

PERSONAL INFORMATION **Dr. Maqsood AHMED**

Associate Professor of Physical Chemistry and X-rays crystallography,  
Institute of Chemistry, The Islamia University of Bahawalpur (IUB), 63100, Pakistan  
Principal Investigator, Materials Chemistry Laboratory (MCL)  
+ Member, National Adhering Body to the IUCr.  
+ Visiting faculty, International Centre for Chemical & Biological Sciences (ICCBS),  
University of Karachi, Pakistan.  
+92 62 9255473 +92 321 6746041, +92 333 8946041

Website: <http://mcl.iub.edu.pk/>

✉ maqsood.ahmed@iub.edu.pk  
maqsoodbwp@gmail.com

Gender Male | Date of birth 01/09/1982 | Nationality Pakistani

Blood Group B+ | Marital Status Married, father of three.

**PHD THESIS TITLE** Ultra High Resolution Crystallography of Small Molecules and Proteins. (Defended May 30, 2012)

**SUPERVISED BY** Prof. Claude LECOMTE and Dr. Christian JELSCH (Université de Lorraine Nancy, France).

**EDUCATION AND WORK EXPERIENCE**

From	To	Position	Institution, City	Country	Degree / remarks
09/2013	date	Assistant Professor	Department of Chemistry, The Islamia University of Bahawalpur.	Pakistan	Full time (Teaching and Research)
06/2012	06/2013	Assistant Professor	Department of Chemistry, GC University Lahore.	Pakistan	Full time (Teaching and Research)
10/2008	05/2012	Doctoral Student	CRM2, Université de Lorraine, Nancy.	France	Fully Funded Overseas Scholarship by the Higher Education Commission (HEC) of Pakistan
07/2008	09/2008	French Language Student	Institut de Langue et de Culture Françaises, Paris	France	French Language Diploma (European level, B1)
01/2008	06/2008	French Language Student	Alliance Française de Lahore	Pakistan	French Language certificate (DELTA A2)
09/2007	12/2007	Research Scholar	The Islamia University of Bahawalpur	Pakistan	Scholarship by The Higher Education Commission (HEC), Pakistan.
09/2005	08/2007	Lecturer (Chemistry)	Federal Government College Bahawalpur	Pakistan	Full time (Teaching)
02/2005	08/2005	No Position	-	Pakistan	Job search and period for selection process for the post of Lecturer
10/2002	01/2005	Student	The Islamia University of Bahawalpur	Pakistan	M. Sc. / 1st division
10/2001	09/2002	No Position	-	Pakistan	Temporary work prior to admission for Master's degree
09/1999	09/2001	Student	Government Sadiq Egerton College Bahawalpur	Pakistan	B. Sc. / 1st division
09/1997	08/1999	Student	Government College Lahore	Pakistan	F. Sc. / 1st division
04/1995	08/1997	Student	Government Arabic Model High School, Pakpattan	Pakistan	Matric/ 1st division

## LANGUAGE SKILLS

Mother tongue	Punjabi				
Other languages	UNDERSTANDING		SPEAKING		WRITING
	Listening	Reading	Spoken interaction	Spoken production	
Urdu	C2	C2	C2	C2	C2
	National language and medium of education				
English	C2	C2	C2	C2	C2
	Official language and medium of education				
French	B1	C1	B1	B1	B1
	DELF B1				

Levels: A1/2: Basic user - B1/2: Independent user - C1/2 Proficient user  
Common European Framework of Reference for Languages

## Computer Skills

- Subject Related:**  
CCDC tools (ConQuest, Mercury, Mogul, IsoStar), CCP4 Package, CRYSTAL17, Gaussian09 GAMESS, MoPro, WinGx Package, Olex2, PyMOL, COOT, Phenix, CrysAlisPro, HKL2000, APEX2, pubCIF etc.
- General:**  
MS Office, ORIGIN, Linux and Windows operating systems.

## Training workshops and Schools (attended and conducted)

- ‘Professional Courses for University Management’ 23-26 February, 2021**, a four day training at NUST, Islamabad funded by The Islamia University of Bahawalpur.
- 4<sup>th</sup> International Workshop on X-rays Crystallography in Structural Biology February 25-27, 2020 at The Islamia University of Bahawalpur**. Organizer and resource person. Funding was received from the IUCr, The Higher Education Commission of Pakistan (HEC), Pakistan Science Foundation (PSF) and commercial sponsors. 60 participants, mainly PhD students and faculty members from across the country were provided hands on training on all aspects of protein structure determination.
- 3<sup>rd</sup> International Workshop on X-rays Crvstallography in Structural Biology** co-organizer and official resource person of a four day training workshop to be conducted at ICCBS, University of Karachi from **October, 8-10, 2018**.
- 43<sup>rd</sup> International Nathiagali Summer College on Physics and Contemporary Needs, July 2018**
- 2<sup>nd</sup> International Workshop on X-rays Crvstallography in Structural Biology** co-organizer and official resource person of a four day training workshop to be conducted at Foramen Christian College (A Chartered University), Lahore, Pakistan from **October, 8-10, 2016**.
- A workshop on Privacy, Digital Data Safety, Communication and Collaboration**, The Islamia University of Bahawalpur, 29 September, 2016
- 1<sup>st</sup> X-rays Crystallography in Structural Biology”** co-organizer and official resource person of a three day training workshop to be conducted at National Institute of Biology and Genetic Engineering (NIBGE) Faisalabad from **November, 12-14, 2015**. No. of Participants 30 with a funding from HEC and foreign agencies.
- “Basic concepts and applications of X-rays diffraction techniques”** an online course delivered at International Center for Chemical and Biological Sciences, University of Karachi and relayed live across Pakistani Universities through HEC’s Virtual Educational Server from August **24-02 September, 2015**.

9. **“Uses and applications of Cambridge Crvstallographic Database” 15 December, 2014** organized at The Islamia University of Bahawalpur. There were 50 participants from various Departments.
10. **IUCr-UNESCO Open Factory in Darmstadt and Grenoble, 10-19 September, 2014.**
11. **IUCr-UNESCO Open Lab in Karachi, Pakistan, April 30- May 08, 2014** as official resource person. Taught basic and advanced topics in crystallography and provided ‘hands on’ training to 50 participants from eight nationalities.
12. **International workshop on crvstallography and nano-technology, GC University Lahore Pakistan, October 19-21, 2011** as resource person to conduct a session on charge density refinement with MoPro.
13. **2<sup>nd</sup> Bio-crvstallography School June 25-July 2010, Marseille France.**
14. **MathCryst2010 (1<sup>st</sup> part), June 22- July 2, Nancy France** Summer School on Mathematical Crystallography
15. **4<sup>th</sup> Crvstallography School October 5-9, 2009, Abbe-des-Prémontrés, Pont à Mousson, France** entitled “*Structural Analysis Using Single-Crystal X-ray Diffraction and Crystallography under Constrains*”.

## Award and Honours

1. Co-advisor, IUB Science Society
2. Focal Person and Mentor in IUB for Science Talent Farming Scheme (STFS) of The Pakistan Science Foundation
3. Officially nominated from Pakistan to participate in the 65<sup>th</sup> Lindau Nobel Laureates Meeting, 2015.
4. Principle Investigator of The Islamia University of Bahawalpur’s mega research project worth PKR 92.1 million for the establishment of an X-rays diffraction laboratory. (Approved, 2014).
5. Fully funded overseas scholarship for PhD in France awarded by The Higher Education Commission of Pakistan (HEC) for the period 2008-2012.
6. ‘Rising Star Award’ by The Asian Crystallographic Association (AsCA) in 2013 in Hong Kong.
7. IUCr travel grant for the 11<sup>th</sup> meeting of Asian Crystallographic Association (AsCA) in 2012 in Adelaide.
8. A grant worth US\$ 5000 from the IUCr President’s fund to host first meeting of Pakistan Crystallographic Association in October 2011.
9. IUCr travel grant for the 2<sup>nd</sup> IUCr Congress and General Assembly Madrid, 2011.
10. “Roll of Honor” as best student in high school for the period 1992-97.

## Conferences Attended

1. International Chemistry Conference, 27-29 March, 2019, Bahaudine Zakariya University, Multan. (Poster presentation)
2. **16<sup>th</sup> SESAME User’s meeting**, 15-16 December, 2018, Amman, Jordan, Secured travel grant from Loundsberry Foundation for Oral Talk.
3. **Poster Presentation at 43<sup>rd</sup> Intl. Nathiagali Summer College** National Center for Physics, Islamabad, 16-28 July, 2018.
4. **Oral Presentation International Conference on Teaching and Learning (ICOTAL, 2018)**, Department of Education, IUB, Bahawalpur. 19-20 March, 2018
5. **Invited Lecture 1st South Esat Asia Conference on Crvstal Engineering (SEACCE)**, University of Jeyawardhenapur, Colombo, Srilanka, 05-09- September, 2016
6. **65<sup>th</sup> Lindau Nobel Laureate Meeting** 28 June-04 July, 2015, Lindau, Germany.
7. **Oral presentation (10 minutes) as Invited Speaker** entitled “*Crystallography in Pakistan: current status and future prospectus*” at the IYCr Legacy Conference, Hassan II Academy of

