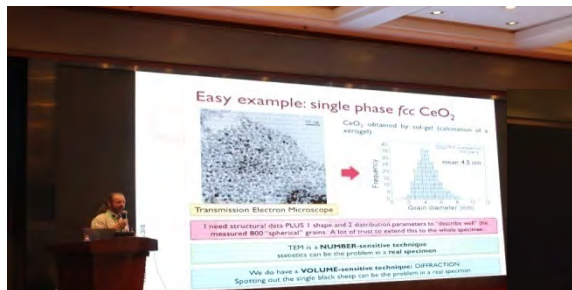


2018 Events

ICDD Workshop and Member Meeting



ICDD Member Meeting



ICDD workshop
ICDD CONFIDENTIAL INFORMATION

2018 Events

First Asia-Pacific Conference on Silicon Carbide and Related Materials

July 5-7, 2018
Beijing



~450 attendees



ICDD CONFIDENTIAL INFORMATION

Page 70 of 108

2018 Events

Chinese Crystallography Society Meeting



Tianjin
Nov. 3-7, 2018

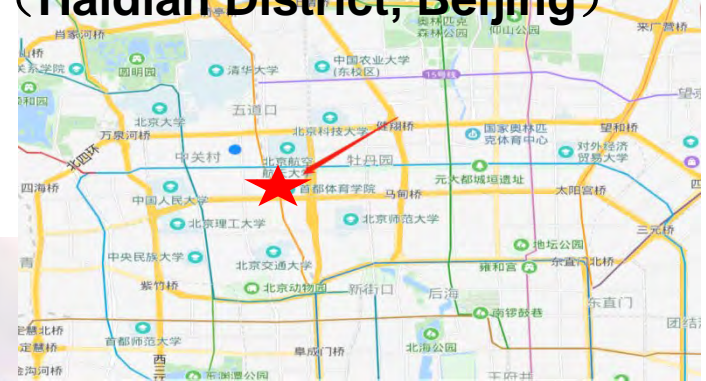
ICDD Representative Office in China

Establish ICDD China RO

ICDD China RO Certificate (Released in January, 2019)



ICDD China RO location (Haidian District, Beijing)



ICDD CONFIDENTIAL INFORMATION

Chunhua Xu at work

- Answer customers' inquiries regarding PDF products
- Advertising ICDD products on Chinese media(free)
- Help customers to purchase ICDD products
- Find good agents
- C...



PDF-4 2019 有机物卡片数据库

报价	60000(元)	APP查看历史信息	产地	美国
型号	PDF-4/Organics 2019		品牌	国际衍射数据中心
样本	下载			

北京嘉德利达科技有限公司 (理学产品代理)

营业执照	已审核	品牌性质	经销商	银牌会员	第11年
信用积分	2956	反馈速度	21-24小时	同类仪器	8星

400-860-5168转2204 仪器信息网认证,请放心拨打

[免费留言咨询](#) [预约在线交流会](#)

ICDD CONFIDENTIAL INFORMATION



PDF 卡片数据库使用说明

作者姓名: 徐春华

职务: 国际衍射数据中心 (ICDD) 中国区代表

联系电话: 13401176510

邮箱: icddchina@163.com

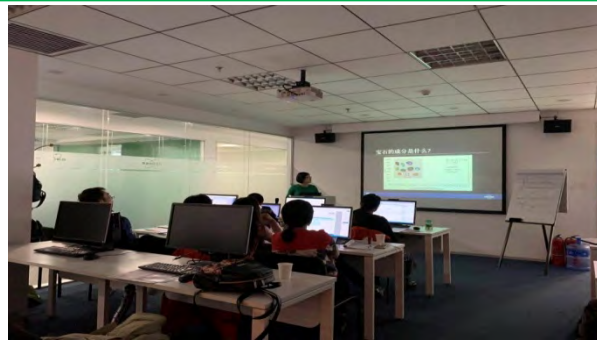
地址: 北京市海淀区西土城路1号7号楼822室

2018年12月 Page 74 of 108

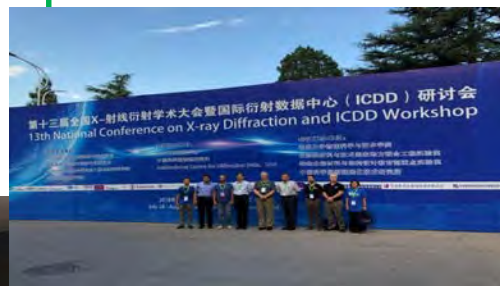
Chunhua Xu at work

Meetings and Workshops

Rigaku and Bruker Users' Workshop



X-ray and Crystal Meetings



ICDD CONFIDENTIAL INFORMATION

Five new distributors



➤ **Shuyun Instruments Co.,Ltd
@ ShangHai**

➤ **Prime Sun @ GuangZhou**
➤ **Beijing Advance Science
& Technology Corporation @ Beijing**

The Rigaku logo is the word "Rigaku" in a bold, blue, sans-serif font.



CCrS

➤ **Beijing Texture Technology Co., Ltd.**

➤ **Neotrident Technology Ltd.
(Very successful in selling
Material Studio software in China)**



- Cooperation with CCRs

- Chinese Crystal Society (CCrS) put ICDD introduction, PDF products on its official website.
- Website address: <http://www.ccrs.net.cn/ICDD/>

ICDD-PDF 数据库



国际衍射数据中心 (ICDD) 概况



国际衍射数据中心 (The International Centre for Diffraction Data, ICDD)

是由成立于1941年的粉末衍射化学分析联合会演变而来，科学组织，致力于收集、编辑、出版和分发标准粉末衍射数据(数据库)，其主要用于结晶材料的物相鉴定。ICDD是全球XRD领域的权威。

PDF-4+ (仅限于PDF-4系列产品)



PDF-4+ 数据库

- 物相鉴定+定量分析
- 最大最全面的无机物相衍射数据库
- 同时含有物相结构数据、衍射数据
- 有机物相衍射数据: 43,516 衍射条目



ICDD CONFIDENTIAL INFORMATION

Page 77 of 108

Feedbacks

PDF users

- One PDF license can be only installed in one computer, hope more substantial discount for slave licenses.
- hope to receive the newest database immediately after new release is available
- Shipping fee is expensive.
- **Additional 5% Customs Tax because of the Sino-US trade friction**
-

Distributors

- Distributors are not willing to handle Multi-years shipping. Hope ICDD database can be downloaded online for the renewal users.
- Multi-years license products should have more discounts.
- The current sales catalog is too complex to understand.
-

Forthcoming Plan

ICDD-PDF users' workshop

Place: Beijing

Time: ~ September 2019

Estimated attendee: ~150

A two-day ICDD users' workshop

Topic

- Overview introduction to ICDD
- Fundamentals of crystal structure
- Fundamentals of powder diffraction
- Capabilities and features of PDF databases
- How to use PDF database and why choose PDF database(over COD and others by examples)
- How to submit PDF Card
- GIA program, awards, fellowship and education
-

Thanks!

REGIONAL CO-CHAIR: Latin America 2018 - 2019

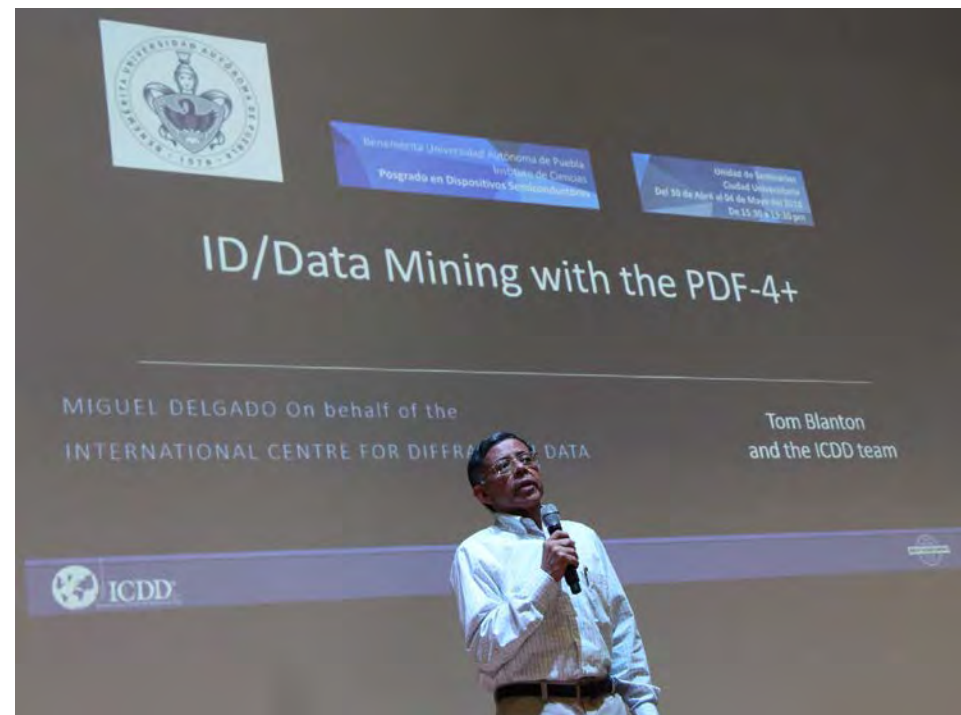
Miguel Delgado

2018



**X-Ray Powder Diffraction Course
BUAP, Puebla, Mexico
April 30 – May 5**

ICDD CONFIDENTIAL INFORMATION



Organizers:

- Prof. Javier Martínez-Juárez (ICDD member)
- Dra. María Josefina Robles Aguilar

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EL CENTRO DE ESTUDIOS SUPERIORES DE ENERGÍA Y MINAS, CESEM INVITA A PARTICIPAR EN EL

SEMINARIO CRISTALOGRAFIA Y DIFRACCION DE RAYOS X

PARA SU USO EN LA CARACTERIZACIÓN DE MATERIALES

COMO PARTE DE LA CREACIÓN DE LA ASOCIACIÓN GUATEMALTECA DE CRISTALOGRAFÍA

IMPARTIDO POR
DR. DIEGO LAMAS/ ARGENTINA
DR. MIGUEL DELGADO/VENEZUELA




Seminars on Crystallography and X-Ray Diffraction
CESEM, Facultad de Ingeniería, USAC – Cementos Progreso.
Ciudad de Guatemala, GUATEMALA, May 7-9, 2018.



ICDD CONFIDENTIAL INFORMATION

Compartimos Sueños. Construimos Realidades.



Seminars on Crystallography and X-Ray Diffraction
CESEM, Facultad de Ingeniería, USAC – Cementos Progreso.
Ciudad de Guatemala, GUATEMALA, May 7-9, 2018.



Founding of the Guatemalan Crystallographic Association

ICDD CONFIDENTIAL INFORMATION

Espoch

I-CIQ-EC-18
1er Congreso Internacional de Química - Ecuador

31 de julio al 2 de agosto de 2018
Espoch, Riobamba

Ada Yonath
Premio Nobel de Química - 2009

Envío de trabajos hasta:
04 de julio de 2018

Aceptación de trabajos:
13 de julio de 2018

Asistentes no expositores

Asistentes no expositores	Costo \$
Profesionales	150
Estudiantes	60

Ponencias

Profesionales:	200
Estudiantes (Pregrado)	100

Posters

Profesionales:	150
Estudiantes (Pregrado)	80

AREAS:

- Química Orgánica
- Química Inorgánica
- Química Física
- Química Analítica
- Bioquímica
- Nanomateriales
- Química Computacional

INVITADOS:

- Diego Lamas - UNSAM (Argentina)
- Mauricio Escudey - USACH (Chile)
- Graciela Díaz de Delgado - ULA (Venezuela)
- Milton Rosero - UCaldas (Colombia)
- Hortensia Rodríguez - Yachay (Ecuador)
- Javier Torres - USFQ (Ecuador)
- José Luis Paz - EPN (Ecuador)
- María Elena Cazar - UC (Ecuador)
- Gianluca Gilardoni - UTPL (Ecuador)
- María Eugenia Lucena - ULA (Venezuela)
- Omar Malagón - UTPL (Ecuador)

Información:
ciq2018@esPOCH.edu.ec
<https://congresoquimicaecuador.wordpress.com>

Riobamba, ECUADOR.
Satellite course "Introduction to Crystallography"
(July 27, 28 and 30)
International Chemistry Congress (July 31-August 2) 2018

