PROGRAM SCHEDULE

Advanced Methods in X-ray Diffraction Analysis: the XD Programming Package
Buffalo NY, 12-17 May 2003
12th May, Monday

Pre-workshop talk by Dr. Charles Campana of Bruker AXS on “Solving difficult structures and analyzing twinned and modulated crystals”

14:00-16:00

Location: Natural Sciences Complex (NSC, Chemistry Building) room 684

Evening

OPENING RECEPTION

At 18:30 a bus* will be available for those who prefer not to walk to the Natural Sciences Complex (abbreviated NSC) where the informal opening reception will take place.

At 21:00 the same bus* will provide transportation from the NSC (at Rensch Loop) back to the motel.

* OPERATED BY “OVER THE FALLS TOURS”

Location of the X-ray Crystallographic Laboratory: Natural Sciences Complex rooms 726-747
TOPIC: REFINEMENT

Free breakfast served 7.30-8.30 at Bert’s (next to NSC lecture halls)

Morning Session 9.00-12.00 Chair: Dr. V. Young

Opening ceremony: 8.45-9.00
Welcoming remarks
H. Hauptman, Nobel Laureate

Introductory lecture: 9.00-10.00
X-ray charge density and chemical bonding: the historical background and future prospects
P. Coppens

Main lecture: 10.15-11.15
The multipolar model and least squares refinement
T. Koritsanszky

Short lectures: 11.15-12.15
Symmetry restraints and chemical constraints
P. Mallinson

The choice of radial functions
P. Macchi

Afternoon Session 13.30-16.30
(tea/coffee will be served 15.00-16.00 in NSC room 216)

Tutorial

Location: Natural Sciences Complex room 218
Presentation by CCR staff
How to access the computer nodes (15 minutes)

Group 1 (beginners)
Teachers: L. Farrugia, P. Mallinson, T. Koritsanszky

getting started with XD (XDINI)
from shelves to XD
from cif files to XD
XDLSM input and output files handling

performing least-squares refinements
worked examples with some datasets
refining multipole variables
refining extinction
refining higher order thermal motion parameters
wave functions and radial deformation functions
refining against neutron data

description of the new features of XDLSM and XDINI
choice of radial functions
extinction
improved code performances
refining difficult parameters
examples provided by the students

Group 2 (advanced)

Teachors: P. Macchi, A. Volkov

Location: Hochstetter Hall room 139

Location: Hochstetter Hall room 141

THIS SESSION CONTINUES ON THE NEXT PAGE!
Poster Session P10X, 16.30 -17.30, NSC room 218
poster presentations (10 minutes each), experimental techniques

Evening: Informal Dinner at Brewpub

At 18:30 a bus* will provide transportation from the Natural Sciences Complex to the Brewpub (6861 Main Street, Williamsville, NY 14221)
At 21:30 the same bus* will provide transportation from the Brewpub back to the motel

* operated by “OVER THE FALLS TOURS”
14th May, Wednesday

TOPIC: Fourier methods and analysis of the results

Morning Session 8.30-12.00

Location: Natural Sciences Complex room 218

Main lecture: Fourier methods in X-ray charge density;
8.30 - 9.30
The rho-cif dictionary
P. Mallinson

coffee break at NSC room 216

Tutorial 9.45-12.00

(tea/coffee will be served 11.00-12.00 in NSC room 216)

Group 1 (beginners) Group 2 (advanced)

Location: Hochstetter Hall room 139 Location: Hochstetter Hall room 141

Teachers: P. Macchi, A. Volkov Teachers: P. Mallinson, T. Koritsanszky

usage of XDFOUR
computing residuals maps with XDFOUR
computing experimental deformation density maps

usage of XDFFT
Fast Fourier peak search and graphical visualization of peaks
+ short presentation by L. Farrugia

usage of XDGRAPH
graphical visualization of maps (XDGRAPH)

usage of XDGEOM
computing geometries (XDGEOM)
producing cif files

usage of XDWTAN
analysis of refinement
+ short presentation by L. Farrugia

Afternoon: Tour of Niagara Falls

At 14:00 a bus will meet participants at MOTEL6. Operated by the Niagara Majestic Tours.
15th May, Thursday

