



ePCCr

An online conference organized jointly with the African Light Source and the African Physical Society

<https://events.saip.org.za/event/170/>

FINAL REPORT
26 April 2022

Introduction

The first Pan-African Conference on Crystallography, PCCr1, was held in Dschang, Cameroon in 2016. This highly successful meeting attracted 192 participants from 32 countries, including 20 African countries. PCCr2 followed in 2019, with over 200 participants from 35 countries. This was a joint meeting with AfLS, and was hosted in Accra, Ghana. PCCr3, which will take place in Nairobi, Kenya, was scheduled for 2021. Unfortunately, due to the pandemic, this meeting had to be postponed. The Steering Committee of the African Crystallographic Association, along with the Local Organizing Committee of PCCr3, decided to hold an online meeting in order to continue the momentum and sense of community generated during the first two PCCr meetings. ePCCr was therefore organized.

The theme of ePCCr was '*Crystallography, an interdisciplinary science for the Africa of the future*'. Submissions were invited in the following thematic areas:

- Crystallography Databases
- Inorganic Materials and Industrial Minerals
- Crystal Engineering and Structural Chemistry
- Crystallography and Life Sciences
- Large Facilities for Emerging Countries
- Diffraction Physics and Phase Transitions.

The meeting was held entirely online *via Zoom*. The conference ran from 15-19 November, 10h00-17h00 Central African Time.

ePCCr organising committee

Gift Mehlana (Chair), Midlands State University, Zimbabwe
Susan Bourne (Secretary), University of Cape Town, South Africa
Dickson Andala, Multimedia University of Kenya, Kenya
David Dodoo-Arhin, University of Ghana, Ghana
Delia Haynes, Stellenbosch University, South Africa
Patrice Kenfack Tsobnang, University of Dschang, Cameroon



Joint meeting

The ePCCr was organized as a joint meeting together with the African Light Source (AfLS) and the African Physical Society (AfPS). There is significant overlap of interest between these three groups, as well as overlap of communities. There was also a group of ten co-convenors, also with overlap of interests (Fig. 1).

The joint event was hosted by X-Tech Lab in Benin (<https://www.xtechlab.co/en/>). Each day had two plenary sessions which were common to all delegates. The Opening and Closing Ceremonies were also organized jointly by ePCCr, AfLS and AfPS.



Fig 1. The companion Pan-African Conferences and the co-convenor organisations that worked together for the joint event.

Delegates

The joint meeting had a total number of 554 registered delegates. Of these, 208 delegates were specifically registered for the ePCCr meeting.

A total of 42 nationalities were represented at ePCCr, with delegates affiliated with institutions in 39 countries. The largest numbers of delegates were affiliated with institutes in South Africa (41), Cameroon (26), Nigeria (13), the UK (13) and France (11). 59% of registered delegates were male, 36% were female and the remaining 5% did not specify a gender. 106 delegates were academics, 81 were students, 15 from industry and 6 registered as observers.



Scientific sessions

The ePCCr was characterized by great talks from plenary lectures to keynote addresses. These talks covered aspects of crystal engineering, inorganic materials and structural chemistry and biology where crystallographic tools have been applied in the characterization of different materials that are used in our everyday lives. Plenary lectures and keynote addresses were presented by scientists from Africa and other parts of the world.

Polymorphism was a key feature in some of the talks that were presented by renowned and emerging scientists. Professor Susan Reutzel-Edens had an inspiring plenary talk on *Inspiring Medicines Design Through Solid State Chemistry* (Fig 2). In her presentation she highlighted methods for identifying drug polymorphs using computational and experimental methods. This was a well-timed presentation given the fact that the world is facing pandemics which need to be eradicated through developing new drugs and vaccines. Professor Bill Jones of the University of Cambridge gave a presentation on *Crystallization methods and disappearing polymorphs*. This further reinforced the importance of understanding the occurrence of polymorphic materials. This knowledge is very useful especially in pharmaceutical industries involved in the manufacture of drugs. In a keynote address Dr Eunice Nyawade stressed the importance of single crystal X-ray diffraction in characterization of polymorphic ruthenium complexes. Dr Tetteh Samuel of the University of Cape Coast in Ghana showed how polymorphism could be predicted using the Cambridge Structural Database (CSD). His presentation acted as a forerunner to the CSD workshop, for which 58 delegates registered, that looked at structural visualization with Mercury and Searching the Cambridge Structural Database using ConQuest. This workshop was attended by students and early career researchers.