Support from IUCr, ICDD, and LACA

I-CIQ-EC-18
1er Congreso Internacional de Química - Ecuador 2018
Curso Pre-Congreso 1
Introducción a las Técnicas Cristalográficas

27, 28 y 30 de julio, Riobamba, Ecuador

Diego Lamas
Universidad Nacional de San Martín
Argentina

Graciela Díaz de Delgado
Universidad de los Andes
Venezuela

José Miguel Delgado
Universidad de los Andes
Venezuela

Dirigido a: estudiantes de pregrado, estudiantes de Maestría o Doctorado, investigadores, interesados en el tema
Costo: 30 dólares (40 horas + aprobación)
Contacto: jorge.silvay@uta.edu.ec



Cancún México
August 19-24, 2018

D6. Characterization of Nanomaterials Using Diffraction and Combined Techniques

Organizers: Lauro Bucio Galindo (UNAM-Mexico)
Thomas N. Blanton (ICDD, USA)
José Miguel Delgado (ULA, Venezuela)

Symposium Topics:

- Structural Characterization of Nanomaterials.
- Pair Distribution Function (PDF) analysis.
- Characterization of Microstructure in Nanomaterials.
- In-situ Characterization of Nanomaterials.
- Use of X-ray and Electron Diffraction techniques.
- 3D Electron Diffraction Tomography.
- Neutron Scattering study of Nanomaterials.
- Structure and Microstructure of Nanomaterials using spectroscopic techniques.
- Structure-Property correlations in Nanomaterials

Invited Speakers

- Fábio Furlan Ferreira (UFABC, Brazil)
- Miguel Angel García Aranda (ALBA, Spain)
- Jacob Jones (North Carolina State Univ., USA),
- Matteo Leoni (University di Trento, Italy) ←
- Beatriz Millán Malo (UNAM, México)
- Scott T. Misture (Alfred University, USA)
- Stavros Nicolopoulos (NanoMEGAS, Belgium)
- Eric Mauricio Rivera Muñoz (UNAM, México)

Video presentation



IMRC Daily News

Day 4. Wednesday, August, 22 | 2018

❖ Plenary 4: MOLECULAR MACHINES



With a very broad participation of the congressperson, this awaited conference was carried out. Prof. Ben L. Feringa, Nobel Prize in Chemistry 2016, using simple wording and interesting videos showed as the molecular motors and machines that sustain life offer a great source of inspiration to the molecular explorer at the nanoscale. In his presentation, he showed that it can be possible to design switches and motors in which molecular motion is coupled to specific functions. It was an inspirational conference.

❖ ORAL SESSIONS

During this day, 16 symposia were done, in which an abundant concurrence, continued their oral presentation. Several topics such as Solar Hydrogen Production, Machine Learning and Data Science in Materials Synthesis, Characterization and Modeling, Functional Surfaces and their Interactions with Biological Systems, Characterization of Nanomaterials Using Diffraction and Combined Techniques, amount others. Speakers from many countries shared their scientific ideas and discuss their results.



Technical Session



You are Invited to the International Centre for Diffraction Data (ICDD) Technical Session at the International Materials Research Congress 2018



Materials Characterization Using XRD and the ICDD PDF-4+ Database

- Presenters
- Thomas Blanton, ICDD
 - Miguel Delgado, Universidad de los Andes

Wednesday, 22 August, 14:00 to 15:45
JW Marriott – Palenque Room

Questions?
Contact Benjamin Hish – Hish@icdd.com



**MEXICAN SOCIETY
OF CRYSTALLOGRAPHY**



IX NATIONAL CONGRESS OF CRISTALLOGRAPHY

XII NATIONAL MICROSCOPY CONGRESS

MEETING OF SYNCHROTRON LIGHT USERS



PROGRAM



0

**SMCr. IX National Congress of Crystallography
XII National Congress of Microcopy
Meeting of Synchrotron Light Users
October 20-25, 2018. Oaxaca, Mexico.**

