4th Winter School of Computational Chemistry Program

Monday 12 Feb 2024		Tuesday 13 Feb 2024		Wednesday 14 Feb 2024		Thursday 15 Feb 2024	
9:00 – 9:45	Computational and Quantum Chemistry: Unraveling Molecular Insights **Dr. Zahra Jamshidi**	**9:00 – 9:45**	Exact and Approximate Wave Functions **Dr. Zahra Jamshidi**	**9:00 – 9:45**	The Standard Models, Part III **Dr. Zahra Jamshidi**	**9:00 – 9:45**	The Explicitly Corrected Wavefunctions: Looking beyond the Orbital-based Ab-initio Computational Method, Part II **Dr. Shahbazian**
10:00 – 10:45	Potential Energy Surface and Geometry Optimization **Dr. Zahra Jamshidi**	**10:00 – 10:45**	Matrices and Quantum Chemistry **Dr. Mohammad Azami**	**10:00 – 10:45**	Matrices and Quantum Chemistry **Dr. Mohammad Azami**	**10:00 – 10:45**	Transition State **Exercise**
10:45 – 11:15	**Break**						
11:15 – 12:00	Tutorial ORCA	**11:15 – 12:00**	The Standard Models, Part I **Dr. Zahra Jamshidi**	**11:15 – 12:00**	The Explicitly Corrected Wavefunctions: Looking beyond the Orbital-based Ab-initio Computational Method, Part I **Dr. Shahbazian**	**11:15 – 12:00**	TBA **Prof. Siamak Nourizadeh**
12:15 – 13:00	Tutorial ORCA	**12:15 – 13:00**	The Standard Models, Part II **Dr. Zahra Jamshidi**	**12:15 – 13:00**	Molecules in a Strong Magnetic Field. **Prof. Trygve Helgaker**	**13:00 – 14:30**	Molecular Dynamics after Photoexcitation, including non-Born-Oppenheimer Effects, Part II **Prof. Horst Köppel**
13:00 – 14:00	**Break**						
14:00 – 16:00	Geometry Optimization and Frequency calculation, **Exercise**	**14:00– 16:00**	Post Hartree-Fock **Exercise**	**14:00 – 16:00**	Hartree-Fock and Population Analysis **Exercise**	**14:30 – 16:00**	UV-Vis spectroscopy, absorption spectrum, **Exercise**
16:00 – 16:30	**Break**						
16:30 – 18:00	Potential Energy Surface **Exercise**	**16:30 – 18:00**	Highly Accurate Quantum-Chemical Calculations **Prof. Trygve Helgaker**	**16:30 – 18:00**	Molecular Dynamics after Photoexcitation, including non-Born-Oppenheimer Effects, Part I **Prof. Horst Köppel**	**16:30 – 18:00**	Fluorescence and Phosphorescence **Exercise**