

The Shanghai International Crystallographic School- Workshop on Chirality in Solid-State Physics and Quantum Materials

was successfully conducted from June 15th (Saturday) to 21st (Friday) 2024, in Rooms 413 and 201 of Building D and J, Baoshan Campus, Shanghai University. With the theme of "*Computational Crystallography and Chiral Quantum Materials Physics*," this workshop attracted renowned experts, scholars, researchers, and young students from different fields of crystallography, chemistry, physics, and quantum materials science around the world to jointly discuss and exchange theoretical knowledge, cutting-edge technologies in crystallography, and the latest research achievements in quantum materials. The workshop was hosted by the Materials Genome Institute and International Centre for Quantum & Molecular Structures of Shanghai University, aiming to establish an international academic exchange platform for crystallography and promote academic innovation and technological progress in the field of computational crystallography.



The purpose of the school was to introduce the group theoretical methods and computational tools necessary for developing and applying symmetry principles productively in solid-state materials science. Special emphasis was placed on in-depth training and learning on the use of the Bilbao Crystallographic Server (BCS) (www.cryst.ehu.es) for computational crystallography in the study of solid-state physics problems, such as phase transitions and their symmetry-mode analysis, comparisons between crystal structures, magnetic symmetry, and the description of magnetic structures. The workshop closely integrated with the new frontiers of quantum materials science research, discussing topics such as chirality in solid physics, continuous symmetry measures, chirality in magnetism, chiral phonons, and chirality and relativity. The scientific program was mainly designed by Alessandro Stroppa in collaboration with Wei Ren and Mois Aroyo, with feedback from each of the lecturers. The event continues the series of schools started in 2017, promoted by Alessandro Stroppa, to boost and favor

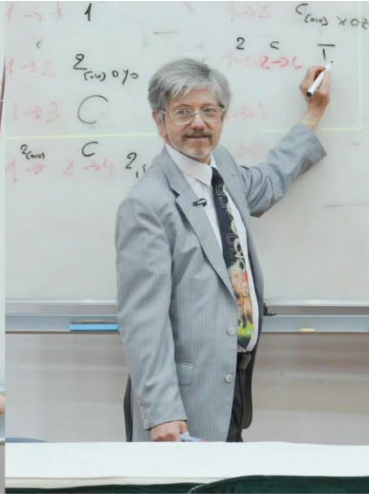
international scientific collaborations between China and Europe and western countries in general.



At the opening ceremony, Nie Qing, Vice President of Shanghai University, delivered a welcome speech on behalf of the University. She introduced the advantages and achievements of organizing academic schools and other international exchanges with Shanghai University, emphasized the remarkable achievements made by the university in the field of crystallography, and expressed hope that international experts might build a bridge of friendship, strengthen long-term cooperation with all parties of Shanghai University, and contribute more to the development of the field of crystallographic and structural science.



The host, Wei Ren, Executive Deputy Dean of the Materials Genome Institute of Shanghai University, introduced the guests attending the symposium, including Prof. Mois Aroyo from the University of Basque Country (Spain), Dr. Alessandro Stroppa from the CNR-SPIN (Italy), Prof. Massimo Nespolo from the University of Lorraine (France), Prof. J. Manuel Perez-Mato from the University of Basque Country (Spain), Distinguished Professor Sang-Wook Cheong (Editor-in-Chief of npj Quantum Materials) from Rutgers University (United States), Prof. Gustavo Aucar from the Northeast University of Argentina (Argentina), Prof. Zhang Lifa from Nanjing Normal University (China), Dr. Matteo Cavalleri from the American Physical Society Publishers (United States), Dr. Juan Rodriguez-Carvajal from the Laboratoire Léon Brillouin (France), as well as Prof. David Avnir from the Hebrew University of Jerusalem (Israel) and Prof. Branton Campbell from Brigham Young University (United States) who both participated online. There were also participants from different universities and research institutions around the world, including the University of L'Aquila in Italy, Rutgers University in the United States, the University of Warwick in the United Kingdom, the University of Cagliari in Italy, M.V. Lomonosov Moscow State University in Russia, the University of Vienna in Austria, the Institute of Physics and the Institute of Semiconductors of the Chinese Academy of Sciences, the Hong Kong University of Science and Technology, the Guangdong Provincial Academy of Sciences, the Southern University of Science and Technology, the University of Science and Technology of China, Beijing Institute of Technology, East China University of Science and Technology, Hangzhou Dianzi University, Fudan University, Southeast University, Nanjing University, and Jilin University.





