

Asian Charge Density Workshop

Analysis of Experimental and Theoretical Electron Densities:
Extracting Properties from a Multipole Refinement

February 23-26, 2015

Indian Institute of Science, Bangalore, Karnataka INDIA

Scientific and Social Program



Sponsors



University
of Glasgow



Sunday February 22nd

14:00 – 16:30 Arrival & Registration at Solid State and Structural Chemistry, IISc

19:00 – 21:00 Welcoming Reception by RSC – CVH Dining Hall

Monday, February 23rd *The Multipole Model & Refinement*

09:00-12:30 *Morning session: Chair - Claude Lecomte*

09:00-09:10 Opening remarks

09:10-09:55 **L1 – Philip Coppens** “A Birds Eye Introduction to X-ray Charge Density Analysis and Some Recent Developments”

09:55-10:20 Tea/coffee break

10:20-11:05 **L2 – Piero Macchi** “General Aspects of Multipole Modelling”

11:05-11:35 **L3 - Jacob Overgaard** “Importance of Modelling H-Atoms”

11:35-12:00 Introduction and preparation for hands on sessions (P. Macchi/C. Jelsch)

12:00-14:00 Lunch & Poster session

14:00-18:30 *Afternoon session: Hands on Workshop*

14:00-16:00 Hands-on Session #1 (Introduction – P. Macchi/C. Jelsch)

16:00-16:30 Tea/coffee break

16:30-18:30 Hands-on Session #1 (continued)

19:30 **Conference Banquet** at Main Guest House Lawns

Tuesday, February 24th *Chemistry from Electron Densities*

09:00-12:30 *Morning session: Chair –Wolfgang Scherer*

09:00-09:45 **L4 – Dietmar Stalke** “Only good data can challenge chemical concepts”

09:45-10:15 **L5 - T.N. Guru Row** “ σ - and π -holes from Charge Densities: Relevance to Chemistry”

10:15-10:45 Tea/coffee break

10:45-11:15 **L6 – Gautam Desiraju** “Charge Densities in Crystal Engineering”

11:15-11:45 **L7 – Pierre Becker** “Important aspects concerning joint refinement of charge/spin electron densities or charge/momentum densities”

12:00-14:00 Lunch & Poster session

14:00-18:30	<i>Afternoon session: Hands on Workshop</i>
14:00-16:00	Hands-on Session #2 (P. Macchi/C. Jelsch)
16:00-16:30	Tea/coffee break
16:30-18:30	Hands-on Session #2 (continued)
19:30	Dinner – CVH Dining Hall

Wednesday, February 25th

9:00 – 19:30 Day trip to Jain Shrine Shravanabelagola , Hoysala Temples at Belur and Halebid

Thursday, February 26th *Advanced Techniques*

09:00-12:30	<i>Morning session: Chair –Jacob Overgaard</i>
09:00-09:45	L8 – Claude Lecomte “X , n polarized neutron joint refinement Applications to organic radicals and molecular magnets.”
09:45-10:30	L9 - Wolfgang Scherer “Chemical Bonding in Solid State Compounds”
10:30-11:00	Tea/coffee break
11:00-13:00	Hands-on Session #3 (P. Macchi/C. Jelsch)
13:00-14:00	Lunch
14:00-16:30	<i>Afternoon session: Chairs – Pierre Becker</i>
14:00-14:15	L10 – Dylan Jayatilaka “X-ray wavefunction refinement - Introduction”,
14:15-14:30	L11 - Simon Grabowsky "X-ray wavefunction refinement - Application"
14:30-16:30	Hands-on Session #4 (Dylan Jayatilaka & Simon Grabowsky)
16:30	Concluding remarks