Faculty of Science and Technology

Caribbean Regional X-ray Science Toward Advancement Laboratory (crXstal)

Fundamentals of Crystallography: Theory and Practice

The Inaugural Caribbean Crystallography School

Date: **June 2-7, 2025**

Venue: **The University of the West Indies, Mona Campus**
Kingston Jamaica

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Messages

Professor Michael Taylor

Dean, Faculty of Science and Technology
The University of the West Indies, Mona

I am delighted to extend warm congratulations on the hosting of the Inaugural Caribbean Crystallography School at The University of the West Indies, Mona. This marks a significant milestone not just for our campus, but for the Caribbean region as a whole.

The establishment of a dedicated crystallography school in the Caribbean affirms the region's readiness as a serious player in cutting-edge scientific research. It sends a clear signal that we are not just consumers of knowledge, but creators and contributors. This School represents the power of vision, collaboration, and network-building—bringing together international experts, regional institutions, and local talent in a shared commitment to scientific advancement.

Importantly, this event builds on the momentum generated by the recent opening of the CrXstal Lab, our first X-ray crystallography facility. That lab was a bold step in creating in-region capacity; this School is the next logical—and necessary—step in building the community of practice that can sustain and grow the field.

To all participants, I say welcome. To the organizers and partners, I say thank you. May this inaugural school lay the foundation for a vibrant and connected Caribbean crystallography network for years to come.

Messages

Dr. Marvadeen Singh-Wilmot

Founder of crXstal and Co-Chair of the CCS

It gives me great pleasure to welcome you to the inaugural Caribbean Crystallography School, CCS2025 here at crXstal, the Caribbean Regional X-ray Science Toward Advancement Laboratory, the home of CCS! For the first time in our region's history, we gather as a Caribbean community of users and potential users of X-ray crystallography and start building the future of crystallography in our islands.

Many of you already know the journey: For over two decades, Caribbean researchers longed for a local X-ray lab. Without the opportunity for hands on experience many lost interest even in taking courses in X-ray crystallography. The rest of us shipped priceless crystals across oceans only to face delays, damage, or—even more frustrating—complete loss. Eventually the loss became the spark for something far greater, a proposal and push for a regional hub for X-ray techniques. Energized by Dr. Michele Zema's leadership as then Executive Outreach Officer for the IUCr and co-chair of LAAAMP, inspired by the X-Tech Lab model in Benin, and buoyed by generous support from instrument manufacturers, Bruker, Deans of the FST UWI-Mona and Cave Hill, thePrincipal's Office UWI-Mona, LAAAMP, Prof. Sekazi Mtingwa, CSD's FAIRE grant, the RSC, Juici Beef Limited, UNESCO's Participation Programme, CAS Jamaica and the University of Bologna's Global South Fund, we channelled every setback into momentum. On October 3, 2024, we officially launched crXstal, a regional hub for X-ray diffraction with clear goals to build regional X-ray crystallography capacity, stimulate research, popularize crystallography and cultivate a collaborative Caribbean network of users.

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The CCS is one of the main mechanisms for achieving these goals and I am eternally gratefully for the overwhelming support from the local and international community, especially our main sponsor, the IAEA, who have made this crucial regional capacity building intervention possible. Thanks to the PIOJ for endorsing this event under Jamaica's country programme framework with the IAEA and to all other sponsors and supporters of the CCS. Thanks also to the solution-oriented organizing team whose dedication and commitment to excellence made this all possible.

To the trainees in this school I say, get ready for an intense but rewarding programme, covering the theory of X-ray crystallography with hands-on experience for each participant in growing single crystals, collecting diffraction data, solving crystal structures, using structural databases and preparing publications. Get ready to be taught by international experts who are among the best in the world, representing the International Union of Crystallography, the Italian Crystallography Association, the Latin American Crystallography Association, the International Science Council, Bruker and the Cambridge Structural Database. Get ready to make connections across the region, the world, across generations, and disciplines. Share your diverse perspectives and experiences and forge new relationships to co-author papers, and develop materials that address local and global challenges. Get ready to turn diffraction into discovery and take those crystals all the way to publication by the end of CCS2025!

Messages

Professor Michele Zema

University of Bari, Italy
Chair of Lightsources for Africa, the Americas, Asia, Middle East and Pacific (LAAAMP)
Co-founder of crXstal and Co-chair of the Caribbean Crystallography School

It is a pleasure to welcome you to the first edition of the Caribbean Crystallography School. This event marks an important step in the growth of a crystallography community in the region, and I'm glad we can begin this journey together.

The creation of crXstal, a new crystallography hub for the Caribbean, is part of a broader vision supported by LAAAMP to expand access to advanced scientific infrastructure through regional centres of excellence. Over the past year, we've worked to bring that vision to life—drawing inspiration from the X-TechLab in Benin, launched in 2018. In that spirit, crXstal aims to foster research, training, collaboration, and long-term development, while also helping to build a scientific bridge between Africa and the Caribbean.

I am especially grateful to Dr Marvadeen Singh-Wilmot, who has been a driving force throughout this process. Her leadership, energy, and clear vision have been central to both the establishment of the crXstal facility and the organisation of this inaugural event. I would also like to thank everyone at her home institution, the University of the West Indies, Mona Campus, for their support and foresight in hosting crXstal and backing this regional initiative. Without their commitment—and without Marvadeen's outstanding contribution—none of this would have come together.

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Many individuals and institutions have supported this effort. I am particularly thankful to Bruker AXS and the Cambridge Crystallographic Data Centre (CCDC) for their generous support, as well as to all the partners who helped make crXstal a reality.

This school is more than a training event—it is the first step in building a strong, connected, and internationally engaged crystallographic community in the Caribbean. I'm pleased to welcome participants from across the region, as well as lecturers from Central and South America, and other parts of the world, including Italy, my home country. I hope this is just the beginning of a lasting scientific collaboration, supported also by the Italian Crystallographic Association (AIC).

Thank you for being part of this inaugural edition. I look forward to the exchanges, ideas, and connections that will emerge in the days ahead.

CCS
Organizers

International Scientific Committee

- Chair: Dr. Marvadeen Singh-Wilmot (F, Jamaica)
- Co-Chair: Prof. Michele Zema (M, Italy)
- Dr. Christopher Cahill (M, USA)
- Dr. Javier Alcides Ellena (M, Brazil)
- Prof. Lucia Maini (F, Italy)
- Dr. Suzanna Ward (F, UK)

Organizing Committee

- Dr. Marvadeen Singh-Wilmot (F, University of the West Indies, Mona Campus, Jamaica, Chair)
- Mrs. Terry-Ann Collins Fray (F, administrator)
- Mrs. Sabraham Green-Smith (F, administrator)
- Mr. Jermaine Smith (M, The University of the West Indies, Mona)
- Dr. Zeyar Min (M, University of Technology, Jamaica)
- Dr. Richard Taylor (M, University of the West Indies, St. Augustine
- Campus, Trinidad and Tobago)
- Prof. Avril Williams (F, The University of the West Indies, Cave Hill Campus, Barbados)
- Ms. Andrea Rhule (F, The University of the West Indies, Mona)

CCS2025 Online Preschool

In anticipation of CCS2025 June 2-7 2025, we hosted two one-hour online pre-school sessions, May 19 and 21 under the leadership of Prof. Lucia Maini, Mariagiovanna Zoccali, and Giacomo Montanari from the University of Bologna Italy.

The sessions were designed to align participants' understanding of crystallographic symmetry and its mathematical representation before the in-person school. The first session focused on symmetry in 2D and 3D space, for which attendees were required to complete Units 3.1–3.4 of the MOOC The Fascination of Crystals and Symmetry, review other documents on introduction to symmetry, and prepare 3D models illustrating crystal systems from cubic through triclinic. The second session addressed symmetry from a mathematical perspective, prompting participants to study the "Math Basics" guide and an introduction to matrix representations of symmetry operations.

The sessions were well attended with nineteen (19) participants in session one and nineteen (19) in session two. In each session participants were divided into groups with group leaders assigned who came back to the main room at the end of the sessions and reported on group activities. The sessions were very interactive and the post session reviews revealed that students appreciated the intervention.

Our Lecturers

Dr. Marvadeen Singh-Wilmot

Founder of crXstal and Co-Chair of the CCS

Dr. Marvadeen Singh-Wilmot is a Senior Lecturer in Inorganic Chemistry at the University of the West Indies, Mona Campus, who conceptualized and co-founded the Caribbean Regional X-ray Science Toward Advancement Laboratory (crXstal). Dr. Singh-Wilmot's research centers on the design, synthesis and detailed characterization of lanthanide-based coordination polymers and metal–organic frameworks (MOFs) for functional applications, underpinned by spectroscopic and crystallographic methods. She investigates how variations in ligand identity, lanthanide ionic radius and synthetic conditions (e.g., solvothermal vs. sonochemical routes) influence framework topology, polymorphism and supramolecular assembly—particularly through halogen···halogen and hydrogen-bonding interactions—to enable rational crystal engineering and the development of luminescent sensing platforms for metal ions and nitroaromatic compounds.

Dr. Singh-Wilmot is a member of the executive committee and Caribbean representative on the Greater Caribbean Light Source/LAMISTAD Project which aims to educate scientists and students of science about synchrotron sciences and ultimately build a synchrotron facility for regional collaboration. She is part of the team developing the International Union of Pure and Applied Chemistry (IUPAC) Guiding Principles for the Responsible Practice of Chemistry, promoting ethical conduct, safety, and sustainability. She contributed to the Royal Society of Chemistry's focus group on race and ethnicity in chemical sciences and The World Academy of Sciences (TWAS) working group for refugees and displaced scientists. Her contributions extend to strategic planning for interventions to advance chemical sciences in Commonwealth countries and external review of chemistry teacher education.

Dr. Marvadeen Singh-Wilmot cont'd

Singh-Wilmot's work has been recognized locally and internationally, including membership in the Global Roster of Experts for the International Science Council, Fellow of the Caribbean Academy of Sciences, the IUPAC Committee for Ethics, Diversity, Equality, and Inclusion (CEDEI) and TWAS' Young Affiliate Network (TYAN). She is also a reviewer for many international chemistry journals and for TWAS' Global Science Diplomacy Course.

Singh-Wilmot is dedicated to mentoring and uplifting future generations of young scientists. She conceptualized the "Walking in Her/His Footsteps" STEM Mentorship Programs, which empower young women/men to step boldly into scientific careers and is working to achieve the projects expansion into a national STEM mentorship programs in 2025. As a Jury Member for the L'Oréal Young Talents Caribbean for Women in Science Programme and Appointed Member of the International Union of Pure and Applied Chemists (IUPAC) Committee for Ethics, Diversity, Equality, and Inclusion (CEDEI), she champions equity in STEM. She has served the Faculty of Science and Technology, UWI-Mona, as Associate Dean for Student Experience 2021-2023.

Professor Michele Zema

University of Bari, Italy
Chair of Lightsources for Africa, the Americas, Asia, Middle East and Pacific (LAAAMP)
Co-founder of crXstal and Co-chair of the Caribbean Crystallography School

Chemist and crystallographer with over 25 years of research and teaching experience, Prof. Michele Zema is Associate Professor at the University of Bari, Italy and Fellow of the African Academy of Sciences. Coordinator of the activities for the UN International Year of Crystallography in 2014, he acted as Executive Outreach Officer for the International Union of Crystallography from 2015 to 2024. He is co-founder and Chair of the Executive Committee of LAAAMP (Lightsources for Africa, the Americas, Asia, Middle East and Pacific), and serves on the Executive Committees of the International Mineralogical Association and the African Light Source. Founding member and advisor to the Executive Committee of the African Crystallographic Association, he acted as facilitator for the foundation of several crystallographic associations worldwide.

An expert in global science diplomacy and advocacy and in human resources and scientific infrastructure capacity building assessment, he initiated actions, such as the IUCr-UNESCO OpenLab, and directed several international schools and meetings. He is co-founder of the X-TechLab, a Western African hub for education and research in structural science, based in Benin, and of crXstal, the regional crystallography hub for the Caribbean islands, based in Jamaica.
His research activity mainly deals with complex intracrystalline phenomena occurring under variable physicochemical conditions in minerals and inorganic solid solutions.

Professor Serena C. Tarantino

Associate Professor at the University of Pavia, Italy, and Associate Researcher at the Italian National Research Council

Serena C. Tarantino (BSc in Chemistry - 1997; PhD in Mineralogy, Petrology and Crystallography - 2001) is Associate Professor at the University of Pavia, Italy, and Associate Researcher at the Italian National Research Council. Her research interests reside at the intersection of mineralogy, solid-state chemistry, and materials science, with the objective of correlating short- and long-range crystal structures to the macroscopic behaviour of mineral solid solutions and other complex materials. Recent interests encompass the examination of materials recovery processes and secondary raw materials.

She is a member of the Commission on Inorganic and Mineral Structures of the International Union of Crystallography, has served on the Council of the European Crystallographic Association as representative of Individual Members and has been Regional Editor of the IUCr Newsletter. She has directed two AIC International Crystallography Schools in 2016 and 2019, has chaired the organizing committee of the 1st European Crystallography School in 2014 and has participated in several scientific and organising committees for international schools and meetings.

Yinka Olatunji-Ojo

User Support Scientist and member of Training, Education and Outreach team, the Cambridge Crystallographic Data Centre (CCDC).

Yinka Olatunji-Ojo is a User Support Scientist and a member of the Training, Education and Outreach team at the Cambridge Crystallographic Data Centre (CCDC). Yinka joined the US operations of CCDC in 2019 after completing a postdoc at the University of California, Berkeley and working as the Lead Computational Scientist at a medical device startup. Her doctoral studies focused on utilizing computational methods to study inorganic and organometallic systems for various applications. As part of the T, E & O team, Yinka works on creating workshop materials and delivering training at various schools and summer courses.

Professor Leopoldo Suescun

Associate Professor at Univ. de la República in Montevideo, Uruguay
Chair of the Uruguayan National Committee of Crystallography

Leopoldo Suescun received his Doctorate degree in 2003 from Universidad de la República, Facultad de Química in Montevideo, Uruguay. He made a 3-year postdoctoral stay at the Materials Science Division in Argonne National Laboratory from 2005 to 2008. During his undergrad and Masters studies he performed single-crystal small molecule crystallographic studies of organic and metal-organic compounds and during this doctorate and postdoc he studied ceramic samples using neutron and X-ray powder diffraction applying the Rietveld method. Since his first publication in 1996 he has contributed more than 200 structures to the CSD and more than 150 to the ICSD, some solved using PXRD data.

He has been active at the International Union of Crystallography being a member (2014-2023) and Chair (2021-2023) of the Mathematical and Theoretical Crystallography Commission of the IUCr and founder of the Latin American Crystallographic Association representing Uruguay in 2014. Among other dissemination activities he has been one of the organizers of the National Crystal Growing Competition of Uruguay running its 12th consecutive edition since 2014. Currently, he is an Associate Professor at Univ. de la República in Montevideo, Uruguay lecturing in Crystallography and Materials Chemistry. He is the Chair of the Uruguayan National Committee of Crystallography and member of the Board of Directors of the International Centre for Diffraction Data.

Dr. Javier Ellena

Vice-Coordinator of the Center for Characterization of Mineral Species
Vice-President of the Brazilian Crystallographic Association, Chair of the Structural Chemistry Commission of the International Union of Crystallography (IUCr), and Co-editor of Acta Crystallographica E

Dr. Javier Ellena holds a Ph.D. in Physics with a specialization in Crystallography from the Universidad Nacional de La Plata, where he also earned his Bachelor's degree in Physics in 1993. He completed his doctoral studies in 1998 and, since 2002, has been a faculty member at the São Carlos Institute of Physics (IFSC) at the University of São Paulo. He served as Vice-President of the IFSC Graduate Commission from 2016 to 2018 and is a former President of the same commission. Currently, Dr. Ellena is the Coordinator of the Structural Crystallography Laboratory (LaMuCrEs) at IFSC-USP—the oldest structural crystallography laboratory in Brazil. He is also a Level 1B Researcher with the National Council for Scientific and Technological Development (CNPq). Dr. Ellena's primary research focuses on the development and characterization of new multi-component solid forms of active pharmaceutical ingredients aimed at improving pharmacokinetic and pharmaco-technical properties. His additional research interests include the design and characterization of Metal–Organic Frameworks (MOFs), the study of natural minerals, and the experimental and theoretical analysis of electron charge density in compounds with biological activity or nonlinear optical properties.

He currently serves as Vice-Coordinator of the Center for Characterization of Mineral Species. Dr. Ellena has authored over 540 peer-reviewed scientific publications indexed in Web of Science and 1,183 on Google Scholar, accumulating more than 6,900 citations on Web of Science and 8,900 on Google Scholar, with an H-index of 39 and 44, respectively.

Dr. Javier Ellena cont'd

He is Vice-President of the Brazilian Crystallographic Association, Chair of the Structural Chemistry Commission of the International Union of Crystallography (IUCr), and Co-editor of Acta Crystallographica E, published by IUCr Journals. He has also served as a member of the X-ray Diffraction Committee of the National Synchrotron Light Laboratory.

Dr. Ellena has co-organized several major scientific events, including the I and II Latin American Symposium on Polymorphism and Crystallization in Drugs and Medications (LAPOLC 2007 and LAPOLC 2009), the IUCr High-Pressure Workshop in 2015, and the 1st and 3rd Latin American Crystallographic Association Schools on Small Molecule Crystallography. He actively contributes as a reviewer for numerous international scientific journals and serves as an ad hoc consultant for governmental institutions, in addition to advising various academic and industrial organizations.

Professor Lucia Maini

Department of Chemistry
University of Bologna

Lucia Maini is a full professor of chemistry at the Department of Chemistry " G. Ciamician" at the University of Bologna. She has a strong background in structure determination from single-crystal and powder X-ray diffraction and in solid state characterization. Her research covers a range of areas within the field of crystal engineering: polymorphs, co-crystals, coordination polymers, organic materials. She is involved in the promotion of mechanochemistry. She actively collaborates with historians of science through the replication of ancient recipes. She organizes and participates in public engagement activities and educational events for schools and cooperation project.

Ilaria Gimondi

Senior Training, Education and Outreach Officer at the Cambridge Crystallographic Data Centre (CCDC)

Ilaria Gimondi is Senior Training, Education and Outreach Officer at the Cambridge Crystallographic Data Centre (CCDC). Ilaria joined the CCDC in 2020, after completing her PhD in Chemical Engineering at University College London (UK) during which she studied polymorphic transition using computational techniques. At the CCDC, Ilaria contributes to the creation of training resources on the use of the Cambridge Structural Database (CSD) and associated software both for researchers and educators, and she is involved with the planning and delivery of workshops. In her role, she also participates in education and outreach activities and supports initiatives such as the Frank H. Allen International Research and Education (FAIRE) Programme for underrepresented communities and the CCDC Engagement Grants.

Professor Graciela Diaz de Delgado

Crystallography Laboratory, Universidad de Los Andes (ULA)
Vice-President of the International Union of Crystallography (IUCr)
Section Editor of Acta Crystallographica E, member of the Board of Directors of the International Centre for Diffraction Data (ICDD), and member of ISC's Liaison Committee of the Regional Focal Point for Latin American and the Caribbean

Graciela Diaz de Delgado was born in Maracaibo, Venezuela, she studied Chemistry at Universidad de Los Andes (ULA) in Mérida, Venezuela, and obtained her Ph.D. in Chemistry at Brandeis University, USA, in 1988. In 1989 she joined the Crystallography Laboratory at ULA as Assistant Professor and has been a Full Professor since 2002. In 2023 she was elected Vice-President of the International Union of Crystallography (IUCr).

She is Section Editor of Acta Crystallographica E, member of the Board of Directors of the International Centre for Diffraction Data (ICDD), and member of ISC's Liaison Committee of the Regional Focal Point for Latin American and the Caribbean. She was awarded a National Prize in Science from the Ministry of Science and Technology of Venezuela in 2023. Her research interests include the structural characterization by single crystal and powder diffraction techniques of active pharmaceutical ingredients, commercial pharmaceutical products, and natural products isolated from medicinal plants of the Venezuelan Andes.

Dr. Araya Sibaja

Researcher at LANOTEC (Costa Rica)
President of the Latin American Crystallographic Association (LACA)

Andrea Mariela Araya Sibaja holds a Master's degree in Pharmacy from the Federal University of Santa Catarina (Brazil) and has pursued doctoral studies in Engineering through the Interuniversity Program between the Costa Rica Institute of Technology (TEC) and the University of Costa Rica (UCR). As part of her doctoral training, she completed a research internship with the Bill Jones Group in the Department of Chemistry at the University of Cambridge, United Kingdom, where she focused on cocrystallization through mechanochemistry. Dr. Araya Sibaja is currently a researcher at LANOTEC (Costa Rica), where she focuses on crystallization and nanomaterials. Her research aims to improve the solubility, dissolution, and bioavailability of small organic molecules and poorly water-soluble bioactives, as well as to develop advanced drug delivery systems. She has authored scientific publications in these areas, particularly on the crystallization of biomolecules and their encapsulation in nanostructured systems. In addition to her research work, Dr. Araya Sibaja has organized and actively participated in numerous scientific events, workshops, and schools related to crystallography across Latin America, fostering collaboration and education in the field. She has served as President of the National Committee of Crystallography of Costa Rica and currently serves as President of the Latin American Crystallographic Association (LACA).