It was a very intense week of training and lively discussions among the students and the lecturers, but also among the lecturers themselves on the exciting frontiers in materials research. This was clearly a sign of the high and interdisciplinary interests towards the topics discussed in the school. Lectures were given from 08:30 am to 13:00 (morning session) and from 14:30 to 19:00 (evening session). A post-dinner session from 20:00 to 22:00 was actively used for more discussions about the topic of the day.





The initial two days of school (pre-school days) were devoted to align the students' background to a common basic knowledge of group theory and crystallographic science. A social dinner for the organizers and speakers was held in Shanghai city near the Bund. During the dinner, new trends in materials topics and future event organization were discussed.

At the closing ceremony, the organizers presented Shanghai University souvenirs to the diligent presenters, awarded outstanding posters and participation certificates to outstanding trainees, and distributed international crystallographic textbooks as rewards. The organization of this Shanghai International Crystallographic School not only provided a platform for academic exchanges for global crystallographers, but also injected new vitality into crystallography research and industrial development.



This workshop attracted a large number of doctoral students and young researchers interested in in-depth and practical knowledge of group theory and crystallography applications. The maximum participation limit was set at 70 on-site, while the total number of viewers on the online live broadcast platforms Koushare Video, Bilibili, and Koushare Platform reached 44624, clearly suggested the high interest towards the topic of the school.



Conference website: <https://conferences.koushare.com/shu>

Scientific program

Shanghai International Crystallographic School

Workshop on chirality in solid state physics and quantum materials

International Centre for Quantum and Molecular
Structures

Shanghai University, Shanghai, China,

15-21 June 2024

Organizers:

Wei Ren (Shanghai University - 266 Jufengyuan Rd, Baoshan, Shanghai, Cina, 200444)

Alessandro Stroppa (CNR-SPIN, Via Vetoio, 67100, L'Aquila, Italy)

Mois I. Aroyo (Department of Physics, University of the Basque Country, UPV/EHU, Apto. 644, 48080 Bilbao, Spain)

SCIENTIFIC PROGRAM

Lecturers:

Mois I. Aroyo (MIA) (Department of Physics, University of the Basque Country, UPV/EHU, Apto. 644, 48080 Bilbao, Spain)

J. Manuel Perez-Mato (JMPM) (Department of Physics, University of the Basque Country, UPV/EHU, Apto. 644, 48080 Bilbao, Spain)

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David Avnir (DA) (Institute of Chemistry, The Hebrew University of Jerusalem, Jerusalem, Israel 9190401)

Branton J. Campbell (BJC) (Department of Physics & Astronomy, Brigham Young University, Provo, UT 84602, USA).

Lifa Zhang (LZ) (Nanjing Normal University, Nanjing, 210023, China)

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Gustavo Aucar (GA) (Northeastern University of Argentina)

Matteo Cavalleri (MC) (Publisher, Strategy and Portfolio Development, AIP Publishing)

Aims and scope

The aim of the school is to provide an introduction to group theoretical methods and computational tools necessary for appropriate applications of symmetry properties in solid-state materials science. Special emphasis is given to the applications of computational crystallography using the Bilbao Crystallographic Server (BCS) (www.cryst.ehu.es) for the study of specific problems in solid-state physics, like phase transitions and their symmetry-mode analysis, comparison between crystal structures, magnetic symmetry and its applications in the description of magnetic structures, etc. Special topics like chirality in solid-state physics, continuous symmetry measures, chirality in magnetism, chiral phonons, chirality and relativity will be discussed in the context of new frontiers in materials science research.

