

2nd Winter School of Computational Chemistry Program

Monday 28 February 2022

Tehran Local Time	EU Local Time	Topic	
10:45 – 11:00	8:15 – 8:30	Opening	
11:00 – 11:50	8:30 – 9:20	Dr. Julien Toulouse	Basic Density-Functional Theory
11:50 – 12:00	9:20 – 9:30	Break	
12:00 – 13:00	9:30 – 10:30	Dr. Julien Toulouse	Basic Density-Functional Theory
13:00 – 14:00	10:30 – 11:30	Break	
14:00 – 15:00	11:30 – 12:30	Dr. Haratian	Practical Session (ORCA)
15:00 – 15:15	12:30 – 12:45	Break	
15:15 – 16:30	12:45 – 14:00	Dr. Haratian	Practical Session (ORCA)
16:30 – 16:45	14:00 – 14:15	Break	
16:45 – 18:00	14:15 – 15:30	Dr. Haratian	Practical Session (ORCA)
Tuesday 1 March 2022			
11:00 – 11:50	8:30 – 9:20	Dr. Julien Toulouse	Approximation in Density-Functional Theory
11:50 – 12:00	9:20 – 9:30	Break	
12:00 – 13:00	9:30 – 10:30	Dr. Julien Toulouse	Approximation in Density-Functional Theory
13:00 – 13:40	10:30 – 11:10	Break	
13:40 – 15:20	11:10 – 12:50	Dr. Haratian	Practical Session (VASP)
15:20 – 15:30	12:50 – 13:00	Break	
15:30 – 16:30	13:00 – 14:00	Dr. Klaas Giesbertz	Density Functional Approximations from the Perspective of Dissociating Molecular Hydrogen
16:30 – 16:45	14:00 – 14:15	Break	
16:45 – 18:00	14:15 – 15:30	Dr. Klaas Giesbertz	Meaning of Kohn-Sham Orbital Energies
18:00 – 18:15	15:30 – 15:45	Closing	