**TOPIC:**
Properties from the electron density

**Morning Session 9.00-12.00**

Main lecture:
9.00-10.00
*Electron density from multipolar model and the derived properties; the electrostatic potential*

P. Macchi

coffee break at NSC room 216

Short lectures:
10.15-12.00
*Theoretical vibrational mode constraint (module XDVIB)*

T. Koritsanszky

*Static deformation densities and their analysis*

P. Macchi

*Atomic and molecular partitioning*

A. Volkov

**Afternoon Session 14.00-18.00**

**Tutorial 14.00-17.00**
*(tea/coffee will be served 15.00-16.00 in NSC room 216)*

**Group 1 (beginners)**

Location: Hochstetter Hall room 139

Teachers: P. Mallinson, T. Koritsanszky, L. Farrugia, P. Macchi

*usage of XDPROP:*
- computing static deformation densities
- reconstructing the total electron density and Laplacian
- reconstructing partial densities (core/valence etc.)
- computing multipole moments (from atomic moments and from Stockholder partitioning)
- extracting d-orbital populations
- computing the electrostatic potential

*usage of XDGRAPH*
- graphical visualization of maps (XDGRAPH)

**Group 2 (advanced)**

Location: Hochstetter Hall room 141

Teachers: C. Gatti, A. Volkov

*use of TOPXD*
- searching critical points of the electron density
- integration of the density in the atomic basins (TOPXD)
- producing and visualizing maps
- worked examples also for advanced users

**Poster Session P20X, 17.00 -18.00, NSC room 218**

*poster presentations (10 minutes each), charge density results and interpretation*
16th May, Friday

**TOPIC:**
Topological Analysis of the charge density

**Morning Session 9.00-12.00**

**Location:** Natural Sciences Complex room 218

- **Main lecture:**
  9.00-10.00  
  The topology of charge density in crystals  
  C. Gatti

- **coffee break at NSC room 216**

- **Short lectures:**
  10.15-12.00  
  TOPXD: Merging TOPOND and XD  
  A. Volkov
  
  Search of critical points of the density  
  C. Gatti
  
  Algorithms for integration, optimization of the performances  
  A. Volkov
  
  Interpretation of results  
  C. Gatti

**Afternoon Session 14.00-18.00**

**Tutorial 14.00-17.00**

(Tea/coffee will be served 15.00-16.00 in NSC room 216)

- **Group 1 (beginners)**
  - **Location:** Hochstetter Hall room 139
  - Teachers: C. Gatti, A. Volkov

  - **use of TOPXD**
    - searching critical points of the electron density
    - integration of the density in the atomic basins (TOPXD)
    - producing and visualizing maps

  - **topological analysis with XDPROP**
    - analysis of properties along bond paths
    - visualization of results

- **Group 2 (advanced)**
  - **Location:** Hochstetter Hall room 141
  - Teachers: P. Mallinson, T. Koritsanszky, P. Macchi, L. Farrugia

  - **new features of XDPROP**
    - computing multipole moments (from atomic moments and from Stockholder partitioning)
    - extracting d-orbital populations
    - mathematics on the grid files (+ short presentation)
    - application to user’s data

**Poster Session P30X, 17.00-18.00, NSC room 218**

- poster presentations (10 minutes each), charge density results and other techniques
17th May, Saturday

Morning session 9.00-12.00  
Chair: Prof. A. Pinkerton

<table>
<thead>
<tr>
<th>Time</th>
<th>Session</th>
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<tbody>
<tr>
<td>9.00-10.00</td>
<td>Main lecture: <em>Statistical analyses and analyses of geometrical and thermal parameters</em> L. Farrugia</td>
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<tr>
<td>10.15-10.30</td>
<td>Technical discussion: <em>Choice of a default compiler for the XD package</em> A. Volkov</td>
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<td>10.30-11.15</td>
<td>Open presentation: <em>New results obtained at the meeting</em></td>
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<td>11.15-12.00</td>
<td>Open discussion: <em>Comments from the participants</em> Bug reports General questions</td>
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<td>12.00-12.30</td>
<td>Closing remarks: P. Coppens</td>
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Location: Natural Sciences Complex room 218