Dr. Ashley (Weiland) Schmidt

Applications Scientist, Single Crystal
X-Ray Diffraction Division, Bruker

Dr. Ashley (Weiland) Schmidt received her B.S. in Environmental Chemistry from Duquesne University in Pittsburgh, PA, where she developed a keen interest in crystallography and solid-state chemistry under the guidance of her research advisor Jennifer Aitken. Dr. Schmidt then pursued her Ph.D. in Inorganic Chemistry at the University of Texas at Dallas, where she encountered and solved numerous difficult crystallographic problems while studying rare earth intermetallics with Julia Chan. During her doctoral studies, she spent four months at the Advanced Photon Source, where she worked with Saul Lapidus at the high-resolution powder diffraction beamline, 11-BM. After completing her Ph.D., Dr. Schmidt did her postdoctoral work at Los Alamos National Laboratory, where she worked on Uranium-based superconductors and other low-dimensional materials. As an Applications Scientist in the Single Crystal X-Ray Diffraction Division at Bruker, Dr. Schmidt is dedicated to sharing her expertise in crystallography to train and educate.

Our Tutors

Jermaine Smith

PhD student in Inorganic Chemistry
(Supervisor: Dr. Marvadeen Singh-Wilmot)
Department of Chemistry, Faculty of Science and Technology,
The University of the West Indies, Mona Campus

Jermaine Smith is a PhD student in Inorganic Chemistry under the supervision of Dr. Marvadeen Singh-Wilmot in the Department of Chemistry, Faculty of Science and Technology, The University of the West Indies, Mona Campus. His area of focus is the synthesis, characterization and potential applications of hybrid organic-inorganic materials called Metal-Organic Frameworks (MOFs). MOFs are a new class of porous coordination polymers (CPs) with well-defined topologies that continue to intrigue scientists not only because of their appealing structural architectures, but also because of their potential applications in gas storage and separation, sensing of small molecules, catalysis and biomedicine.

Dr. Zeyar Min

Head of the Division for Research Development and Consultancy
Lecturer in Advanced Physical Chemistry and Materials Chemistry
University of Technology (UTech), Jamaica

Dr. Zeyar Min serves as the Head of the Division for Research Development and Consultancy and is also a Lecturer in Advanced Physical Chemistry and Materials Chemistry at the University of Technology (UTech), Jamaica. In addition to his academic roles, he coordinates the General Chemistry 1 Laboratory Module, during which he has revised the Laboratory Manual and Curriculum, updated the Student Lab Safety Guidelines, and directed the production of a new Laboratory Safety Video. His interest in sustainability has further led him to explore and promote greener laboratory practices as part of a broader initiative to address gaps in the local and regional educational landscape.

Dr. Min's professional roles allow him to integrate his passion for materials science with strong leadership and management skills. His early research focused on the design and synthesis of Hybrid Organic-Inorganic Frameworks within the field of materials science. Over time, his research interests have expanded to encompass the Blue Economy and Water Systems and Management—particularly issues related to Non-Revenue Water and Water Loss—as part of a strategic approach to addressing critical local and regional challenges.

Committed to education, Dr. Min adopts a teaching philosophy that is attuned to the unique needs and learning preferences of Generation Z students. He is particularly engaged in the integration of gamification techniques, especially feedback loops, into pedagogical practices. This innovative approach supports a more dynamic and interactive learning environment while allowing him to remain responsive to the evolving demands of modern education.

Schedule of **Activities**

Day 0 | Sunday, June 1, 2025			
Arrival of Participants at Jamaica Pegasus Hotel			
7:00 pm - 9:00 pm	Networking and Cocktail Reception		Jamaica Pegasus Hotel
Day 1 | Monday, June 2, 2025			
8:30 am - 9:00 am	Registration		Chemistry Lecture Theatre 5
9:00 am - 11:00 am	Opening Ceremony		Chemistry Lecture Theatre 5
	Teaching Begins		
11:00 am - 11:30 am	Crystallizing the CCS Network Facilitators: **MSW, MZ, LS**		
11:30 am -1:00 pm	History of crystallography and introduction to crystal symmetry Facilitator: **MZ**		Chemistry Lecture Theatre 5
1:00 pm - 2:00 pm	Lunch		
Chair: JE			
2:00 pm - 3:00 pm	Principles of crystallization and crystal growth Facilitator: **MSW**		Chemistry Lecture Theatre 5
3:00 pm - 4:00 pm	The D8 Quest Eco diffractometer and crystal mounting techniques Facilitator: **AS**		Chemistry Lecture Theatre 5
4:00 pm - 4:20 pm	Coffee break		
4:20 pm - 4:30 pm	Groups' formation: **BLUE**; **GREEN**; **PURPLE**; **BROWN**		Chemistry Lecture Theatre 5
4:30 pm - 6:30 pm	Laboratory Activity		
	In the lecture room (**LS**, **LM**; MZ, SCT, GDD) 4:30 pm - 5:30 pm **BLUE** & **GREEN** Symmetry in crystals with exercises (symmetry operations; lattices) 5:30 pm - 6:30 pm **PURPLE** & **BROWN** Symmetry in crystals with exercises (symmetry operations; lattices)	In the chemistry lab (**MSW**, **AA**; JS, ZM) 4:30 pm - 5:30 pm **PURPLE** Crystal growing techniques 5:30 pm - 6:30 pm **BLUE** Crystal growing techniques	In the XRD lab (**AS**, **JE**; MZ, JS, ZM) 4:30 pm - 5:30 pm **BROWN** Crystal selection and mounting, XRD data collection 5:30 pm - 6:30pm **GREEN** Crystal selection and mounting, XRD data collection