- Science, Rabat, Morocco from 22-24 April, 2015.
8. **Oral presentation (15 minutes)** entitled “*Ultra high resolution crystal structure of protein Cholesterol oxidase*” presented at the 12<sup>th</sup> International Conference of Pakistan Society for Biotechnology and Molecular Biology held at the Islamia University of Bahawalpur, Pakistan from 4-7 December, 2014.
  9. **Oral presentation (20 minutes)** entitled “*Crystallography at ultra high resolution; Charge density analysis of small molecules and proteins*” presented as invited speaker at the IUCr-UNESCO South Asia Summit held at ICCBS, University of Karachi from 28-30 April, 2014 in connection with celebrating 2014 as International Year of Crystallography.
  10. **Oral presentation (20 minutes)** entitled “*An experimental and theoretical charge density analysis of Bromoethyl sulphonium triflate; atomic charges and their implications for reaction mechanism*” presented at the 12<sup>th</sup> Meeting of the Asian Crystallographic Association (AsCA), held at Hong Kong University of Science and Technology, Hong Kong December 7-10, 2013. Travel grant (USD 800) provided by AsCA.
  11. **Oral presentation (20 minutes)** entitled “*Ultra high resolution X-rays structure of protein Cholesterol oxidase*” at 12<sup>th</sup> SESAME synchrotron users meeting to be held at Amman, Jordan, November 20-22, 2013. Invitation with full funding from SESAME.
  12. **Oral presentation (30 minutes)** entitled “*Ultra high resolution X-rays crystallography and X-rays charge density analysis: the ultimate tool in a chemists hands*” presented at “12<sup>th</sup> International and 24<sup>th</sup> National Conference of The Pakistan Chemical Society held at Bahauddin Zakariya University Multan, October 28-30, 2013.
  13. **Oral presentation (50 minutes)** entitled “*Ultra high resolution crystallography & Experimental electron density analysis: A tool to study intermolecular interactions*” invited to present at the International workshop on crystallography & nano-technology and the First meeting of Pakistan Crystallographic Association at GCU, Lahore 19-21 October 2011.
  14. **Oral presentation (15 minutes)** entitled “Structural studies and charge density analysis of thiophene based compounds” presented at the 22<sup>nd</sup> IUCr Conference and General Assembly August 22-29, Madrid, Spain.
  15. **Poster Presentation** entitled “Structural studies and charge density analysis of thiophene based compounds” presented at the 22<sup>nd</sup> IUCr Conference and General Assembly August 22-29, Madrid, Spain.
  16. **Poster Presentation** entitled “Stereochemistry and charge density of hydrogen bonds with oxygen acceptors” at the Doctoriales de Lorrains, May 22-27, 2011, Ventron, France.
  17. **Poster Presentation** entitled “Stereochemistry and charge density of hydrogen bonds with oxygen acceptors” at the DocSciLor (young researchers), June 23, 2011, Nancy, France.
  18. **Oral Presentation (15 minutes)** entitled “*Stereochemistry and charge density of hydrogen bonds with oxygen acceptors*” at the “First North African Crystallographic Conference (NACC-1)” November 23-26, 2010 Casablanca, Morocco.
  19. **Oral Presentation (15 minutes)** entitled “*Stereochemistry and charge density of hydrogen bonds with oxygen acceptors*” at Colloque de AFC (Association Française de cristallographie) July 7-10, 2010 Strasbourg, France.
  20. **Poster Presentation** entitled “*Electron density analysis of atomic polarization in protein Cholesterol Oxidase*” at the Young researchers Day conference at the University of the Greater Region, March 19-20,

# Curriculum Vitae

Dr. Maqsood AHMED

2010 Saarbrücken, Germany.

21.