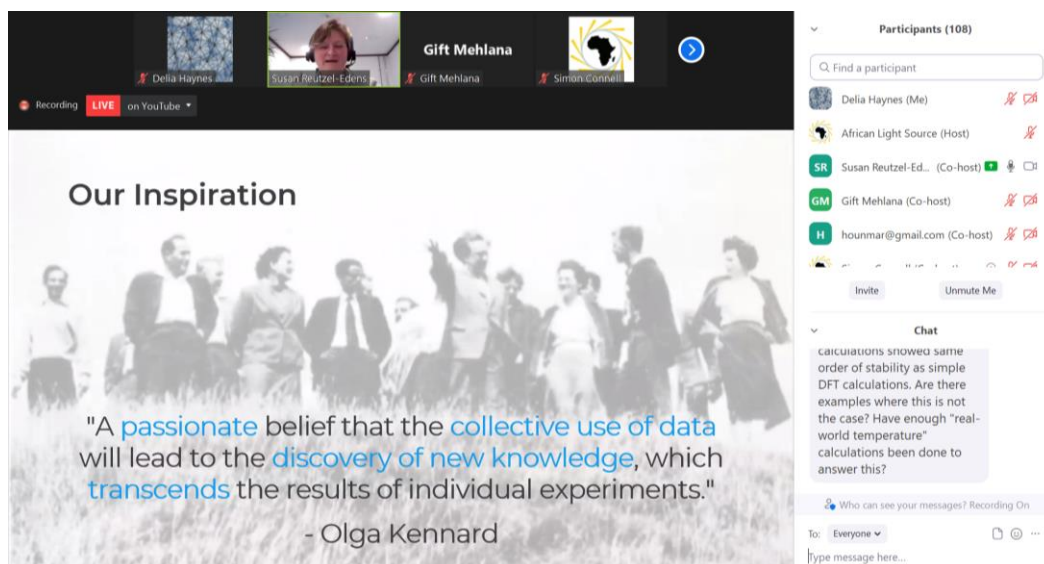


Fig 2. A screenshot from Susan Reutzel-Edens' presentation.



A plenary lecture on protein crystallography was presented by Professor Richard Garratt from the University of São Paulo. He spoke about the unravelling the complexities of septin filaments using crystallography. He also spoke about the importance of infrastructure development in advancing science in Brazil, particularly in terms of the construction of the first synchrotron in Latin America, and how this has changed science in the region. Another excellent plenary lecture was given by Professor Seham Abdel-Aal from Cairo University, who presented her work on hybrid perovskite materials and their properties.

Metal-organic Frameworks (MOFs) are a topical issue and as such their research is moving fast in directions as diverse as indoor climate and biotechnology. This was evidenced by keynote addresses by Neil Champness and Tendai Gadzikwa. The importance of these new materials in gas storage to catalysis was also highlighted. Dr Gadzikwa outlined how these materials can be used as scaffolds for enzyme-inspired catalysis paving way for their potential application in biotechnology. In a related presentation, Prof Lars Öhrström of Chalmers University of Technology explained how MOFs can be made by design and how their structures could be reduced to simple nets which we read about everyday in general chemistry textbooks. He further explained how MOF research has completely changed the way we look at the solid state, what we can do with it, how we can investigate it and how it pushes the limits of experimental techniques. Cyrielle Dazem Fogou from the University of Yaoundé briefly presented topological analysis in metal oxalates. Both Dazem Fogou and Öhrström explained the importance of topological analysis in the context of solving structures from powder X-ray diffraction data, and success has been achieved with covalent organic frameworks. Other presentations in the MOF area included structural transformations mediated by solvents. These talks were presented by Dr Christophe Ndamyabera and Alan Eaby of the University of Cape Town and Stellenbosch University respectively.

