PROGRAM

4. – 6. November 2020, Max-Planck-Institut für Kohlenforschung

Day I: November, 4th

12:00 - 13:00   Arrival, Coffee
13:30 - 14:00   Welcome
14:00 - 14:30   Getting started with ORCA 4.2
14:30 - 15.00   optimizing transition states
15.00 - 15.30   Core level Spectroscopy with ORCA
15:30 - 16:00   Coffee break
16:00 - 17.30   Tutorial I - Geometries, transition states, frequencies, visualization
19.00           Evening Programme - Get together in Muelheim

Day II: November, 5th

09:00 - 09:45   Recent developments in multiscale simulations
09:45 - 11:15   Tutorial II - LED and electronic structure analysis
11:15 - 11:45   Coffee break
11:45 - 12:15   TDDFT Basics
12:15 - 12:45   Solvation methods in ORCA
13:00 - 14:30   Group photo and Lunch break
14:45 - 15:15   Ab-Initio Molecular Dynamics features in ORCA
15:30 - 17:00   Tutorial III - EPR spectroscopy
17:00 - 17:30   Coffee break
17:30 - 18:00   What makes my ORCA fast? (Grids, COSx and Integrals)
18.00 - 18.30   Calculating NMR properties in ORCA
19:00 - 22:00   Dinner, Poster session

Day III, November 6th

09:00 - 09:30   Excited State Dynamics in ORCA
09.30 - 10.30   CAS clinic - CASSCF intro and solutions
10.30 - 11.00   Modeling solids in ORCA
11:00 - 11:30   Coffee break
11:30 - 13:00   Tutorial VI - Treating transition metals with ORCA
13:00           Farewell

Lecturers: