European Crystallographic Association

ECA

Report for school financial support

1. Date, location and title of meeting:

Title meeting	Tools for Chemical Bonding 2019
Location	House of Science, Bremen, Germany
Date	July 14, 2019 - July 19, 2019
Website address	https://www.tcb2019.com/

2. Please describe how the bursary was used.

The bursary of 1000 Euros was used as travel bursary for students to attend the workshop. It was split into two awards to cover travel and accommodation for the two students that made the most compelling case how they depend on the travel bursary. The organizing committee [Simon Grabowsky, Bremen; Thorsten M. Gesing, Bremen; Jens Beckmann, Bremen; Paulina M. Dominiak, Warsaw; Alessandro Genoni, Metz; Amir Karton, Perth] decided on the successful candidates. Ekaterina A. Radiush (Novosibirsk) and Michael Patzer (Mülheim) won the travel bursaries. Their individual reports are attached.

3. Report (min. 250 words, max. 500 words, will be published on the ECA web site)

This hands-on workshop was organized with two different purposes in mind:
i) Bridging the communities of quantum crystallography and quantum chemistry. In quantum crystallography, experimental electron density measurements are interpreted with respect to chemical-bonding questions, whereas in quantum chemistry theoretical wavefunctions are interpreted with exactly the same aim. Both communities can greatly benefit from adopting strategies and philosophies of the other.
ii) Publication of a new compound or synthesis strategy normally requires both a crystal structure and a geometry optimization, but the wealth of chemical-bonding information in diffraction measurements and wavefunction calculations is rarely exploited beyond the discussion of bond distances and angles. So in this workshop, various popular software suites for chemical bonding analysis were introduced at a beginners' level. There will be a textbook based on the workshop materials in the deGruyter publishing house for university students at graduate level entitled "Complementary Bonding Analysis" available in summer 2020.
The workshop was very well attended with 55 participants and 20 teachers from all over the world. From the organizers' perspective, we were very happy with the engagement of the participants and the mingling of teachers with participants. We hope that this new format will see new editions in the future.
A photo of the workshop during a software session is added on the next page.