

### Workshop topics:

The general topic of the 4<sup>th</sup> TOPAS User's meeting will be on the development and application of MACROS using the unique algebraic language of TOPAS/TOPAS academic in Launch mode. A key topic is 'advanced microstructural analysis', where WPPM in theory and practice are taught within and beyond the MACRO language of TOPAS.

Following this workshop, proceedings are planned in form of a "macro tutorial" for Topas.

### List of speakers/instructors and topics:

- **Bill David, Rutherford Appleton Laboratory, Didcot (confirmed)**
  - TOPAS computer algebra applied to optimised molecular conformation, vibrational analysis and disorder,
  - "beyond least-squares" refinement,
  - generalised sample-dependent broadening and particle size analysis.
- **Robert Dinnebier, Max Planck Institute for Solid State Research, Stuttgart (confirmed)**
  - Kinetic data from sequential and parametric refinements
  - Data presentation and interface to external programs

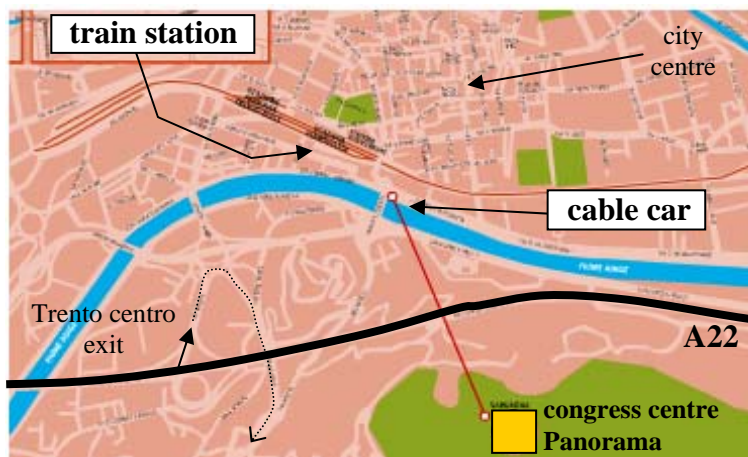
- **John Evans, University of Durham (confirmed)**
  - Parametric refinements
  - Surface refinements
  - Symmetry-motivated distortion-mode amplitudes (ISODISPLACE) Rietveld Refinement
- **Bernd Hinrichsen, Bruker AXS, Karlsruhe (confirmed)**
  - Charge flipping with Topas: fundamentals and applications
- **Arnt Kern, Bruker AXS, Karlsruhe (confirmed)**
  - Introduction and syntax of the TOPAS macro language
  - Profile analysis
  - 3<sup>rd</sup> SDPD round robin results (SA und Charge Flipping)
- **Andreas Leineweber, Max Planck Institute for Metal Research, Stuttgart (confirmed)**
  - Physical interpretation of anisotropic line broadening
  - User defined convolutions - exotic peak shape function
- **Ian Madsen, CSIRO, Melbourne (to be confirmed)**
  - Full quantitative phase analysis with TOPAS in theory and practice
  - Description and assessment of a number methods for the QPA of amorphous material
  - Issues in precision and accuracy
- **Pamela Whitfield, National Research Council, Ottawa (confirmed)**
  - Global optimization methods
  - Preferred orientation and other physical effects
  - Restraints and penalty functions
  - Rigid bodies
- **Peter Stephens, SUNY at Stony Brook (confirmed)**
  - Robust refinement with impurity phases using Topas
  - Refinement of molecular geometry using the Z-matrix formulation in Topas
  - Phenomenological description of line profiles
- **Paolo Scardi, University of Trento (confirmed)**
  - Some theoretical and practical issues in line profile analysis
  - From pattern *fitting* to pattern *modelling*: an introduction to WPPM
- **Matteo Leoni, University of Trento (confirmed)**
  - WPPM in practice. Software and applications

## Location:

Centro Congressi Panorama:  
Strada alla Funivia n. 66  
38040 Sardagna (Trento)  
Tel: 0461.261671  
Fax: 0461.261686  
Email: panorama@operauni.tn.it

