

|       | Jun-03<br>Fri | Jun-04<br>Sat   | Jun-05<br>Sun  | Jun-06<br>Mon  | Jun-07<br>Tue  | Jun-08<br>Wed  | Jun-09<br>Thu  | Jun-10<br>Fri   | Jun-11<br>Sat |  |
|-------|---------------|---|--|--|--|--|--|---|---------------|--|
| 08:30 |               | INTRODUCTION  |  |  |  |  |  |   | DEPARTURES    |  |
| 09:00 |               | Helen Maynard-Casely<br>Introduction to HP crystallography  | Diffpy-CMI (1)<br>YELL (1)<br>Recipocalspaceship (1)                                 | Diffpy-CMI (2)<br>YELL (2)<br>MD simulations part 1 (1)              | GUDRUN (1)<br>PDFGETX (1)<br>MDX-LIB (1)                       | RMCProfile (1)<br>DEBUSSY (1)<br>MD simulations part 1 (2)                         | RMCProfile (2)<br>DISCUS (1)<br>MD simulations part 2 (1)                        | DISCUS (2)<br>DEBUSSY (1)<br>MD simulations part 2 (2)    |               |  |
| 09:45 |               | Dave Keen<br>Historical context of diffuse scattering   | Diffpy-CMI (1)<br>YELL (1)<br>Recipocalspaceship (1)                                 | Diffpy-CMI (2)<br>YELL (2)<br>MD simulations part 1 (1)              | GUDRUN (1)<br>PDFGETX (1)<br>MDX-LIB (1)                       | RMCProfile (1)<br>DEBUSSY (1)<br>MD simulations part 1 (2)                         | RMCProfile (2)<br>DISCUS (1)<br>MD simulations part 2 (1)                        | DISCUS (2)<br>DEBUSSY (1)<br>MD simulations part 2 (2)    |               |  |
| 10:30 |               | COFFEE  | COFFEE   | COFFEE   | COFFEE   | COFFEE   | COFFEE   | COFFEE  |               |  |
| 11:00 |               | H Ginn<br>X-ray diffraction theory  | Diffpy-CMI (1)<br>YELL (1)   | Diffpy-CMI (2)<br>YELL (2)<br>Image simulators (1)                   | Matt Tucker<br>Diffuse scattering<br>in high pressure research | RMCProfile (1)<br>DEBUSSY (1)<br>MDX-LIB (2)                                       | RMCProfile (2)<br>DISCUS (1)<br>SPINVERT part 1 (1)                              | DISCUS (2)<br>SPINVERT part 2 (1)<br>DEBUSSY (1)          |               |  |
| 11:45 |               | Simon Billinge<br>The pair distribution function  | Diffpy-CMI (1)<br>YELL (1)   | Diffpy-CMI (2)<br>YELL (2)<br>Image simulators (1)                   |  | RMCProfile (1)<br>DEBUSSY (1)<br>MDX-LIB (2)                                       | RMCProfile (2)<br>DISCUS (1)<br>SPINVERT part 1 (1)                              | DISCUS (2)<br>SPINVERT part 2 (1)<br>DEBUSSY (1)          |               |  |
| 12:30 |               | LUNCH   | LUNCH  | LUNCH  |  | LUNCH  | LUNCH  | LUNCH   | LUNCH         |  |
| 14:30 |               | A Peck<br>Models of protein<br>diffuse scattering   | Nick Sauter (ZOOM)<br>Interpreting macromolecular<br>diffraction                     | Dectris<br>Detectors   | EXCURSION  | D Wych<br>Analysis of MD<br>simulations of protein crystals                        | Alexei Bosak<br>Tandem use of diffuse and<br>inelastic x-ray scattering          | Nozomi Ando<br>Protein correlated motion                  |               |  |
| 15:15 |               | Anotnella Guagliardi<br>X-ray scattering in nanomaterials and<br>Debye Scattering Equation method         | Joe Paddison<br>Magnetic diffuse<br>scattering                                       | S Meisburger<br>Lattice dynamics in<br>biological diffuse scattering |  | Karena Chapman<br>in situ and operando<br>total scattering studies                 | K Ayer<br>Biological diffuse scattering<br>at XFELs                              | A Goodwin<br>Diffuse scattering in<br>materials chemistry |               |  |
| 16:00 |               | COFFEE  | COFFEE   | COFFEE   |  | COFFEE   | COFFEE   | COFFEE  | COFFEE        |  |
| 16:30 |               | Arkadiy Simonov<br>What data can tell you: 3D-APDF method<br>to solve the crystal diffuse scattering data | M Wall (ZOOM?)<br>Molecular dynamics simulations<br>of biological diffuse scattering | Dave Keen<br>Data correction   |  | Kirsten Jensen<br>Pair Distribution Function analysis<br>of nanomaterial structure | D Hekstra<br>Time-resolved macromolecular<br>crystallography                     | Outlook<br>and conclusions                                |               |  |
| 17:15 |               | Hans-Beat Bürgi<br>Workflow for interpreting disorder<br>diffraction - NaLaF4 as an example               | Ray Osborn<br>Real Space Maps of Structural<br>Correlations in Quantum Materials     | Matt Tucker<br>reverse Monte Carlo methods                           |  | Reinhard Neder<br>Science with DISCUS  | Silvia Capelli<br>Single-crystals, Laue and time-of-flight<br>the SXD experience |   |               |  |
| 18:00 |               | INTRO TO ERICE  | POSTER SESSION<br>ODD NUMBERS  |  |  | POSTER SESSION<br>EVEN NUMBERS   |  |   |               |  |
| 20:00 | ARRIVALS      | WELCOME BUFFET  | DINNER AT POSTERS  |  | DINNER AT POSTERS  |  | FAREWELL DINNER  |   |               |  |