Schedule of **Activities**

<table>
<tr><th colspan="4">Day 2 | Tuesday, June 3, 2025
Chairs: AA (Morning Session) & GDD (Afternoon Session)</th></tr>
<tr><td>8:30 am - 9:30 am</td><td colspan="2">Point and space groups in crystals

Facilitator: LM</td><td>Chemistry Lecture Theatre 5</td></tr>
<tr><td>9:30 am - 10:30 am</td><td colspan="2">The International Tables for Crystallography Vol. A

Facilitator: LS</td><td>Chemistry Lecture Theatre 5</td></tr>
<tr><td>10:30 am - 11:00 am</td><td colspan="3">Coffee break</td></tr>
<tr><td rowspan="3">11:00 am - 1:00 pm</td><td colspan="3">Laboratory Activity</td></tr>
<tr><td><u>In the lecture room</u>
(LS, LM; SCT, MZ, GDD)

11:00 am - 12:00 pm
PURPLE & BROWN
Determination of plane and space groups with exercises

12:00 pm - 1:00 pm
BLUE & GREEN
Determination of plane and space groups with exercises</td><td><u>In the chemistry lab</u>
(MSW, AA; JS, ZM)

11:00 am - 12:00 pm
GREEN
Crystal growing techniques

12:00 pm - 1:00 pm
BROWN
Crystal growing techniques</td><td><u>In the XRD lab</u>
(AS, JE; MZ, JS, ZM)

11:00 am - 12:00 pm
BLUE
Crystal selection and mounting, XRD data collection

12:00 pm - 1:00 pm
PURPLE
Crystal selection and mounting, XRD data collection</td></tr>
<tr><td colspan="3"></td></tr>
<tr><td>1:00 pm - 2:00 pm</td><td colspan="3">Lunch</td></tr>
<tr><td>2:00 pm - 3:00 pm</td><td colspan="2">Cell determination and data collection strategies using Apex 6

Facilitator: AS</td><td>Chemistry Lecture Theatre 5</td></tr>
<tr><td>3:00 pm - 4:00 pm</td><td colspan="2">X-ray diffraction, Bragg's law, Reciprocal space

Facilitator: JE</td><td>Chemistry Lecture Theatre 5</td></tr>
<tr><td>4:00 pm - 4:30 pm</td><td colspan="3">Coffee break</td></tr>
<tr><td rowspan="2">4:30 pm - 6:30 pm</td><td colspan="3">Practical Activity</td></tr>
<tr><td colspan="3">In Computer Resource Lab

All Groups: Tutorial on Apex 6

AS; MZ; JE; AA, LM, SCT, GDD, JS, ZM</td></tr>
</table>

Schedule of **Activities**

Day 3 | Wednesday, June 4, 2025 Chairs: GDD (Morning Session) & MZ (Afternoon Session)		
8:30 am - 10:30 am	Practical Activity: Tutorial #1 on the use of the Cambridge Structural Database Facilitator: **IG and YO**	In Computer Resource Lab
10:30 am - 11:00 am	**Coffee break**	
11:00 am - 12:00 pm	Structure factors Facilitator: **SCT**	Chemistry Lecture Theatre 5
12:00 pm - 1:00 pm	Structure Solutions Method Facilitator: **JE**	Chemistry Lecture Theatre 5
1:00 pm - 2:00 pm	**Lunch**	
2:00 pm - 3:00 pm	Data integration, scaling and space group determination using Apex6 Facilitator: **AS**	Chemistry Lecture Theatre 5
3:00 pm - 4:30 pm	Structure refinement step by step – live demo with real data Facilitator: **LM**	Chemistry Lecture Theatre 5
4:00 pm - 4:30 pm	Coffee break	
4:30 pm - 6:30 pm	Laboratory Activity	
	In the lecture room (**LM**; JE, MZ, LS, GDD) All groups Structure refinement with SHELXL	In the XRD and chemistry labs (**AS**, **MSW**, **AA**; JE, SCT, JS, ZM) Activity continues as needed

Schedule of **Activities**

Day 4 | Thursday, June 5, 2025 Chairs: LM (Morning Session)		
8:30 am - 10:30 am	Practical Activity: Tutorial #2 on the use of the Cambridge Structural Database Facilitators: **IG and YO**	In Computer Resource Lab
10:30 am - 11:00 am	**Coffee break**	
11:00 am - 12:00 pm	Structural computing and analysis using Mogul and Crystal explorer- live demo with real data Facilitator: **JE, IG**	In Computer Resource Lab
11:00 am – 1: 00 pm	In the XRD and chemistry labs (**AS**, **MSW**, AA; LM, MZ, SCT, JS, ZM): Activity continues as needed	
12:00 pm - 1:00 pm	Use of ITA for structural analysis: a case study Facilitator: **LS**	Chemistry Lecture Theatre 5
1:00 pm - 2:00 pm	**Lunch**	
2:00 pm	Excursion	