Congress centre Panorama is a yellow building on a rocky spur directly above Trento. It is connected to the city by a cable-car service operated every 15 minutes from 7.00 am to 10.30 pm, within the local transportation network (need a bus ticket). The cable-car station is near a bridge on Adige river, not far from the train station and city centre. If you travel by car, from the Trento Centro of Autostrada A22, follow indications to Monte Bondone / Sardagna (7 km)

Web site (in Italian !!): <http://www.operauni.tn.it/cms-01.00/articolo.asp?IDcms=79&s=29&l=>



## Registration fee:

220 Euro RegularCost:  
110 Euro Student

Registration fee includes coffee break, lunch and reception. Accommodation is not included, reservations are to be made directly with the conference center (see below). Limited funds for students willing to present their work (poster or short talk) are available upon request

## Accommodation

The Centro Congressi Panorama offers sleeping rooms (breakfast included):

16 single bed (33 euro),  
2 twin-bed (55 euro),  
4 kingsize bed (55 euro).

Twin and Kingsize used as single: 40 Euro.

Alternative inexpensive accommodation downtown (on the order of 40 Euro per night, breakfast included):

Hotel Venezia

Piazza Duomo, 45 - Via Belenzani, 70 - 38100 Trento, Italia

Tel/Fax: +39/0461 234114 +39/0461 234559

E-mail: [info@hotelveneziatn.it](mailto:info@hotelveneziatn.it)

[www.hotelveneziatn.it](http://www.hotelveneziatn.it)

Hotel Aquila d'Oro  
Via Belenzani, 76 - 38100 Trento  
Tel 0461 986282  
info@aquiladoro.it  
<http://www.aquiladoro.it/>

New International Youth Hostel, Giovane Europa Trento  
Via Torre Vanga, 9 - 38100 TRENTO, Italia  
Tel 0461 263484  
Fax 0461 222517  
[info@gayaproject.org](mailto:info@gayaproject.org)  
<http://www.viamundis.com/en/new-international-youth-hostel-giovane-europa.html>

### **Time**

Thursday , June 18, 13:00 – 18:00  
Friday, June 19, 9:00 – 18:00  
Saturday June 20, 9:00 - 18:00

### **Hand's on sessions**

The workshop is divided in theoretical sessions (approx. 1 hr) and practical tutorials (approx. 2 hrs). Contemporary laptop (Windows XP) with working USB ports and administrator rights (or pre-installed Topas Version 4.1) is required.

### **Requirements**

Basic knowledge in crystallography and physics. Some practical experience with the TOPAS program.

### **Sponsors**



**Bruker AXS GmbH, Karlsruhe**

## Registration

**The number of participants is limited to 40.** Early booking is advised.

Please mail or fax the completed registration form to:

Prof. Paolo Scardi  
Department of Materials Engineering and Industrial Technologies,  
University of Trento  
38100 via Mesiano 77 (TN) - Italy  
Tel: +39 0461 882417 / 882467 / 881915 881919 (switchboard)  
Fax: +39 0461 881977 (881999)  
E-mail: [Paolo.Scardi@unitn.it](mailto:Paolo.Scardi@unitn.it)  
WWW: <http://www.ing.unitn.it>

**4<sup>th</sup> TOPAS Users Meeting**  
**University of Trento, June 18-20, 2009**  
**Organizers: Paolo Scardi, Robert Dinnebier & Arnt Kern**

**REGISTRATION FORM**

**Name** .....

**Affiliation** .....

**Address** .....

**E-mail:** .....

**Tel.** .....

**Student** ..... (y/n - if yes, please provide a certification of the student status)

**Registration fee:**     **220,00 €(Regular Cost), 110,00 € (Student)**

**To be paid NO LATER THAN MAY 15 by:**

<p><b>Bank transfer to: University of Trento</b> <b>Bank: Banca di Trento e Bolzano - Via Mantova 19 - Trento</b> <b>IBAN: IT92 H 03240 01801 0000 10000496</b> <b>Swift code: BAT BIT 2TB 01</b> <b>Reason for payment: 4th TOPAS Users' meeting + Your Name</b></p>
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**INVOICE**

**Please provide data for the invoice: even if you don't need it, this is formally required to complete the registration process. Data can be different from your data, i.e., you can bill to your company, department, etc. . Payment is not refundable.**

**Name** .....

**Address** .....

**Tax Number and/or VAT number** .....