

Lecture course on “Topology and Group Theory “

August 23-26, 2018, Donostia - San Sebastian

The aim of the course is to provide the group-theoretical background necessary for the understanding and application of symmetry methods and techniques in topological-matter problems. The lectures will be complemented by exercises to help the participants to get some practical knowledge in crystallographic groups and their representations. Through numerous examples and hands-on sessions the participants will gain experience in the use of the online tools of the Bilbao Crystallographic Server (BCS) to solve specific problems related to topological properties of solids.

Time table: morning sessions: 8:30 – 10:30, 11:00 – 13:00
afternoon sessions: 14:30 – 16:30, 17:00 – 19:00
coffee breaks: 10:30 - 11:00. 16:30 - 17:00
lunch break: 13:00 - 14:30

Remarks:

Please note that the depth of treatment of the listed topics and the time for their presentation will depend strongly on participants' knowledge of crystallographic groups and their representations.

For the practical hands-on sessions a laptop is required.

Part 1. Group theory, representations and their applications in solid state (10 hours)

Thursday, 23rd: the whole day

Friday, Aug 24th: 8:30 - 10:30

Lecturer Juan Luis Mañes Palacios

1. Symmetries, degeneracies and representations.
2. Irreducible representations as building blocks. Application to molecular vibrations.
3. Operations with representations: Physical properties and spectra.
4. Spin and double valued representations. Splitting of atomic orbitals in crystals.
5. Representation theory and electronic bands.

Part 2. Crystallographic groups and their representations: Online tools of the Bilbao Crystallographic Server (10 hours)

Friday, Aug 24th: 11:00-13:00; afternoon session

Saturday, Aug 25th: morning session

Lecturer Mois I. Aroyo

1. Overview of crystallographic point groups. Wyckoff positions. Double point groups. Point-group symmetry tools of BCS.
2. Symmetry operations and their descriptions. Space groups and their structure. General and special Wyckoff positions, site-symmetry groups, crystallographic orbits. Double space groups. Online tools of BCS for space-group symmetry data.
3. Representations of crystallographic groups. Subduced and induced representations. Direct product representations.

Representations of a group in terms of the representations of an invariant subgroup. Time-reversal symmetry.

4. Representations of space groups. Symmetry in reciprocal space: Brillouin zones and wave-vector symmetry types: wave-vector star and little groups. Irreducible representations of space groups and their construction. Double space groups and their representations. Brillouin-zone database of BCS. Basic computer tools for single- and double-valued space-group representations.
5. Subduced and direct-product representations of space groups. Compatibility relations and electronic energy bands. Site-symmetry approach and band representations.

Part 3. Topological quantum chemistry: symmetry approach

Saturday, Aug 25th (afternoon session)

Sunday, Aug 26th (the whole day)

**Lecturers: Barry Bradlyn
Jennifer Cano**

1. Connectivity of bands and band representations; graph connectivity
2. Wannier functions: symmetry, polarization, connection to band representations
3. Chemical bonding, hybridization, non-equivalent atomic limits
4. Topological insulators: overview
5. Topological quantum chemistry
6. Algorithms for finding topological materials and using the BCS