



bilbao crystallographic server



Utilisation des outils du Bilbao Crystallographic Server :
application aux transitions de phase

Programme prévisionnel

[Mardi 01/10] - [Mercredi 02/10] - [Jeudi 03/10] - [Vendredi 04/10]

Lundi 30 septembre

- 19h00 Arrivée
20h00 - Dîner

Mardi 1er octobre

- 8h15 - 8h45 Introduction
- 8h30 - 10h30 **Revision 1. Matrix calculus applied to crystallography** [Mois Iliá Aroyo (Bilbao)]
- Isometries and crystallographic symmetry operations
 - Crystallographic point- and space-group symmetry operations. Matrix-column presentation of symmetry operations
 - Symmetry elements: geometric elements and element sets
- 10h30 - 11h00 *Pause café*
- 11h00 - 13h00 **Revision 2. Space-group symmetry** [Mois Iliá Aroyo (Bilbao)]
- Space groups and their descriptions in International Tables for Crystallography, Vol. A and in the Bilbao Crystallographic Server (BCS)
 - Transformations of the coordinate systems: change of origin and orientation. Conventional and non-conventional descriptions of space groups; ITA-settings
 - BCS computer databases and access tools to crystallographic symmetry data for space groups (GENPOS, WYCKPOS, IDENTIFY GROUP)
- 13h00 - 14h30 *Pause déjeuner*
- 14h30 - 16h30 **Crystal-structure tools of the Bilbao Crystallographic Server** [Mois Iliá Aroyo (Bilbao)]
- Crystal-structure descriptions. Descriptions of crystal structures with respect to different ITA settings of the space groups (the program SETSTRU)
 - Equivalent crystal structure descriptions (the programs EQUIVSTRU). Crystal-structure descriptions compatible with symmetry reduction (the program TRANSTRU). Comparison btw different structure descriptions (the program COMPSTRU)
 - BCS: Hands-on session with the computer tools for crystal-structure descriptions
- 16h30 - 17h00 *Pause café*
- 17h00 - 19h00 **Landau theory of phase transitions** [Philippe Rabiller (Rennes)]
- 19h30 - 20h00 *Cocktail de bienvenue*
20h00 - *Dîner*

Mercredi 2 octobre

- 8h00 - 10h00 **Group-subgroup relations** [Mois Ilia Aroyo (Bilbao)]
- Group-subgroup relations between space groups. Domain-structure analysis in structural phase transitions.
 - BCS: Hands-on session with the computer databases and computer tools in the study of group-subgroup relations of space groups (SUBGROUPGRAPH, HERMANN, WYCK-SPLIT, MINSUP, SUPERGROUPS)
- 10h00 - 10h30 *Pause*
- 10h30 - 13h00 **Crystal-structure relationships** [Juan Manuel Perez-Mato (Bilbao)]
- Structural pseudosymmetry. Pseudosymmetry search for new ferroics. Application in structural phase transitions. (PSEUDO)
 - Crystal-structure relationships. Family trees (Baernighausen trees) of crystal structures: arystotype (basic) and hettotypes (derivative structures) (STRUCTURE RELATIONS, SUBGROUPS (1st part))
- 13h00 - 14h30 *Pause déjeuner*
- 14h30 - 15h30 **Revision 3: Representations of crystallographic groups (part 1)** [Mois Ilia Aroyo (Bilbao)]
- Review of basic definitions. Simple examples of point-group representations
 - Identity representation: Symmetry adapted crystal tensors (the program TENSOR)
- 15h30 - 15h45 **Sponsor presentation** [Bruker AXS]
- 20h00 - *Dîner*

Jeudi 3 octobre

- 8h30 - 9h30 **Revision 3: Representations of crystallographic groups (part 2)** [Mois Ilia Aroyo (Bilbao)]
- Review of basic definitions. Simple examples of point-group representations
 - Identity representation: Symmetry adapted crystal tensors (the program TENSOR)
- 9h30 - 10h30 **Representations of space groups (part 1)** [Mois Ilia Aroyo (Bilbao)]
- Representation of the translation group. Symmetry in reciprocal space: Brillouin zones and wave-vector symmetry types. Star of a representation. Little groups and small representations. Full-group representations of space groups
 - Representations of symmorphic and non-symmorphic groups. Subduced and direct-product representations of space groups
 - Hands-on session with the computer tools of representations of crystallographic groups of the Bilbao Crystallographic Server (KVEC, Representations SG, REPRES)
- 10h30 - 11h00 *Pause café*
- 11h00 - 12h00 **Representations of space groups (part 2)** [Mois Ilia Aroyo (Bilbao)]
- Representation of the translation group. Symmetry in reciprocal space: Brillouin zones and wave-vector symmetry types. Star of a representation. Little groups and small representations. Full-group representations of space groups
 - Representations of symmorphic and non-symmorphic groups. Subduced and direct-product representations of space groups
 - Hands-on session with the computer tools of representations of crystallographic groups of the Bilbao Crystallographic Server (KVEC, Representations SG, REPRES)
- 12h00 - 13h00 **Symmetry analysis of phase transitions (part 1)** [Juan Manuel Perez-Mato (Bilbao)]
- Representation theory tools in the analysis of phase transitions. Primary and secondary order parameters, couplings and hierarchy of modes
 - Order parameter direction and isotropy subgroups. Ferroelectric and ferroelastic phase transitions. Sequence of phase transitions (MECHANICAL REP, Get_irreps, SUBGROUPS (2nd part))
- 13h00 - 14h30 *Pause déjeuner*
- 14h30 - 15h30 **Symmetry analysis of phase transitions (part 2)** [Juan Manuel Perez-Mato (Bilbao)]
- Representation theory tools in the analysis of phase transitions. Primary and secondary order parameters, couplings and hierarchy of modes
 - Order parameter direction and isotropy subgroups. Ferroelectric and ferroelastic phase transitions. Sequence of phase transitions (MECHANICAL REP, Get_irreps, SUBGROUPS (2nd part))
- 15h30 - 16h30 **Symmetry-mode description of distorted structures (part 1)** [Juan Manuel Perez-Mato (Bilbao)]
- Symmetry-mode description of distorted structures
 - Hands-on session with the computer tools of symmetry analysis of structural phase transitions of the Bilbao Crystallographic server (AMPLIMODES)
- 16h30 - 17h00 *Pause café*

- 17h00 - 18h00 **Symmetry-mode description of distorted structures (part 2)** [Juan Manuel Perez-Mato (Bilbao)]
- Symmetry-mode description of distorted structures
 - Hands-on session with the computer tools of symmetry analysis of structural phase transitions of the Bilbao Crystallographic server (AMPLIMODES)
- 18h00 - 18h45 **Symmetry-mode description of distorted structures (part 3)** [Juan Manuel Perez-Mato (Bilbao)]
- Visualization of distortion modes with VESTA and/or Jmol
- 18h45 - 19h00 **Sponsor presentation [Rigaku]**
- 20h00 - 21h30 *Dîner de gala*

Vendredi 4 octobre

- 8h00 - 9h00 Symmetry-mode description of distorted structures (part 4) [Pierre-Emmanuel Petit (Nantes)]
- Structure refinement using symmetry modes: Combined use of AMPLIMODES and FullProf
- 9h00 - 10h00 Final session with BCS program and tools (part 1) [Juan Manuel Perez-Mato and Mois Ilia Aroyo (Bilbao)]
- Final additional hands-on session with BCS programs and tools (programs to be decided depending on the interest of the participants)
- 10h00 - 10h30 *Pause*
- 10h30 - 11h30 Final session with BCS program and tools (part 1) [Juan Manuel Perez-Mato and Mois Ilia Aroyo (Bilbao)]
- Final additional hands-on session with BCS programs and tools (programs to be decided depending on the interest of the participants)
- 11h30 -
11h45 - *Récupération des paniers-repas*
Départ de la navette pour la gare de La Rochelle