2018 International Workshop on Density Functional Theory First Principles Simulations in Materials Science

Exciting Shanghai School - Hands-on workshop on density functional theory- First-principles simulations in materials science was successfully held in Shanghai University - Baoshan Campus on 18th-22nd November 2018. The idea to start with such a series of workshops in Shanghai was put forward by Alessandro Stroppa, from CNR-SPIN Institute.

The event was organized in collaboration with Prof. Wei Ren from the International Center for Quantum and Molecular Structures of Shanghai University, Professor of Physics, Faculty of Science, Shanghai University.

The school was organized in the framework of the international collaboration between CNR-SPIN and Shanghai University aiming to promote common research projects in computational material science and

young student exchanges between China and Italy, hosted by SPIN institute.

World-renowned scientists from prestigious research centers and institutes attended the school such as Prof. Matthias Scheffler (Director of the Fritz Haber Institute-Max Planck Society-Germany), Prof. Claudia Draxl, (Humboldt-Universität zu Berlin), Prof. Weitao Yang (Duke University), Prof. Lucia Reining (École Polytechnique, Paris), Prof. Guo Hong (McGill University), Prof. Jiang Hong (Peking University), Prof. Jiawang Hong (Beijing Institute of Technology), and Dr. Miao Liu (Institute of Physics, Chinese Academy of Sciences), and many others.

The school was attended by about 100 teachers and students from Beijing Institute of Applied Physics and Computational Mathematics, University of Chinese Academy of Sciences, Shanghai University, Fudan University, Shanxi University, Jilin University, Zhejiang University, Inner Mongolia University, University of Science and Technology, Beijing Institute of Technology, Harbin Institute of Technology, Beijing University of Science and Technology, Huazhong University of Science and Technology, Shanghai Institute of Silicate, Fujian Institute of Physical Structure and many other institutions of higher learning.

The event was supported by the Materials Genome Institute and the Computing Center and Academic Affairs Office of Shanghai University, the Physics Department of Shanghai University, the *exciting* software team of Humboldt University in Berlin, the NOMAD project (European Novel Materials Discovery project), and the Suzhou Computation Services Ltd.

The school started at 8:45 am on 18th November 2018. The opening ceremony was given by Prof. Wei Ren. Prof. Jeffrey Reimers from the International Center for Quantum and Molecular Structures of Shanghai University gave a welcome speech. In the first talk, Prof. Matthias Scheffler discussed the latest achievements and developments in electronic structure theory calculations, and he explained in detail the big data-driven

material research paradigm and the European NOMAD project; Prof. Weitao Yang gave an in-depth explanation of the basic principles of density functional theory, introducing the concept of fractional electrons and the latest theoretical developments. Prof. Hong Guo focused on the development of RESCU software based on mathematical algorithms for large-scale systems and its application in materials research. Prof. Jiawang Hong introduced a comprehensive use of first-principles calculations and experimental methods for non-harmonic effects in the lattice dynamics of advanced materials; Prof. Lucia Reining discussed the nature of quasi-particle GW approximation and time-dependent density functional theory (TDDFT); dr. Miao Liu, a researcher focussing on material databases and high-throughput computing examples, explained how to discover new materials through data processing; Prof. Claudia Draxl gave a detailed analysis of the NOMAD project; Prof. Jiang Hong reported on the first principles methods for studying strongly correlated materials containing *d/f* electrons; Dr. Alessandro Stroppa discussed the magneto-optical effects and the second harmonic generation in connection with advanced multi-functional materials. Dr. Andris Gulans introduced the basics of the plane wave combined with the local orbital method (APW+LO) and how to implement the GW method in the *exciting* software. Dr. Pasquale Pavone described how to define the crystal structure in the *exciting* software, structure relaxations and mechanical elastic properties; Dr. Fabio Caruso introduced the phonons and the electron-phonon interaction, Dr. Sven Lubeck analyzed the accuracy in density functional theory calculations, Dr. Maria Troppenz explains the NOMAD data analysis and cluster expansion methods for solid solutions; Dr. Christian Vorwerk detailed the calculation of the optical spectra within the many-body perturbation theory.

The school adopted the method of lectures and computer tutorials. This combination enables the unpexerienced students to learn how to use the *exciting* package for studying materials properties. The Shanghai University Computing Center was used for the computer tutorials and to discuss in more details the algorithms and practical examples. Many

students exploited the self-study time to discuss after dinner. Students and teachers were very enthusiastic for the teaching/learning experience. The school ended successfully at 6 pm on 22nd November 2018.

It was the first time that the school in electron structure theory based on the *exciting* software was held in China. All the participants expressed their interest in this event. The international school has played an active role in promoting the students in condensed matter physics, first principles simulations and materials science to strenghten their experience and to promote international collaborations.