Monday, May 8th, at 12:00, Aula

Computational Chemistry of Complex Chemical Systems: Status and Perspectives

Walter Thiel

Max-Planck-Institut für Kohlenforschung, Kaiser-Wilhelm-Platz 1, 45470 Mülheim, Germany

Theoretical calculations and computer simulations continue to gain importance in chemistry. Due to the synergy between improved computational methods and increasing hardware performance, the computations become ever more accurate and can be applied to ever more complex systems so that chemical problems can nowadays often be solved by the interplay of experiment and theory [1-3]. The lecture will present an overview over these developments and address the current status and the perspectives of quantum chemistry. Current applications include highly accurate ab initio calculations on the spectroscopy of small molecules, density functional studies of transition metal catalyzed reactions, semiempirical excited-state dynamics simulations, and QM/MM modeling of complex biomolecules. The lecture will cover all these types of applications using examples from our own research [3-8]. The focus will be on simulations of chemical and enzymatic reactions to demonstrate how computational chemistry can contribute to a detailed understanding of reactivity and (bio)catalysis.

[1] W. Thiel, *Angew. Chem. Int. Ed.* **50**, 9216-9217 (2011).
[2} H. M. Senn, W. Thiel, *Angew. Chem. Int. Ed.* **48**, 1198-1229 (2009).
[3] W. Thiel, *Angew. Chem. Int. Ed.* **53**, 8605-8613 (2014).
[4] S. Shaik, S. Cohen, Y. Wang, H. Chen, D. Kumar, W. Thiel, *Chem. Rev.* **110**, 949-1017 (2010).
[5] M. Leutzsch, L. M. Wolf, P. Gupta, M. Fuchs, W. Thiel, C. Farès, A. Fürstner, *Angew. Chem. Int. Ed.* **54**, 12431-12436 (2015).
[6] B. Karasulu, W. Thiel, *ACS Catal.* **5**, 1227-1239 (2015).
[7] A. Owens, S. N. Yurchenko, W. Thiel, V. Spirko, *Phys. Rev. A* **93**, 052506 (2016).
[8] D. Fazzi, M. Barbatti, W. Thiel, *J. Am. Chem. Soc*. **138**, 4502-4511 (2016).