Schedule of **Activities**

Day 5 | Friday, June 6, 2025 Chairs: IG (Morning Session) & MSW; LS (Afternoon Session)		
8:30 am - 9:30 am	Polymorphism in organic crystals Facilitator: **AA**	Chemistry Lecture Theatre 5
9:30 am - 10:30 am	Polymorphism and phase transitions in inorganic crystals Facilitator: **SCT**	Chemistry Lecture Theatre 5
10:30 am - 11:00 am	Coffee break	
11:00 am - 1:00 pm	Laboratory Activity	
	In the Computer Resource Lab (LM, MZ, LS, AA) Structure refinement with SHELXL: new data	In the XRD and chemistry labs (AS, MSW, AA: JE; SCT, JS, ZM) Activity continues as needed
1:00 pm - 2:00 pm	Lunch	
2:00 pm - 3:20 pm	**Students' presentations** (20 min/GROUP; each group nominates their delegates to present the results of their work)	Chemistry Lecture Theatre 5
3:20 pm - 4:00 pm	Q & A Session on the work presented by groups All lecturers and students	Chemistry Lecture Theatre 5
4:00 pm - 4:30 pm	Coffee break	
4:30 pm – 6:30 pm	A Crystallography Symposium Chemistry Lecture Theatre 5	
	Special topics: • Metal-Organic Frameworks: **MSW, JS, ZM** • Organic molecular materials: **LM** • Polymorphism in Pharmaceuticals: **GDD** • Bioactive compounds from crystal engineering to drug delivery: **AA** • Quantum Crystallography: **JE** • Single crystal X-ray diffraction at variable T and P: **MZ** • Spinels: **SCT** • Perovskites: **LS**	

Schedule of **Activities**

Day 6 | Saturday, June 7, 2025 Chairs: MZ (Morning Session)		
8:30 am - 9:30 am	Structure validation, preparation of CIF file, CIF tools Facilitator: **GDD**	Chemistry Lecture Theatre 5
9:30 am - 10:30 am	Round table: All lecturers are students	Chemistry Lecture Theatre 5
10:30 am - 11:00 am	Coffee break	
11:00 am - 1:00 pm	Laboratory Activity	
	In the Computer Resource Lab (**LM**: JE, GDD, MZ, LS) Structure refinement with SHELXL: new data	In the XRD and chemistry labs (**MSW, AA**: JE; SCT, JS, ZM) Activity continues as needed
1:00 pm - 2:00 pm	Lunch	
2:00 pm - 3:00 pm	IUCr sponsored lecture Publishing with IUCr Journals Facilitator: **GDD**	Chemistry Lecture Theatre 5
3:00 pm - 4:00 pm	Presentation of Certificates of Attendance and Awards (ICDD, AIC, RSC, IUCr; UNESCO Office for the Caribbean Facilitator: **MZW**	Chemistry Lecture Theatre 5
4:00 pm - 4:30 pm	Closing Remarks	

Key to Lecturers and Tutors

Andrea Araya-Sibaja (**AA**)	Lucia Maini (**LM**)	Michele Zema (**MZ**)
Ashley Schmidt (**AS**)	Yinka Olatunji-Ojo (**YO**)	Jermaine Smith (**JS**)
Javier Alcides Ellena (**JE**)	Marvadeen Singh-Wilmot (**MSW**)	Zeyar Min (**ZM**)
Graciela Diaz de Delgado (**GDD**)	Leopoldo Suescun (**LS**)	
Ilaria Gimondi (**IG**)	Serena C. Tarantino (**SCT**)	

Thanks to
Sponsors and Partners

for contributing to the hosting of the Inaugural Caribbean Crystallography School 2025

1. Caribbean Regional X-ray Science Toward Advancement Laboratory (crXstal) School, Department of Chemistry, Faculty of Science and Technology, The University of the West Indies, Mona;
2. Lightsources for Africa, the America, Asia, Middle East and the Pacific (LAAAMP)
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5. The University of Bologna Global South Program (UniBo)
6. Cambridge Crystallographic Data Centre (CCDC)
7. Bruker AXS
8. Italian Crystallography School (AIC). Please visit the AIC website to explore available grants.
9. International Science Council
10. Juici Beef Limited
11. Royal Society of Chemistry
12. International Union of Crystallography (IUCr). Financial support has been received from the IUCr. Please visit the IUCr meeting website to view the availability of funds to assist young scientists.
13. LearnSci
14. American Crystallography Association
15. International Centre for Data Diffraction

Endorsement

Thanks to the following partners for their Generous Support/Endorsement of the School.

1. The Latin American Crystallography Association
2. IUCr Commission on Structural Chemistry
3. George Washington University

Thanks to Sponsors and Partners

for contributing to the establishment of Caribbean Regional X-ray Science Toward Advancement Laboratory (crXstal)
(Launched October 3, 2024)

1. UNESCO Participation Programme
2. Office of the Principal, The University of the West Indies, Mona
3. Faculty of Science and Technology, The University of the West Indies, Mona
4. Faculty of Science and Technology, The University of the West Indies, Cave Hill
5. Lightsources for Africa, the America, Asia, Middle East and the Pacific (LAAAMP)
6. Royal Society of Chemistry
7. The University of Bologna Global South Program (UniBo)
8. Caribbean Academy of Science Jamaica
9. Juici Beef Limited
10. Bruker AXS
11. Bristol Myers
12. Prof. Sekazi Mtingwa