Large facilities and presentations from our sponsors

During the conference, several instrument manufacturers had the opportunity to showcase their products. Vernon Smith of Bruker, James Gordon of Rigaku and Marcus Mueller of Dectris presented on some of the instruments useful in material characterization, with a focus on crystallographic-oriented research. Dr Tom Blanton of ICDD presented on material characterization using powder diffraction techniques and the powder diffraction file. By using the Powder Diffraction file (PDF), it is possible to identify all phases that are present in a material making the PDF an invaluable tool in mining and pharmaceutical industries.

ePCCr had a total of 9 invited lectures (3 plenary lectures and 6 keynote lectures). 5 of the invited speakers are African, with 3 currently based in Africa. 4 of the 9 invited speakers are female. There were an additional 20 talks selected from submitted abstracts, of which 9 were given by students or young researchers, and 6 by female delegates. An additional 5 presentations were given by sponsors.



ePCCr invited speakers

Dr Susan Reutzel Edens, CCDC

Prof Seham Abdel-Aal, Cairo University

Prof Neil Champness, University of Birmingham

Prof Bill Jones, University of Cambridge

Dr Emile Engel, KTH Royal Institute of Technology

Dr Tendai Gadzikwa, Kansas State University

Prof Richard Garratt, University of São Paulo

Dr Eunice Nyawade, Jomo Kenyatta University of Agriculture and Technology

Prof Bernard Omondi Owaga, University of KwaZulu-Natal

The ePCCr also involved several lively poster sessions, which were held online in *Gather Town*. A total of 26 posters were accepted.

Thanks to generous sponsorship (see below), 6 poster prizes and 3 speaker prizes were awarded. The winners of poster and speaker prizes, selected from participants in the ePCCr conference by a panel of judges, were announced at the conference closing ceremony. The winners are listed below. All prize winners received a certificate and a USD200 prize.

Poster prizes

Crystal Growth & Design poster prizes

Akin Olaleru from Yaba college of Technology, Nigeria

Optimal conditions for preparation of perovskite crystals and thin film

Eddy F. Yusslee from the University Malyasia Sabah, Malaysia

Transformation of kalsilite from kaolinite via hydrothermal method

CCDC poster prizes

Tristan Theunissen from the University of Cape Town, South Africa

Silver(I) complexes with picoline derivative ligands: Synthesis, characterization, DFT and QTAIM calculation study

Hannah van Dyk from the University of the Free State, South Africa

The application of functionalized salicylidene Schiff base ligands in catalysis, luminescence, and radiopharmacy.

CrystEngComm poster prizes

Samantha Le Roux from Stellenbosch University, South Africa

Dithiadiazolyl radical co-crystal formation

Abraham Zigla Atour from the University of Maroua, Cameroon

Design, characterization and investigation of CO catalytic oxidation over Mg-modified Co_3O_4 catalyst



Speaker prizes

CrystEngComm speaker prizes

Cyrielle Dazem Fogou from the University of Yaounde 1, Cameroon

Topological diversity in Metal Oxalates and Structural Variability of Copper(II) oxalate anion associated with Pyridinium Derivatives Cations

Alan Eaby from Stellenbosch University, South Africa

Solvent-Mediated Elasticity in Flexible Single Crystals

ICDD speaker prize

Najlaa Hamdi from University Sidi Mohamed Ben Abdellah, Morocco

Crystal characterization and application of a new vanado-phosphate material

Launch of AfCA

A special session was organized on Wednesday morning of the ePCCr in order to constitute the African Crystallographic Association. The session involved presentations on the history leading up to the formation of an African Crystallographic Association, as well as addresses by representatives from the International Union of Crystallography, the European Crystallographic Association, the International Science Council and UNESCO. This session was very well-attended by delegates as well as observers.