C o u r s e s

Introducción a la Microscopía Electrónica de Barrido y Técnicas de Análisis EDS

Carlos Segovia, *Micra Ingeniería S.A., México*

Enrique Enríquez, *Micra Ingeniería S.A., México*

SAXS a Power Tool for Nano-Structure Analysis

Gerd Langenbacher, *Anton Paar the Americas, U.S.A.*

Radiación Sincrotrón

Abel Moreno & Colegas

Observación e Interpretación de Imágenes Crio TEM y Tomografía

Abraham Hernández, *Hospital Infantil de México Federico Gómez, México*

Luis Felipe Jiménez, *Facultad de Ciencias, UNAM, México*

Resolviendo Estructuras por TEM & STEM

Arturo Ponce, *University of Texas, San Antonio, U.S.A.*

Uso de la Base de Datos PDF-4+. Minería de Datos

Lauro Bucio, *Instituto de Física, UNAM, México*

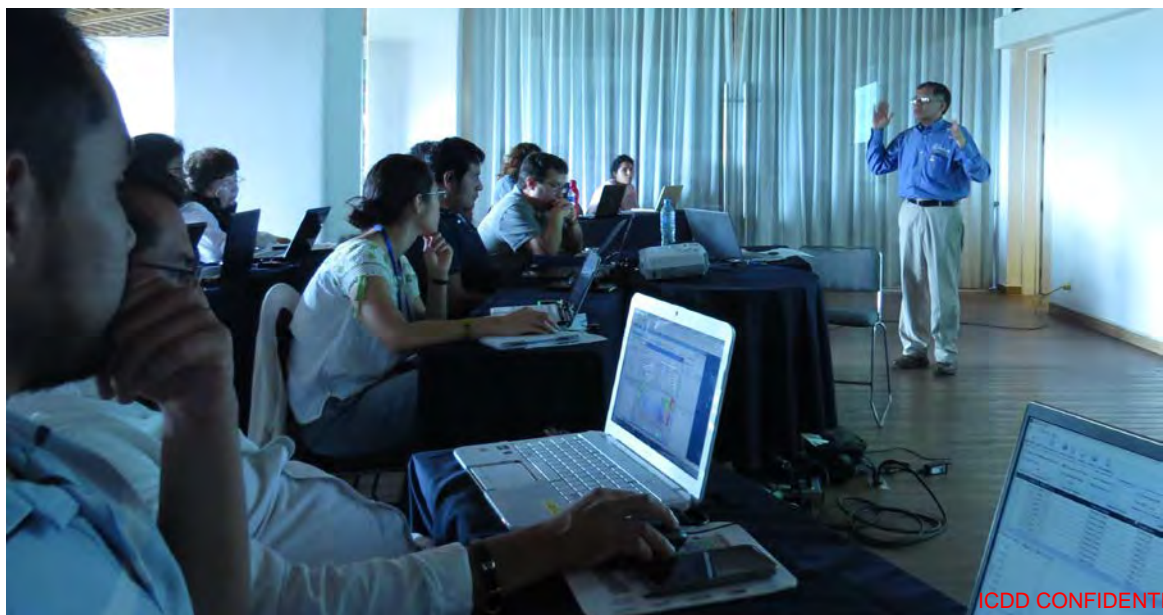
Miguel Delgado, *Universidad de los Andes, Mérida, Venezuela*



Curso Pre-Congreso: “Uso de la base de datos PDF-4+ en el Análisis de Materiales por Difracción. Minería de datos”

INSTRUCTORES: Prof. Miguel Delgado (Lab. Cristalografía, ULA, Venezuela)
Prof. Lauro Bucio (Inst. de Física, UNAM, Ciudad de México)

October 20-21, 2018




IUCr in Mexico in 2026?

SMCr (2018-2021)

- President: Abel Moreno-Cárcamo
- Javier Martínez-Juárez
- Gonzalo González

LACA (2019-2021)

- President: José Reyes Gasga (México)
- Vice President: Miguel Delgado (Venezuela)
- General Secretary: José Roberto Vegas (Costa Rica)
- Adjunct Secretaries: - Natalia Alvarez (Uruguay)
- Mauricio Fuentealba Carrasco (Chile)
- Treasurer: Iris Torriani (Brasil)
- Past President: Diego Lamas (Argentina)



III REUNIÓN DE LA ASOCIACIÓN LATINOAMERICANA DE CRISTALOGRAFÍA I ENCUENTRO DE LA AChCr

III Meeting of the
Latin American Crystallographic Association, LACA
October 8-12, 2018
Valparaiso, Chile.





