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General Theory Issues

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In this talk I would like to draw attention to the recent theoretical challenges quantum chemistry has. Undisputedly, theoretical calculations are part of chemical research: the results of these are used to understand chemical phenomena, to interpret experiments, predict properties, and support engineering.

Thanks to the effort of theoreticians, today easy to use computer codes are available which enable chemists to use theoretical methods in their every day work. The traditional role of theoreticians is challenged, since our help in these calculations are often not necessary. Still, development of these techniques is constantly needed: the type of systems and events chemists (and even biologists) want to study increase. Therefore, we have to work on theory and upgrade our codes to fulfill these requests.

In this talk I will try to give a personal view of this matter. I will cover the following challenges:

Theoretical methods:

- Dynamics at all level
- DFT: search for functionals, hybrid methods etc.
- Wave function methods: dilemma of accuracy vs. system size
- Inclusion of environmental effects
- Fragment methods
- Role of machine learning

Systems:

- Surface processes
- Excited states
- Electron transfer
- Quantum control

Implementation:

- Modern architectures
- Role of clouds

Clearly, it is impossible to cover all challenges, but I hope that my presentation will be provocative enough and will initiate deep discussions during the Perugia edition of EuCo-CTC.

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