PROGRAM

5th ORCA USER MEETING

28. – 30. April 2020, Max-Planck-Institut für Kohlenforschung

Day I: April, 28th

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: April, 29th

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, April 30th

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: