bilbao crystallographic server

cnrs

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 Ilia 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 Ilia 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 Ilia 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)]

- Crystal-structure relationships. Family trees (Baernighausen trees) of crystal structures: arystotype (basic) and hettotypes (derivative structures) (STRUCTURE RELATIONS, SUBGROUPS (1st part))
- Structural pseudosymmetry. Pseudosymmetry search for new ferroics. Application in structural phase transitions. (PSEUDO)

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 presenation [Bruker AXS]

20h00 -   *Dîner de gala*

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
- Structure refinement using symmetry modes: Combined use of AMPLIMODES and refinement programs (FullProf, JANA)

18h45 - 19h00   Sponsor presenation [Rigaku]

20h00 - 21h30   *Dîner*

Vendredi 4 octobre

8h00 - 9h00 **Symmetry-mode description of distorted structures (part 4)** [Pierre-Emmanuel Petit, Olivier Hernandez (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 - *Récupération des paniers-repas*
11h45 - *Départ de la navette pour la gare de La Rochelle*