Advanced Crystallography: theory and experiments (20 h)

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The course illustrates selected topics related to crystallography, crystallochemistry and crystallophysics. On the basis of the students' interests, the final program will be defined by selecting the desired items among those proposed below:

1. Geometry of the crystals
   i. Crystallographic axes
   ii. Miller indexes
   i. Zone axis equation
2. Point group symmetry
   ii. Symmetry elements, symmetry operations and symmetry operators
   iii. Point groups
   iv. Symmetry in 2 dimensions
   v. 3-dimensional Point groups
3. Fundamental concepts of crystallography (symmetry elements: identity, rotation, inversion, reflection, roto- reflection; Schoenflies and Hermann-Maugin notations; crystal lattice; unit cell; crystal systems; Bravais lattices)
4. Group Theory: an introduction
5. Point and Space Groups
6. International Tables of Crystallography (symmetry operations, generators, positions, multiplicity, Wyckoff notation, site symmetry, reflections conditions, sub-groups and super-groups)
7. The reciprocal lattice; TEM and electron diffraction
8. Powder diffraction (X-ray and neutron radiation)
9. Structural refinement: the Rietveld method
10. Diffraction line profile analysis: structural strain, coherent diffraction domains size and chemical homogeneity.
11. Distorsive structural transition; symmetry relationships; soft modes; spontaneous strain
12. Symmetry Relationships among crystal structures
13. The anti-symmetry operation; black-white space groups; representational analysis; magnetic moments ordering (magnetic scattering)
14. Molecular Geometry and Crystallochemistry: VSEPR theory; ionic radii; the coordination polyhedron; BVS theory; Pauling's rules
15. Crystallophysics: tensors and physical properties of crystals; Neumann's principle