III REUNIÓN DE LA ASOCIACIÓN LATINOAMERICANA DE CRISTALOGRAFÍA I ENCUENTRO DE LA AChCr



Satellite Meeting
XRPD and the PDF4-ICDD database
9 de Octubre 2018
Universidad Federico Santa María (UFSM)
Dpto. de Ingeniería Metalúrgica y Materiales
Valparaíso, CHILE





Centro de Física Aplicada y Tecnología Avanzada



*UNAM-CFATA, Querétaro, MEXICO, October-November 2018
Prof. Mario Rodríguez and Eric Rivera-Muñoz (ICDD-member)*



*Four weeks intensive graduate course on
"X-Ray Powder Diffraction"*



*One week intensive course on
"X-Ray Powder Diffraction" for nearby Academic Institutions*



Pucón, CHILE
November 4-7, 2018





SARX-WORKSHOP

**CHEMFORS-2018 – Cultural Heritage Materials and Forensic Sciences:
From authentication to crime evidences through analytical tools.
November 8-9, 2018**

Organizers: Ignasi Queralt (CSIC, Barcelona, Spain)
Miguel Delgado (ULA, Venezuela)
Oswaldo Maldonado (Soluciones Analíticas, SAX, Chile)

ICDD CONFIDENTIAL INFORMATION

*To.Sca.Lat.-1.0: Diffraction and Total Scattering Analysis for Advanced Materials and NanoScience,
Vila Fátima, Florianópolis, Brasil, 10-14 December 2018*



ICDD CONFIDENTIAL INFORMATION

Invited Speakers:

- Prof. Norberto Masciocchi, Univ. Insubria, Como, Italy.
- Dr. Antonella Guagliardi, Institute of Crystallography CNR, Como, Italy.
- Prof. Matteo Leoni, Univ. Trento, Italy.
- Dr. Federica Bertolotti, Aarhus University, Denmark.
- Dr. Alexandre Magnus Gomes Carvalho, LNLS/Brasil.

New ICDD Member



PROF. CLAUDIO EDUARDO AGUILAR RAMIREZ
Departamento de Ingeniería Metalúrgica y Materiales
Universidad Técnica Federico Santa María
Avenida España 1680, Valparaíso, CHILE
claudio.aguilar@usm.cl

Organizers of the IV LACA Crystallography School
(Powder Diffraction –*Microstructure*-)

Valparaíso, Chile.

Nov. 30 – Dec. 5, 2020

Prof. Claudio E. Aguilar Ramírez,

Dr. Raúl Cardoso-Gil

(*Max Planck Institut für Chemische Physik fester
Stoffe, Dresden*),

Prof. Miguel Delgado

(*Universidad de Los Andes*).

NEXT MEETINGS



ICDD Booth and Technical session
Justin Blanton and Miguel Delgado

GiA Workshop
IV MEXICAN MEETING ON DIFFRACTION
Pachuca, Hidalgo, November 2019

**IV MEETING OF THE
LATIN AMERICAN
CRYSTALLOGRAPHIC
ASSOCIATION**

OCTOBER 7th-10th, 2019. BUGARAMANGA, COLOMBIA.

I MEETING OF THE
COLOMBIAN
CRYSTALLOGRAPHIC
SOCIETY

II LACA SCHOOL

October 1th-6th, 2019
Piedecuesta, Colombia



 fb.me/LACA2019  IV Reunión LACA 2019  lacacolombia2019@gmail.com

Prof. José Antonio Henao (ICDD member)
Chairman of the Organizing Committee

¡GRACIAS!

Regional Co-Chair Report for the United Kingdom & Ireland

Steve Hillier

Activities since March 2018

- Clay Minerals Society Annual Meeting
 - Urban-Champaign Illinois 11-14 June 2018
- EPDIC
 - Edinburgh 1-4th July 2018
- Mid European Clay Conference
 - Zagreb, Croatia, 17-21st September 2018