A detailed description of the session is given in Addendum A, a copy of an article submitted to the IUCr newsletter.

Sponsors and budget

The ePCCr meeting was supported by several generous sponsors (Fig. 3), listed in the budget summarized on the following page.

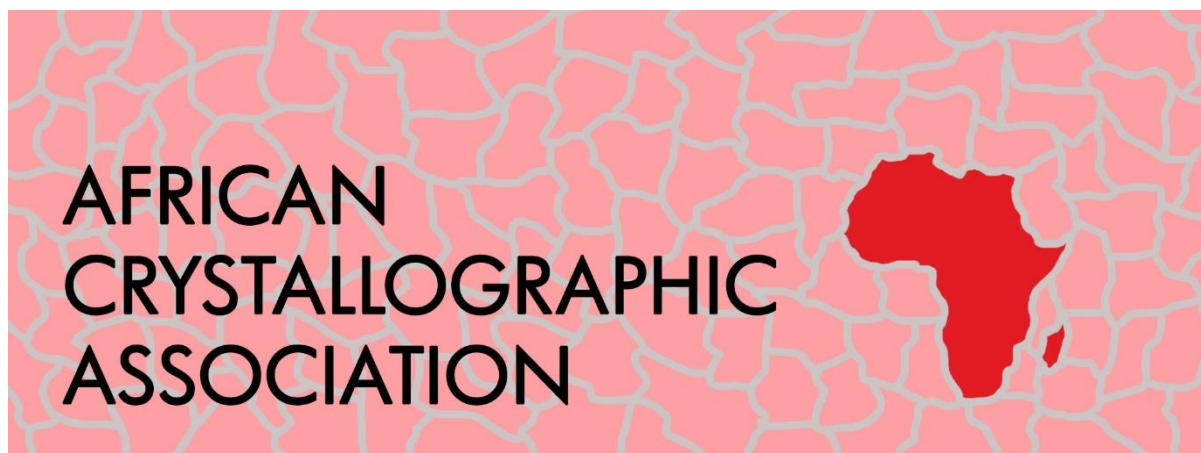
Thank you to our generous sponsors.



Fig 3. Logos of ePCCr sponsors



Addendum A: Article on AfCA launch (submitted to IUCr Newsletter)



It's official – the African Crystallographic Association is born!

After many years of crystallographic activity on the African continent, on 17 November 2021 we witnessed the birth of the African Crystallographic Association (AfCA). This follows years of work by many groups and individuals, including the IUCr Africa Initiative, the IUCr Outreach Program, and the AfCA Steering Committee, with the collaboration of institutions like the United Nations Educational, Scientific and Cultural Organization (UNESCO), the International Science Council (ISC) and many companies like Bruker and the Cambridge Crystallographic Data Center (CCDC).

The Association was launched during the online ePCCr meeting, organised as a joint conference with the African Light Source and the African Physical Society (<https://events.saip.org.za/event/170/>). The ePCCr meeting attracted 205 delegates from 37 countries, including 17 African countries. AfCA was officially constituted during a special session at this online meeting, chaired by Delia Haynes, the chair of the Executive Committee of the AfCA Steering Committee.

The session opened with addresses from the president of the International Union of Crystallography (IUCr) (<https://www.iucr.org/>), Hanna Dabkowska, and the president of the European Crystallographic Association (ECA) (<https://ecanews.org/>), Marijana Đaković. Hanna indicated how, since 2011, under the presidencies of Gautam Desiraju (2011-2014), Mervin L. Hackert (2014-2017) and Sven Lidin (2017-2021), the Union has advanced the promotion of crystallography in Africa. She hopes AfCA will apply for regional membership of the IUCr during the 26th IUCr congress in Australia. In her address, Marijana mentioned that several African countries with active crystallography communities have been members of the European Crystallographic Association, and ECA has been a strong support on the road to forming AfCA.

