

Crystallography Online: Workshop on the use and applications of the structural tools of the Bilbao Crystallographic Server

20 Aug - 21 Aug 2018, Oviedo

20 August

8:30 - 10:30 Space-group symmetry

- 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

10:30 - 11:00 Coffee break

11:00 - 13:00 Group-subgroup relations

- 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

13:00 - 14:30 Lunch break

14:30 - 16:00 Crystal-structure tools of the Bilbao Crystallographic Server

- 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 between different structure descriptions (the program COMPSTRU)
- BCS: Hands-on session with the computer tools for crystal-structure description

16:00 - 16:30 Crystal-structure relationships

- Crystal-structure relationships. Family trees (Baernighausen trees) of crystal structures: arystotype (basic) and hettotypes (derivative structures).
- Structural pseudosymmetry. Pseudosymmetry search for new ferroics. Application in structural phase transitions.
- BCS: Hands-on session with the programs STRUCTURE RELATIONS and PSEUDO

16:30 - 17:00 Coffee break

17:00 - 18:30 Crystal-structure relationships (cont.)

18:30 - 19:30 Representations of crystallographic groups

- Review of basic definitions. Simple examples of point-group representations

21 August

8:30 - 10:30 Representations of space groups

- 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.

10:30 - 11:00 Coffee break

11:00 - 12:00 Symmetry analysis of phase transitions

- Representation theory tools in the analysis of phase transitions. Primary and secondary order parameters; couplings and faintness index. Order parameter direction and isotropy subgroups.

12:00 - 13:00 Symmetry-mode analysis of structural phase transitions

- Symmetry-mode description of distorted structures. Primary and secondary modes. Hierarchy of modes. Ferroelectric and ferroelastic phase transitions. Sequence of phase transitions.

13:00 – 14:30 Lunch break

14:30 - 16:30 Symmetry-mode analysis of structural phase transitions (cont.)

- Hands-on session with the computer tools of symmetry analysis of structural phase transitions of the Bilbao Crystallographic server (SUBGROUPS, AMPLIMODES).
- Visualization of distortion modes with VESTA and/or Jmol.
- Structure refinement using symmetry modes: Combined use of AMPLIMODES and refinement programs (FullProf, JANA).

16:30 – 17:00 Coffee break

17:00 - 19:30 Symmetry-mode analysis of structural phase transitions (cont.)