

CECAM DISCUSSION MEETING
“QUANTUM CRYSTALLOGRAPHY: CURRENT DEVELOPMENTS AND
FUTURE PERSPECTIVES” (Nancy, 19-20 June 2017)

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The CECAM Discussion Meeting “Quantum Crystallography: Current Developments and Future Perspectives” took place in Nancy on the 19th and 20th of June 2017 at the Presidency of the University of Lorraine, with 29 participants coming from 9 different European countries and also from Australia, USA and Canada. In the organization of the meeting we were also able to attract external sponsors that, other than CECAM, financially supported us (Turbomole, Wien2K and Bruker) and whose representatives have actively participated in all the scientific sessions and discussions. They gave us the impression that, from now on, they feel part of our community and will continue to support us. External financial supports were also received from the French Chemical Society (Société Chimique de France, SCF) and from the “Métropole of Grand Nancy”.

The goal of the meeting was dual: 1) discussing the state of the art of “Quantum Crystallography;” 2) discussing on the possibility of re-founding and re-initiating the field, by proposing a new, consistent and commonly accepted definition of “Quantum Crystallography” (QCr).

To accomplish this task, on the first day we had 23 short talks that gave a general overview of the field and, on the second day, three round table discussions, which addressed the following topics: i) the necessity of a new definition of QCr; ii) strategies to build new QCr community; iii) future perspectives and vision for QCr. On the second day, we also organized a “Rebuttal Session”, where everybody had the opportunity to re-express their point of view on current status and directions of the field, also considering the outcomes of the previous discussions.

During the discussions, an overwhelming consensus was reached among the participants on the fact that Quantum Crystallography is the ideal vehicle to drive modern developments in diffraction and scattering science with flow-on effects into materials and life sciences as well as quantum chemistry. Therefore, it was concluded that the definition of QCr as currently present in the literature is too narrow and does

not reflect either all current developments or the reception that QCr has received in the past few years for its diverse applications. Different options for a broader definition were discussed, but intentionally, a new definitive definition was not fixed during the meeting. Rather, the outcomes of the workshop will be summarized in a viewpoint article for “Chemistry – a European Journal” with all participants as co-authors, with the aim to open a debate about the definition in connection to the usefulness of the field and the scope for applications beyond the field. This is supposed to culminate into networking activities, future discussion meetings, and eventually a IUPAC project (within the next three years) to formalize the definition of QCr. Road maps and responsibilities for the organization of activities resulting from this CECAM discussion meeting were fixed and agreed. Therefore, the meeting did not only contribute to scientific progress, but also to the initiation of concrete plans for establishing a new scientific field and a new scientific community.

For more detailed information, we attach to the present report the “Book of Abstracts” of the workshop, where you can find the list of participants, their abstracts and the detailed program of the conference.

Website: <http://qcrystcecam.weebly.com>



Figure 1. Speakers of the CECAM Discussion Meeting on “Quantum Crystallography”