Winter School of Computational Chemistry 2023 Program

Monday 20 Feb 2023		Tuesday 21 Feb 2023		Wednesday 22 Feb 2023	
9:00 – 9:45	Introduction to ORCA	10:00 – 10:45	Basic Stuff	10:00 – 10:45	MCSCF and Excited States
10:00 – 10:45	Introduction to ORCA	11:00 – 11:45	Hartree-Fock	11:00 – 11:45	Density Functional Theory
11:00 – 11:30	Break	12:00 – 12:30	Break	12:00 – 12:30	Break
11:30 – 13:00	Working with ORCA	12:30 – 14:00	Electron Correlation	12:30 – 14:00	Basis set
13:00 – 14:00	Break	14:00 – 14:30	Break	14:00 – 14:30	Break
14:00 – 16:00	Working with ORCA	14:30 – 16:00	Computer exercise	14:30 – 16:00	Theoretical exercise
16:00 – 16:30	Break	16:00 – 16:30	Break	16:00 – 16:30	Break
16:30 – 18:00	Working with ORCA	16:30 – 18:00	Computer exercise	16:30 – 18:00	Theoretical exercise

Thursday 23 Feb 2023		Friday 24 Feb 2023	
10:00 – 10:45	Qualitative models	9:00 – 9:45	Theoretical exercise
11:00 – 11:45	Molecular properties	10:00 – 10:45	Theoretical exercise
12:00 – 12:30	Break	11:00 – 11:30	Break
12:30 – 14:00	Wavefunction Analysis	11:30 – 13:00	Computer exercise
14:00 – 14:30	Break	13:00 – 13:30	Closing
14:30 – 16:00	Computer exercise		
16:00 – 16:30	Break		
16:30 – 18:00	Computer exercise		

Plan A: Yellow Cells
Plan B: Green Cells

Contact us at tccw@ch.sharif.edu