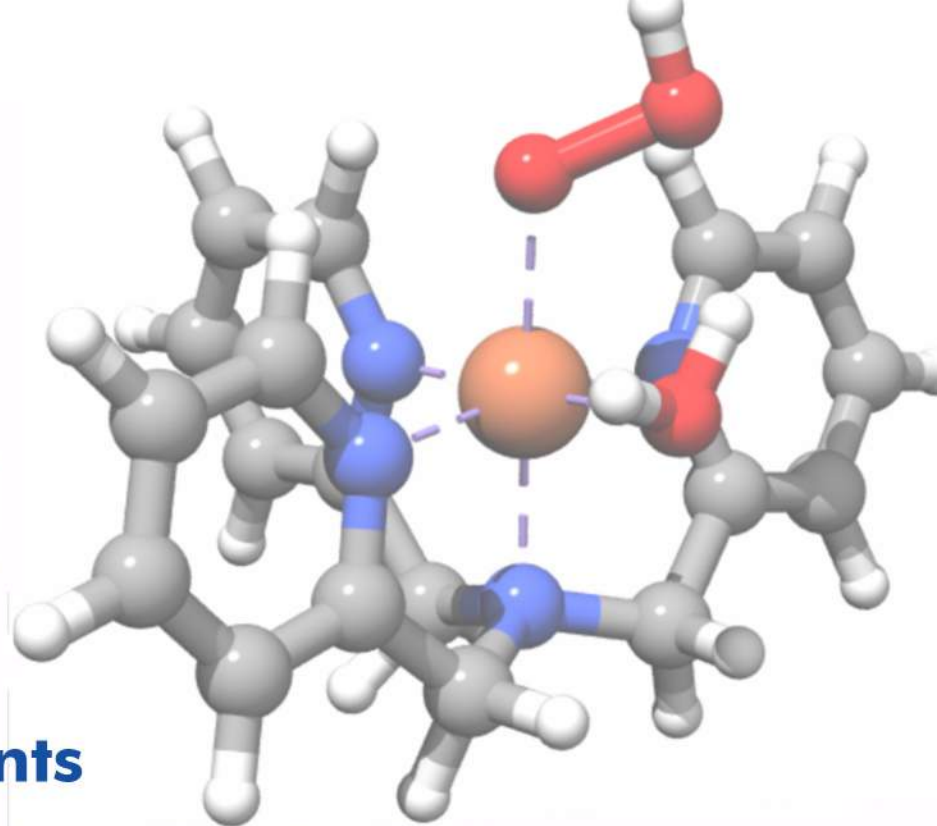


# ORCA User Meeting

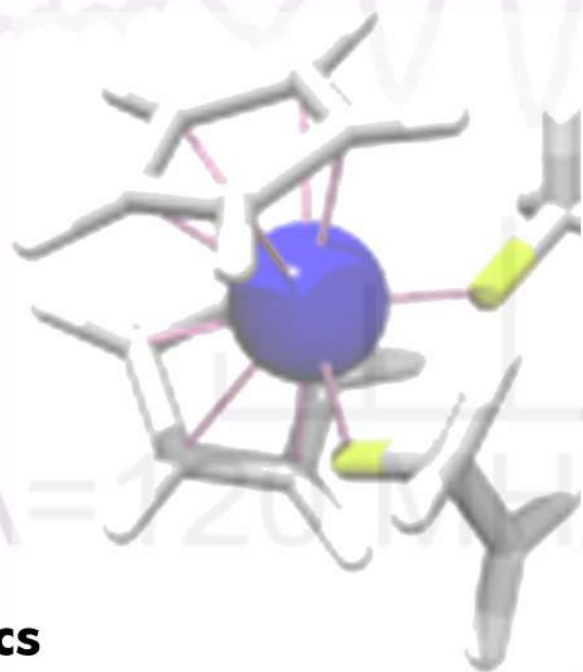


Methods, applications and developments

September 7-8, 2015 - Wissenschaftspark Gelsenkirchen, Germany

The ORCA program package by now has a vastly increasing user community worldwide. In order to facilitate discussion between developers, contributors and users we organize the first ORCA users meeting. The team is looking forward to meeting you there!

$$D_{kl}^{\text{SOC}-(0)} = -\frac{1}{S^2} \sum_{b(S_b=S)} \Delta_b^{-1} \left\langle 0SS \left| \sum_i h_k^{\text{SO}}(i) s_{i,z} \right| bSS \right\rangle \times \left\langle bSS \left| \sum_i \right. \right.$$



## Invited Speakers:

- Prof. Stefan Grimme, Universität Bonn, Germany
- Dr. Christoph Riplinger, Princeton University, US
- Dr. Michael Beck, Bayer CropScience, Germany
- Prof. Martin Korth, Universität Ulm, Germany
- Dr. Andreas Hansen, Universität Bonn, Germany
- Prof. Serena DeBeer, MPI-CEC, Germany
- Dr. Michael Römelts, Ruhr-Universität Bochum, Germany
- Dr. Ragnar Björnsson, University of Iceland, Iceland
- Dr. Dimitrios Manganas, MPI-CEC, Germany
- Prof. Ed Valeev, Virginia Tech, US

## Topics

- the ORCA Input Library, Interfaces
- DFT for large systems
- basis set effects
- fast and accurate PNO calculations
- theoretical spectroscopy
- applications on battery acids, crop protection, environmental effects, catalysis



Deadline for registration: 31 July 2015

More information will be available at <http://www.cec.mpg.de>

Organizers: Alexander Auer, Frank Wennmohs, Robert Izsak



Max Planck Institute for Chemical Energy Conversion