## Publications

1. Arshad Mehmood, Aisha Fahim, **Maqsood Ahmed**, Sajida Noureen (2020). *J. Molecular Structure Regioselectivity of reduction of nitro groups in 3,5-dinitrosalicylic acid monohydrate explored by experimental and theoretical charge density analysis* (Accepted, special issue on charge density analysis)
2. Muhammad U Faroque, Arshad Mehmood, Sajida Noureen, **Maqsood Ahmed** (2020). *J. Molecular Structure* (1214) 128183 *Crystal engineering and electrostatic properties of co-crystals of pyrimethamine with benzoic acid and gallic acid.*  
<https://doi.org/10.1016/j.molstruc.2020.128183>
3. Asma Hasil, Arshad Mehmood, Sajida Noureen, **Maqsood Ahmed** (2020). *J. Molecular Structure* (1216). 128295 *Experimental and theoretical charge density analysis of skin whitening agent Kojic acid* (Published in the special issue on charge density analysis)  
<https://doi.org/10.1016/j.molstruc.2020.128295>
4. Maharzadi Noureen Shahi, Alia Iqbal, Rashida Bibi, Misbah-ul-Ain Khan, **Maqsood Ahmed**, Sajida Noureen (2020). *J. Mol. Structure*, Volume 1206, 127657. *Syntheses and electron density distribution studies in two new imidazole derivatives.*  
<https://doi.org/10.1016/j.molstruc.2019.127657> IF: **2.1**
5. Hasil, A., Mehmood, A. & **Ahmed, M.** (2019). *Acta Cryst. B75*, 750-762. <https://doi.org/10.1107/S2052520619007911>, *Experimental and theoretical charge-density analysis of hippuric acid: insight into its binding with human serum albumin solvent studied using transferred electron-density parameters.* IF: **6.732**
6. M. U. Faroque, S. Noureen, S. H. Mirza, M. N. Tahir & **M. Ahmed** (2019). *Acta Cryst. C75*, 46-53. *Structure and electrostatic properties of the pyrimethamine–3,5-dihydroxybenzoic acid cocrystal in water solvent studied using transferred electron-density parameters.* IF : **0.93**
7. Shahid, A., Aziz, A., Noureen, S., **Ahmed, M.** Yousuf, S. and Choudhary, M. I. (2018). *Acta Cryst, C74*, 534–541. *Biotransformation, spectroscopic investigation, crystal structure and electrostatic properties of 3,7 $\alpha$ -dihydroxyestra-1,3,5(10)-trien-17-one monohydrate studied using transferred electron-density parameters.* IF : **0.93**
8. Muhammad Umer Faroque, Sajida Noureen, **Maqsood Ahmed** and Muhammad Nawaz Tahir, (2018). *Acta Cryst. C74*, 100-107. *Electrostatic properties of the pyrimethamine–2,4-di-hydroxy-benzoic acid cocrystal in methanol studied using transferred electron-density parameters* IF : **0.93**
9. Erum Akbar Hussain, Nosheen Kanwal, Islam Ullah Khan, Sadaf Mutahir, Muhammad Asim Khan, **Maqsood Ahmed**, Arshad Mahmood, Onur Sahin, Mehmet Akkurt, Muhammad Yar. (2018) *Lett. Org. Chem.* **15**(3). 163-170. *Green and Facile Reaction of Gabapentin with Sulfonyl Chlorides to Synthesize Lactams and Sulfonamides Derivatives in Aqueous Medium.* DOI: 10.2174/1570178614666170907143340 IF : **0.93**