Andreas Roodt (South Africa), Claude Lecomte (France) and Patrice Kenfack Tsobnang (Cameroon), then gave presentations. Andreas Roodt, a past president of ECA and the first chair of the AfCA steering committee, outlined the history and development of crystallography on the African continent. He particularly highlighted the key role played by Claude Lecomte, as well as the

importance of meetings held on the African continent, including ECM21 in South Africa and ECM24 in Morocco, as well as the important meetings held during the International Year of Crystallography in 2014. Claude Lecomte then discussed the development of crystallographic activities in Africa, focussing on the installation of diffractometers in several African countries, and well as the highly successful OpenLabs. He finished by presenting a new project involving remote access to diffractometers for the collection of diffraction data. Finally Patrice Kenfack Tsobnang spoke about the Pan African Conferences on Crystallography, the PCCr series. He mentioned that the idea to launch these conferences arose from the declaration signed during the IYCr2014 Pan African and South African Summit meeting (<https://www.iycr2014.org/summits/bloemfontein>), and how the meetings contribute to growing the African community working on crystallography. PCCr1 and PCCr2 were held in Cameroon in October 2016 and Ghana in January 2019 respectively, and PCCr3 (<http://www.pccr3africa.org/>) is planned to take place in Kenya in January 2023.

1. Discuss TIME-LINE Table in five parts (before 1990)

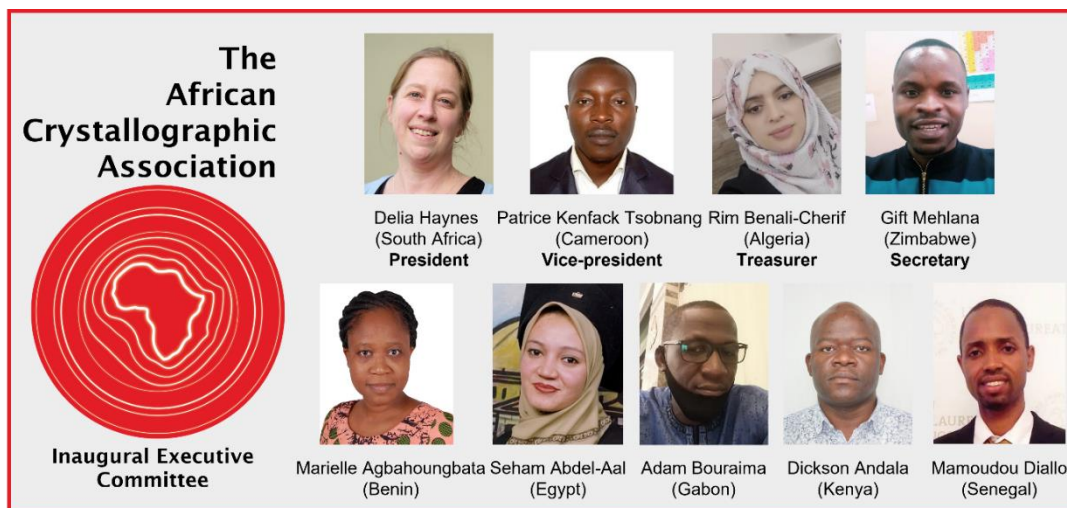
<1990 IUCr/ Académie **Activate Research in Crystallography**

WH Bragg + WL Bragg → RW James (40-50s) → Frank Herbstein (50s) → Jan Boeyens, Luigi Nassimbeni (60-90s) → Joe Leipoldt, John Field

Chat: The Bruker team is proud to be associated with the African Crystallographic Association. We look forward to working together to strengthen science on our continent. Congratulations and all the best!