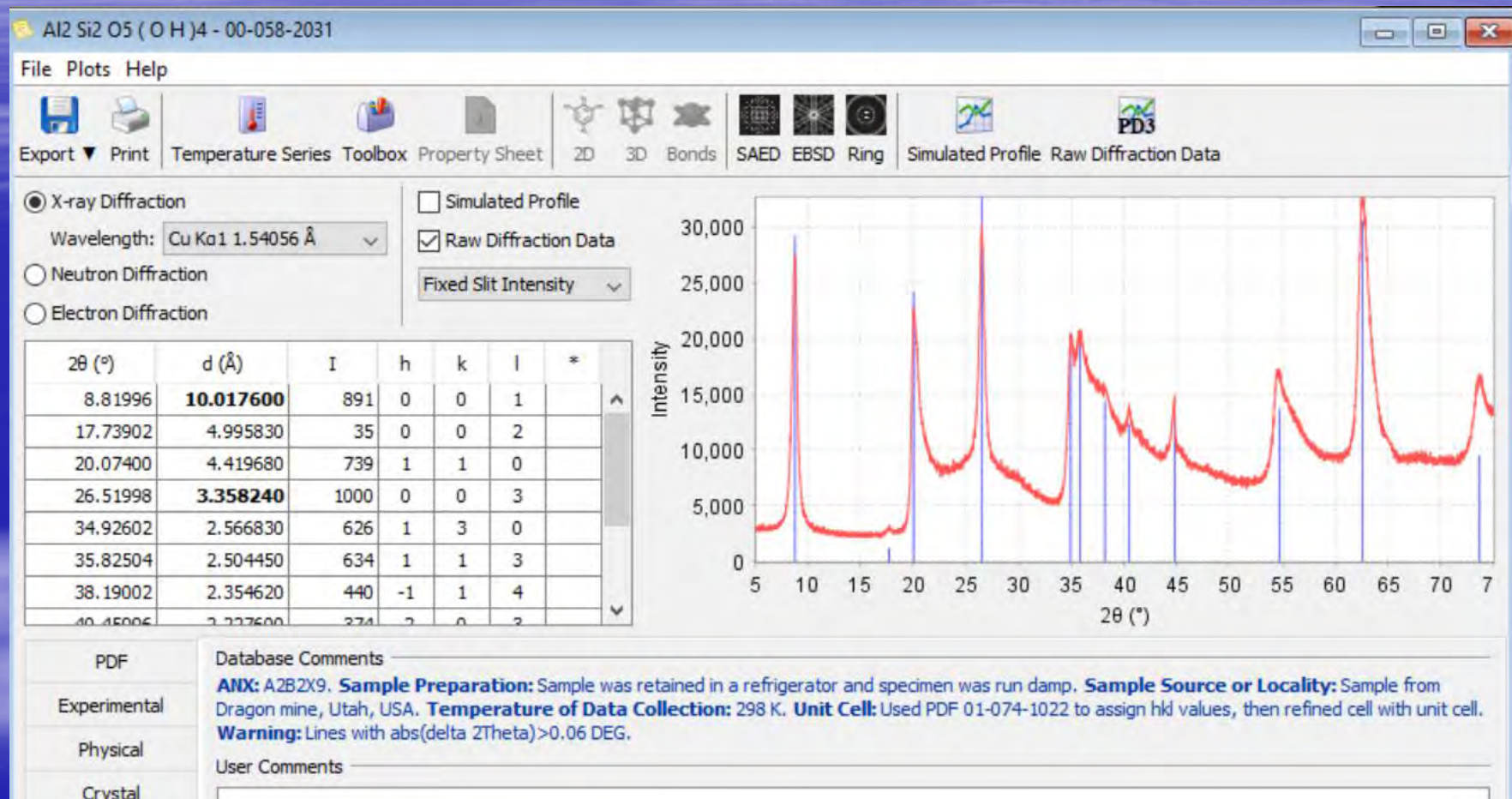
Clay Minerals Task Group

- Review of clay data in PDF
- Some of the issues
 - Representation of clay diffraction bands?
 - Oriented vs Random powder data (PDF has both)
 - Multiple diffraction patterns for different treatments of same sample (could a search consider more than one pattern at a time?) E.g. 00-058-2038, 00-058-2039, 00-058-2040, 00-058-2041