10. Ammara Shahid, Sajida Noureen, Muhammad Iqbal Choudhary, Sammer Yousuf and **Maqsood Ahmed** *Acta Cryst.* (2017). **C73**, 430–436; *Crystal structure and electrostatic properties of prednisolone acetate studied using a transferred multipolar atom model* **IF : 8.667**
11. Ammara Shahid, Sajida Noureen, Muhammad Iqbal Choudhary, Sammer Yousuf and **Maqsood Ahmed** *Acta Cryst.* (2017). **C73**, 430–436; *Crystal structure and electrostatic properties of prednisolone acetate studied using a transferred multipolar atom model* **IF : 8.667**
12. Muhammad Umer Faroque, Sammer Yousuf, Salman Zafar, M. Iqbal Choudhary and **Maqsood Ahmed** (2016). *Acta Cryst.* **C72**, 398–404; *Transferred multipolar atom model for 10 $\beta$ ,17 $\beta$ -dihydroxy-17 $\alpha$  methylestr-4-en-3-one dehydrate obtained from the biotransformation of methyltestosterone* **IF : 4.099**
13. **Maqsood Ahmed, Ayoub** Nassour, Sajida Noureen, Claude Lecomte, Christian Jelsch. (2016). *Acta Cryst.* **B72**, 75-86. “*Experimental and Theoretical charge density analysis of 1,4-bis (5-hexyl-2-thienyl) butane-1,4 dione: Applications of a virtual atom model.* **IF : 2.032**
14. Mariya Al-Rashida, Syeda Abida Ejaz, Sharafat Ali, Aisha Shaukat, Mahwish Hamayoun, **Maqsood Ahmed**, Jamshed Iqbal (2015) “*Diarylsulfonamides and their bioisosteres as dual inhibitors of alkaline phosphatase and carbonic anhydrase: structure activity relationship and molecular modelling studies*”. *Bioorganic & Medicinal Chemistry*, **23**, 2435-2444. **IF: 2.448**
15. Bartosz Zarychta, Artem Lyubimov, **Maqsood Ahmed**, Parthapratim Munshi, Benoit Guillot, Alice Vrielink and Christian Jelsch. (2015). *Acta Crystallographica Section D* **71**, 954-968. “*Ultra high resolution crystal structure and charge density study of cholesterol oxidase.*” [doi:10.1107/S1399004715002382](https://doi.org/10.1107/S1399004715002382). **IF: 2.512**
16. Yar, M., Bajda, M., Shahzadi, L., Shahzad, S. A., **Ahmed, M.**, Ashraf, M., Alam, U., Khan, I. U., Khan. A. F. (2014). *Bioorganic Chemistry*. **54**, 96-104. “*Novel synthesis of dihydropyrimidines for  $\alpha$ -glucosidase inhibition to treat type 2 diabetes: in vitro biological evaluation and in silico docking*” <https://doi.org/10.1016/j.bioorg.2014.05.003> **IF: 2.152**
17. **Ahmed, M.**, Yar, M., Nassour, A., Guillot, B., Lecomte, C., Jelsch. C. (2013). *J. Phys. Chem. A* **117**, 14267-14275. *Experimental and theoretical charge density analysis of a bromoethyl sulphonium salt: Atomic charges and their implications for reaction mechanism.* **DOI: 10.1021/jp410301d** **IF: 2.641**
18. **Ahmed, M.**, Jelsch. C., Guillot, B., Lecomte, C., Domagala, S. (2013). *Cryst. Growth Des.* **13**, 315-325. “*Relationship between stereochemistry and charge density in hydrogen bonds with oxygen acceptors.* **DOI: 10.1021/cg3014656** **IF: 4.153**
19. Tabussum, A., Riaz, N., Saleem, M, Ashraf, M., **Ahmad, M.**, Alam, U., Jabeen, B., Malik, A., Jabbar, A. (2013) *Phytochemistry Letters*. **6**, 614-619 “ *$\alpha$ -Glucosidase inhibitory constituents from *Chrozophora plicata*”.. **DOI: 10.1016/j.phytol.2013.08.005** **IF: 1.575***
20. Jabeen, B., Riaz, N., Saleem, M., **Ahmed, M.**, Naveed, M. A., Tahir, M. N., Pescitelli, G.,

- Ashraf, M., Ejaz, S. A., Ahmed, I., Jabbar, A. (2013). *Zeitschrift fuer Naturforschung B – Chemical Sciences*. 68b, 1041-1048 “Isolation and Characterization of Limonoids from *Kigelia africana*”.. DOI: [10.5560/ZNB.2013-3096](https://doi.org/10.5560/ZNB.2013-3096) **IF: 0.744**
21. Farrukh, M. A., **Ahmed, M.**, Mohamed, S. K., Marzouk, A. A., El-Moghazy, S. M. (2013). *Acta Cryst.* E69, o936-o937 “3-((5(4-chlorophenyl)-3-methyl-1H-pyrazol-1-yl)methyl)-4-tolyl)-1H-1,2,4-triazole-5(4H)-thione”. DOI:[10.1107/S1600536813013494](https://doi.org/10.1107/S1600536813013494)
22. Farrukh, M. A., Mohamed, S. K., **Ahmed, M.**, Marzouk, A. A., El-Moghazy, S. M. (2013). *Acta Cryst.* E69, o295–o296. “4-[5-(4-Chlorophenyl)-3-methyl-1Hydrazol-1-yl]benzenesulfonamide” DOI:[10.1107/S1600536813002134](https://doi.org/10.1107/S1600536813002134)
23. **Ahmed, M.**, Noureen, S., Gros, P. C., Guillot, B., Jelsch, C. (2011). *Acta Cryst.* C67, o329-o333. “2, 2 - (Ethane-1, 2-diyl)bis[2-(5-bromothiophen-2-yl)-1,3-dioxolane] at 100 K refined using a multipolar atom model”. DOI:[10.1107/S0108270111027247](https://doi.org/10.1107/S0108270111027247) **IF : 0.518**
24. Domagała, S., Munshi, P. M., **Ahmed, M.**, Guillot, B., Jelsch. C. (2011). “Structural Analysis and Multipole Modelling of Quercetin Monohydrate – A Quantitative and Comparative Study”. *Acta cryst.* B67, 63-78. DOI:[10.1107/S0108768110041996](https://doi.org/10.1107/S0108768110041996) **IF : 2.286**