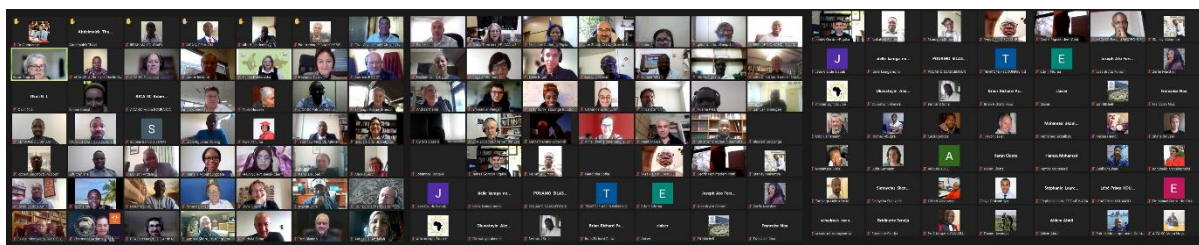
A slide from the presentation given by Andreas Roodt, outlining the history of crystallography in Africa.

These inspiring presentations were followed by the first AfCA Council meeting. Whilst it would have been fantastic to hold this meeting in person, one advantage of the online meeting format is that representatives of crystallography societies and groups from across the continent were easily able to participate in the meeting. Representatives from the founder members in Algeria, Benin, Cameroon, Congo, Côte d'Ivoire, Democratic Republic of Congo, Egypt, Gabon, Ghana, Kenya, Nigeria, Morocco, Rwanda, Senegal, South Africa, Tunisia and Zimbabwe were present. These representatives voted first to approve the constitution and by-laws of the African Crystallographic Association, and to officially constitute the association. This was followed by a vote to approve the proposed AfCA Executive Committee. Both votes were unanimous.



The inaugural AfCA Executive Committee. The committee of nine includes members from the five regions of Africa as defined in the constitution.

The session closed with presentations from Prof Walter Oyawa from the International Science Council, and Dr Jean-Paul Ngome Abiaga from UNESCO. The event was attended by representatives from the European, American, Asian and Latin American Crystallographic Associations, as well as the African Light Source, the African Physical Society and the African Academy of Sciences. Many crystallographers from the African continent and across the globe, also joined this important occasion, as well as representatives from *CrystEngComm*, *Crystal Growth & Design*, the CCDC, ICDD, Bruker and Rigaku.



Attendees at the AfCA session at ePCCr.

The birth of the African Crystallographic Association was a significant and historic moment, both for science in Africa and for crystallography worldwide. In the words of the ePCCr chair, Gift Mehllana, which he shared at the conference closing ceremony,

'Just like a baby, the AfCA will learn to sit, crawl, stand up, walk, and run. During all these stages AfCA will need maximum support from the crystallographic community, African governments, and the world at large. African governments must support science and in particular crystallography through the provision of infrastructure and equipment that is needed to carry out meaningful research. Crystallography has the power to change people's lives.'

We hope to see the AfCA go from strength to strength as it aims to fulfil its objectives, which are to contribute to the advancement of crystallography and structural science in all its aspects, including related topics concerning the non-crystalline states; to promote African cooperation in crystallography

and related areas and to contribute to the development of education and research in crystallography and structural sciences in Africa.

The new AfCA Executive Committee would like to extend particular thanks to the three *ex officio* members of the AfCA Steering Committee, Alessia Bacchi, Claude Lecomte and Michele Zema. They have been incredibly generous with their time and their considerable experience, and this point would not have been reached without their help.

Thank you to all those who contributed to this great event to enable this continent, with abundant resources in minerals and mining, materials science, green chemistry, biotechnology, and archaeology, to have its crystallography association.

Good Luck to AfCA!

**The
African
Crystallographic
Association**