The school is intended for scientists in Materials Science, Solid-State Physics and Crystallography in general and specifically for PhD students and young researchers interested in a deep and practical knowledge of group theory and applied crystallography. The maximum number of participants is limited to 70. Official language of the school is English. The school will take place in Shanghai University (Baoshan Campus) <https://en.shu.edu.cn>

Timetable:

Morning session (4 hours):

Lectures 8:30 – 10:30 // 11:00 – 13:00

Coffee break: 10:30 - 11:00

Lunch: 13:00 – 14:30

Afternoon session (4 hours):

Lectures: 14:30 – 16:30 // 17:00 – 19:00

Coffee break: 16:30 – 17:00

Dinner: 19:00 – 20:30

Evening session (optional): 20:30 – 22:00

Arrival Day (14 June 2024-Friday) - afternoon

15:30 - 19:00 Arrival and registration of the participants

19:00 - 20:30 Welcome Reception

Pre-school Day (15 June 2024-Saturday): morning session (MN,MIA)

8.30 - 10:30 (MN) Revision 1 Crystallographic point groups. Basic properties of groups (group axioms, order, multiplication tables, etc.). Subgroups, index, coset decompositions, Lagrange theorem. Concept of isomorphism and homomorphism. Group actions: conjugation and normalizers.

11:00 - 12:00 (MN) Revision 1 Crystallographic point groups (cont) Wyckoff positions for point groups. Overview of crystallographic point groups and their Hermann-Mauguin symbols.

12:00 - 13:00 (MIA) Revision 2 Matrix calculus applied to crystallography. 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.

Pre-school Day (15 June 2024-Saturday): afternoon session (MIA)

14:30 - 15:30 (MIA) Revision 2 Matrix calculus applied to crystallography (cont.)

15:30 - 16:30 (MIA) Revision 3: Representations of point groups

Representations of crystallographic groups: definition and basic properties. Irreducible and reducible representations.

17:00 - 19:00 (MIA) Revision 3: Representations of point groups (cont)

Subduced and induced representations. Direct product representations. Database of Bilbao Crystallographic Server on point-group representations.

1st Day (16 June 2024-Sunday): morning session (MN)

8:30 - 9:00 Opening of the school

09:00 - 10:30 (MN) Space groups – general introduction:

Periodic structure of the crystalline matter: lattices and their basic properties. Structure of space groups: point groups of space groups. Coset decomposition of the space group with respect to its translation subgroup. Symmorphic and non-symmorphic space groups.

Poster contributions-discussions during the coffee break

11:00 - 12:00 (MN) Space groups – general introduction (cont.) - Classification of space groups

12:00 - 13:00 (MN) Space groups and their descriptions: Symbols of space groups.

1st Day (16 June 2024-Sunday): afternoon session (MN,MIA)

14:30 - 16:30 (MN) Space groups and their descriptions (cont.):

Description of space-group symmetry operations. Space-group diagrams. General and special positions, site- symmetry groups, crystallographic orbits.

Poster contributions-discussions during the coffee break

17:00 - 19:00 (MIA) Representations of space groups:

Representations of the translation group. Symmetry in reciprocal space: Brillouin zones and wave-vector symmetry types. Irreducible representations of space groups and their construction. Subduced and direct-product representations of space groups.

Brillouin-zone database of Bilbao Crystallographic Server. Basic computer tools for space-group representations.

Evening session (optional)

Discussions, questions and comments on the lecture and exercise material of the day

2nd Day (17 June 2024-Monday): morning session (MN,MIA)

8:15 - 9:45 **(MN)** Transformations of the coordinate systems: change of origin and orientation. Conventional and non-conventional descriptions of space groups; ITA-settings.

9:45 - 10:30 **(MIA)** Group-subgroup relations between space groups:
Subgroups of space groups: types of subgroups of space groups; Hermann theorem; maximal subgroups; series of isomorphic subgroups. Coset decomposition. Relations of Wyckoff positions for a group-subgroup pair. Supergroups of space groups.