Student **Participants**

Student Participants	
Country	**Name**
Jamaica	1. Dr. Zeyar Min University of Technology, Jamaica 2. Mr. Ayele Edwards University of Technology, Jamaica 3. Mr. Jermaine Smith The University of the West Indies, Mona 4. Dr. Mark Lawrence The University of the West Indies, Mona 5. Mr. Marcel Denny The University of the West Indies, Mona 6. Mr. Daniel Gillings The University of the West Indies, Mona 7. Dr. Tanya Kerr The University of the West Indies, Mona 8. Dr. Nickeisha Stephenson The University of the West Indies, Mona 9. Dr. Tahjna Roberston The University of the West Indies, Mona 10. Ms. Brianna Levy The University of the West Indies, Mona 11. Ms. Ackeera Campbell, The University of the West Indies, Mona 12. Ms. Crystal Tomlinson The University of the West Indies, Mona 13. Mr. Kirk Wilson The University of the West Indies, Mona 14. Ms. Alexandra DeFreitas The University of the West Indies, Mona
Trinidad and Tobago	15. Dr. Dinesh Pathak The University of the West Indies, St. Augustine 16. Dr. Michael Forde The University of the West Indies, St. Augustine 17. Dr. Varma Rambaran The University of Trinidad and Tobago 18. Dr. Wilson Sue Chee Ming The University of the West Indies, St. Augustine
Belize	19. Dr. Joaquin F. Urbina University of Belize 20. Dr. Apolonio Aguilar University of Belize 21. Mr. Stephen Sangster University of Belize
Barbados	22. Mr. Kahdio Brandon The University of the West Indies, Cave Hill 23. Dr. Keisha Ellis-Holder The University of the West Indies, Cave Hill 24. Dr. Jason Jordan The University of the West Indies, Cave Hill 25. Prof Avril Williams The University of the West Indies, Cave Hill

Faculty of Science and Technology

Caribbean Regional X-ray Science Toward Advancement Laboratory (crXstal)

presents

The Inaugural Caribbean Crystallography School

The Inaugural Caribbean Crystallography School

The Caribbean Crystallography School (CCS) is a premier training initiative hosted by the Caribbean Regional X-ray Science Toward Advancement Laboratory (crXstal) at The University of the West Indies, Mona. Established in October 2024 within the Department of Chemistry, Faculty of Science and Technology, crXstal serves as a regional hub for advancing X-ray crystallography through education and research.

This inaugural school aims to:

1. Expose participants to the fundamental theory of X-ray diffraction and single-crystal X-ray diffraction.
2. Train participants in techniques used for growing single crystals.
3. Collect single-crystal data using the BRUKER D8 Quest Eco.
4. Solve single-crystal structures using various software packages.
5. Prepare crystal structure data for publication.

Participants will have access to state-of-the-art instrumentation, including a Bruker D8 Quest Eco single-crystal diffractometer and an Oxford Diffraction cryostat.

Date: **June 2-7, 2025**

Venue: **The University of the West Indies, Mona Campus**
Kingston Jamaica

Register at:
https://bit.ly/Register-MAST-Courses

Facilitators

Professor Michele Zema
University of Bari, Italy
Chair of Lightsources for Africa, the Americas, Asia, Middle East and Pacific (LAAAMP)
Co-Founder & Co-Chair, Caribbean Crystallography School

Dr. Marvadeen Singh-Wilmot
Senior Lecturer, Dept. of Chemistry, FST, The UWI Mona
Co-Founder & Chair, Caribbean Crystallography School

876-927-1660-9 • fstprofessional@uwimona.edu.jm • www.mona.uwi.edu/fst/new-programmesshort-courses

The Inaugural Caribbean Crystallography School

Opening Ceremony

Monday, June 2, 2025 • 9:00am

Chemistry Lecture Theatre 5
Faculty of Science and Technology The UWI Mona

PROGRAMME

WELCOME/OPENING REMARKS
Dr. Marvadeen Singh-Wilmot
Senior Lecturer, Department of Chemistry
Faculty of Science and Technology, The UWI Mona &
Co-Founder of crXstal and Co-Chair of the Caribbean Crystallography School

GREETINGS
Professor Michael Taylor
Dean, Faculty of Science and Technology,
The UWI Mona

Dr. Donna Minott Kates
Head, Department of Chemistry
Faculty of Science and Technology
The UWI Mona

Professor Densil Williams
Principal and Pro-Vice Chancellor
The University of the West Indies, Mona

Ms. Cecilia De Santis
Honorary Consul, Italy

REMARKS
Professor Michele Zema
University of Bari, Italy
Chair of Lightsources for Africa, the Americas, Asia, Middle East and Pacific (LAAAMP)
&
Co-Founder of crXstal and Co-Chair of the Caribbean Crystallography School

Dr. Bandiougou Diawara
Head of the Natural Sciences Sector
UNESCO Office for the Caribbean

Dr. Andrea Mariela Araya Sibaja
President, Latin American Crystallographic Association

Prof. Graciela Diaz de Delgado
Vice President, International Union of Crystallography &
Member, International Science Council's Liaison Committee of the Regional Focal Point for Latin America and the Caribbean

Prof. Lucia Maini
Executive Committee Member
Italian Crystallographic Association &
Representative, University of Bologna Global South Programme

CLOSING ACTIVITY
Crystallizing the Network

The Inaugural

Caribbean Crystallography School