First Edition (2017) of

Shanghai International Crystallographic School

working with Bilbao Crystallographic server

held

in Shanghai University

"Shanghai International Crystallographic School working with Bilbao Crystallographic Server" was ceremoniously held at Shanghai University in the Siyuan Hall, Lehu new building from June 11st to 17th 2017. Following the idea of Alessandro Stroppa, a computational materials scientist from CNR-SPIN in Italy, the School was organized together with Prof. Wei Ren, professor of physics from the International Center of Quantum and Molecular Structure, Shanghai University and Mois Aroyo, professor of Condensed-Matter physics at the University of Basque in Spain.

The invited lecturers were: Luis Elcoro, Mois Aroyo and Ion Errea, UPV/EHU, Spain; Massimo Nespolo, from CRM2 UL/CNRS, France; Alessandro Stroppa, from CNR-SPIN;

Qiang Zhu from University of Nevada, USA.

Both faculty members and students actively participated to this school, coming from prestigious university such as University of Pennsylvania, the Indian Institute of Technology, the S.N. Bose National Centre for Basic Sciences in India, the Chinese Society of Crystallography, Peking University, Institute of Physics of Chinese Academy of Science, Nanjing University, Fudan University, Nankai University, Harbin Institute of Technology, Xi'an Jiaotong University, Southwest Jiaotong University, Beijing Polytechnic University, Northeast Normal University, Huazhong University of Science and Technology, Shanxi University, East China Normal University, Renmin University of China, Wuhan Institute of Science and University of Science and Technology Beijing.

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The lectures started at 8:30 on June 11, and Professor Wei Ren, the executive director of the International Center for Quantum and Molecular Structure (ICQMS) in Shanghai University, hosted the opening ceremony. Professor Sheng Wancheng, the dean of College of Science, Jeffrey Reimers, the director of the ICQMS, and Mr. Chen Chong, the secretary of the Chinese Crystallography Society, expressed their sincere opening remarks.

During the week, Prof. Mois Aroyo and Prof. Massimo Nespolo mainly taught the matrix calculus in crystallography, the representation of the point and space groups, the symmetry relation of the space group and other basic knowledge, combined with Bilbao Crystallography Server (BCS) which hosts online computing tools useful for the crystal structure relations, magnetic symmetry and other related contents hands-on sessions. Prof.

Luis Elcoro explained the BCS tools such as Subgroups, Amplimodes, Magnext, and Maxmagn. Prof. Ion Errea discussed the calculation of phonon in Density Functional Theory (DFT) and the important role of BCS in supporting and complementing the DFT study of phonons. Prof. Alessandro Stroppa discussed the ferroelectric polarization in solids from inorganic to hybrid organic-inorganic materials, mechanisms and microscopic origins, and he taught how to estimate the electric polarization using the combination of DFT and BCS tools. Prof. Qiang Zhu introduced materials design by using the advanced crystal structure prediction methods. The school was intense and the participants even used the time after dinner for further discussions on daily topics. This certainly contributed to the process of know-how acquisitions. In the evening of June 14th , a poster session was held at the International Center for Quantum and molecular structure at Shanghai University, where scientific discussions with buffet took place, thus allowing to the participants to have closer interactions and to set up new possible collaboration networks.

The school very successfully ended at 6 p.m on June 17, and during the closing ceremony, 30 young scholars were awarded as Young Scholars of International Union of Crystallography.

The school introduced the theory and application of space group symmetry in solid materials science, focusing on the use of computational tools of the Bilbao Crystallographic Server (BCS) (http://www.cryst.ehu.es/) to study structural phase transitions, symmetry mode analysis, crystal structure comparison, magnetic symmetry and other important topics in solid state physics. For the first time, we introduced a DFT part in the BCS school for studying the electric polarization of organic-inorganic crystals, the phonon properties of materials, the prediction and computational design of new materials. The participants also combined their own research experience and conducted an in-depth interactive discussion

focusing on a wide range of subjects. Participants greatly benefited from the school according to their feedback. This international school has played a positive role in promoting different levels of collaborations among all the participants and researchers working in the field of materials science, condensed-state physics , chemistry and crystallography. It also promoted new collaborations between different prestigious research institutions in China and the CNR-SPIN institute in the feature.