International School of Crystallography
52nd Course: - Quantum Crystallography

1 - 10 June 2018, Erice, Italy

Scientific Report for ECA

The 52nd course of Crystallography at the Ettore Majorana Research Foundation in Erice coincided with the inaugural school on Quantum Crystallography.
The school was planned in 2011 by Dylan Jayatilaka and Piero Macchi and submitted for approval to the School director, who scheduled the event in 2018 in conjunction with the school on Electron Diffraction. This combination is in fact very fruitful, because some emerging techniques in electron diffraction enable reconstruction on typical quantum mechanical functions, like the charge density, the electric potential, which are the main subjects of Quantum Crystallography itself. Moreover, wavefunction based methods are nowadays implemented in order to extract the information from experimental electron diffraction.
This synergy has enabled scheduling a few joint sessions with shared lecturers, that was very much appreciated by the students of both courses.

58 students and 25 lecturers/tutors attended the school, filling all the possible seats available for the Quantum Crystallographic School. Ca. 30 additional participants could not be accepted due to lack of accommodation facility. It is therefore envisaged that a future school on the subject may as well attract so many interested participants.

The course on Quantum crystallography consisted in 8 sessions of lectures and 5 of tutorials. More than 25 lecturers and tutors have been invited to deliver high quality lectures and very detailed hands-on sessions using state of the art software.

The lectures followed a rather logic pathway, starting from fundamentals of crystallography (symmetry, diffraction, modelling) and quantum mechanics (Schrödinger equation, wavefunction, physical bases of the models). The lectures then focused on the most adopted methodologies (experimental ad well as computational) to determine the charge and spin electron density, the wavefunction, electric and magnetic properties of crystalline materials. In the last sessions of the meetings, the lecturers presented application of quantum crystallographic studies in fields like material science, chemistry and structural biology. A round table has concluded the meeting, reviewing some topics discussed during the meeting with an outlook on open questions and future studies.

The 5 tutorial sessions consists of 10 workshops, organized on the base of the most broadly adopted and updated programs for multipolar model, X-ray constrained wavefunctions, periodic wavefunction and electric/magnetic properties, such as XD2016, MoPRO, MXN, Olex2-HAR, Tonto, CRYSTAL2017, QuantumExpresso, MoleCoolQT, PolaBer, as well as on many routines and locally modified programs purposes like data reduction and analysis of X-ray diffraction, calculation of X-ray constrained extremely localized molecular orbitals. Overall, each student could attend 5 workshops, each lasting ca. 3 hours.

During each lecture session, sufficient amount of time was allocated for discussion and questions by the students, who interacted quite intensively with the lecturers. The students demonstrated interest also outside the official sessions, during the pauses or the social activities.

Two poster sessions were organized in order to allow the students to present results of their ongoing research activities. Out of the 55 posters, 15 were selected for oral presentations of 10 minutes, including short discussions. The performances of the presenters were exceptionally good and they could well interact with the audience and respond to comments and remarks.

As usual the social program in Erice is extremely rich and pleasant, including social dinners and get together party, music events and excursions to historical sites in the neighborhood. The participants could appreciate these activities and took also opportunities for some extra discussion session, in an informal fashion and much relaxed atmosphere.

Prizes and Award

During the closing ceremony on the last day of the school several prizes were awarded to students: the best poster prizes and the Lodovico prize, awarded to the student most lively and participating inside and outside the lecture hall. The third place for the poster prize was awarded to Alexey Kuzmin, PhD student at Institute of Solid State Physics, Russian Academy of Sciences, (RU), the award for the second place was assigned to Alena Vishina, Postdoc at the Chemistry Department, Chalmers University of Technology, (SE) and the first place was awarded to Emil Damgaard-Møller, Phd student at the Center for Materials crystallography (CMC), Aarhus University (DK). The committee decided to award the Lodovico Prize to Lorraine Andrade-Malaspina, PhD student at the university of Bremen (DE).

At the end of the Course, participants received an electronic survey to evaluate the course and provide comment on the quality of the program. Their responses indicated that a similar meeting should be held at least within 3 - 4 years and that the course had achieved most of its objectives (score 85/100).

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Finacial Report for ECA

The financial support of 1200 euro offered by ECA was used to support the attendance of the following students:

400 Euro

Eleanor Dodd (02/08/1993)
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400 Euro

Florian Kleemiss (b. 28/01/1992)
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400 Euro

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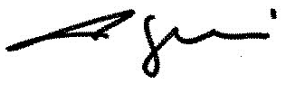
Total 1200€

Sincerely,



Dr. Annalisa Guerri
Executive Secretary
Intenational School of Crystallography

Sesto Fiorentino, 02/07/2018