Poster contributions-discussion during the coffee break

11:00 - 13:00 **(MIA)** Group-subgroup relations between space groups (cont.)

13:00 - 14:00 **(MIA)** Computer databases and access tools to crystallographic symmetry data for space groups. Maximal subgroups data and related computer application in the Bilbao Crystallographic Server.

2nd Day (17 June 2024-Monday): afternoon session

14:30 - 19:00 Excursion in Shanghai

19:30 - 22:00 Dinner in the town

3rd Day (18 June 2024-Tuesday): morning session (MIA)

8:30 - 10:30 **(MIA)** 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 and COMPSTRU). Crystal-structure descriptions compatible with symmetry reduction (the program TRANSTRU).

11:00 - 12:00 **(MIA)** Crystal-structure relationships. Family trees (Baernighausen trees) of crystal structures: aristotype (basic) and hettotypes (derivative) structures (the program STRUCTURE RELATIONS).

12:00 - 13:00 **(MIA)** Structural pseudosymmetry. Pseudosymmetry search for new ferroics. Application in structural phase transitions (the program PSEUDO).

3rd Day (18 June 2024-Tuesday): afternoon session (JMPM)

14:30 – 16:30 **(JMPM)** Group-subgroup relations of space groups and their applications to phase transitions (SUBGROUPS, AMPLIMODES) - First part.

17:00 – 19:00 **(JMPM)** Group-subgroup relations of space groups and their applications to phase transitions (SUBGROUPS, AMPLIMODES)- Second part

Evening session (optional)

Discussions, questions and comments on the lecture and exercise material of the day

4th Day (19 June 2024-Wednesday): morning session (JMPM)

8:30 - 10:30 (JMPM) Magnetic symmetry. Magnetic point operations and point groups, connection to magnetic tensor properties. Magnetic space groups and their presentation in D. Litvin's tables. OG and BNS settings of type-IV magnetic space groups

11:00 -13:00 (JMPM) Representation analysis vs magnetic symmetry description of magnetic structures

4th Day (19 June 2024-Wednesday): afternoon session (JMPM)

14:30 - 16:30 (JMPM) Magnetic symmetry and its applications in the databases and tools of the Bilbao Crystallographic Server. Magnetic point and magnetic space groups. General and special Wyckoff positions. Magnetic symmetry material tensors. Extinction rules for magnetic space groups. Maximal magnetic space groups for a given a propagation vector and resulting magnetic structural models.

17:00 - 19:00 (JMPM) Database of magnetic structures on the Bilbao Crystallographic Server.

Evening session (optional)

Discussions, questions and comments on the lectures and exercise material of the day

5th Day (20 June 2024-Thursday): morning session (LZ)

8:30 - 10:30 (LZ) Chiral Phonons: definitions and theoretical description

11:00 -13:00 (LZ) Emergent phenomena with chiral phonons.

5th Day (20 June 2024-Thursday): afternoon session (MN,DA,BJC)

14:30 - 16:30 (MN) Chirality: from molecules to crystal structures.

17:00 - 19:00 (DA) (on-line) Continuous symmetry and chirality measures: Principles and applications across the natural sciences.

19:00 - 20:00 (BJC) (on-line) A new symmetry-mode based descriptor of chirality. Applications to chiral organic-inorganic hybrid metal-halides.

20:00 - 23:00: Poster session (with bouffet and beer)

6th Day (21 June 2024-Friday): morning session (SC)

8:30 - 10:30 (SC) Chirality and Kinetomagnetism

11:00 -13:00 (SC) Altermagnetism and Kinetomagnetism

6th Day (21 June 2024-Friday): afternoon session (GA,MC)

14:30 - 16:30: (GA) Chirality, Relativity and The Standard Model of Particle physics

17:00 - 18:00: (MC) How to get published and be read

18:00 - 18:30: Conclusion remarks. Final farewell and end of the school.

Acknowledgements

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