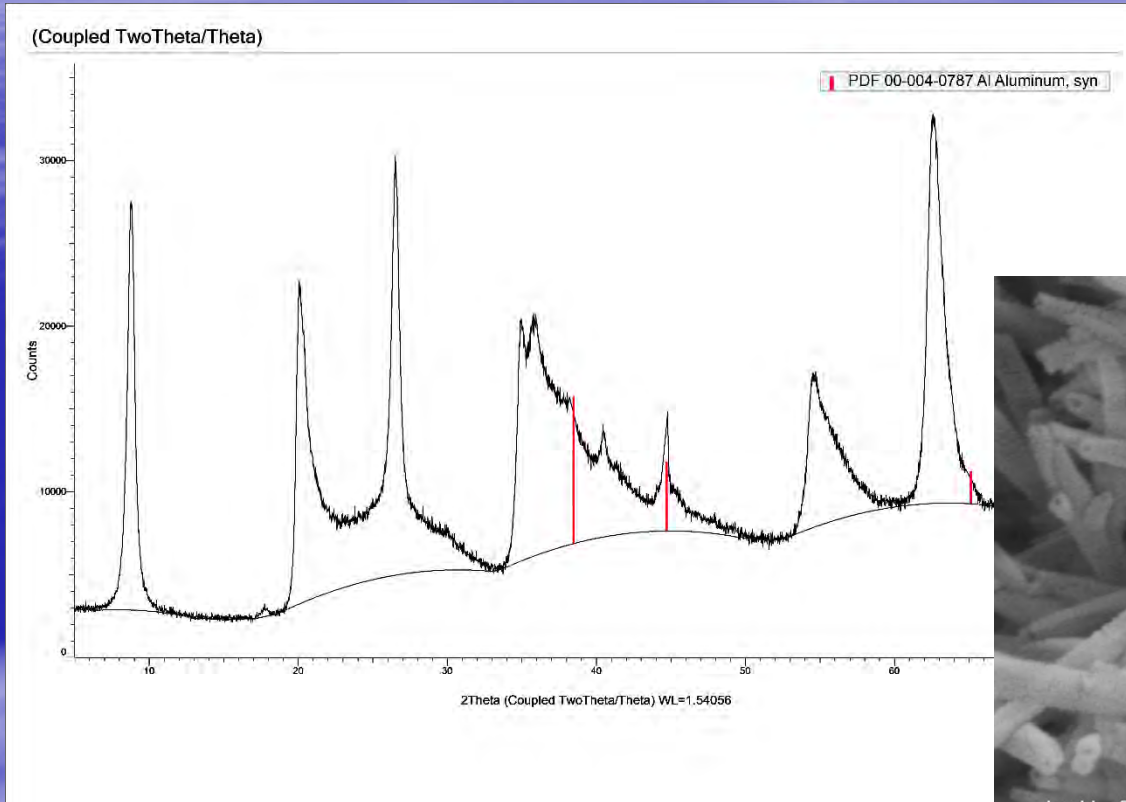
Clay Minerals Task Group

H	J	K	L
MinSubGroup	Clay Comments	Impurities	Quality
DI	Pattern has had Al peaks removed but process has	Aluminium	Bad
DI	Sample height issue -0.1 deg offset. Anatase in me	Anatase	Bad
DI	Sample height issue, -0.08 degree offset	Anatase	
DI	Sample height issue, -0.1 degree offset. Anatase pe	Anatase	Bad
DI	Trace anatase included as a kaolinite peak but u	Anatase	Bad
DI	Gibbsite indexed as kaolinite peak. Oriented patte	Gibbsite	Bad
DI	Significant quartz contamination. Peaks flagged bu	Quartz	Bad
DI	3.34A peak is quartz, incorrectly indexed as dickite	Unknown 7.3	Bad
CTT	002 peak intensity very low		Bad
DI	14A peak indexed but was removed from pattern 60-1517.		
TRI	Air dried		
ANA	Amphibole not a clay group		

Clay Minerals Task Group



Clay Minerals Task Group



Forthcoming Meetings

- Euroclay Paris 1-5 July 2019?
- Eurosoil 2020 Geneva
- World Congress of Soil Science, 30 July 7 August, Glasgow 2022?

- Also Reynolds Cup quantitative clay mineral round robin (10th) runs again next year, Steve Hillier organising. ICDD helped advertise it to potential participants previously (9th RC) 10th?

Regional Co-Chair

