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## Program

The summer school will start on Sunday 24/9 and will close on the evening of Friday 29/9.  
A preliminary program is provided below.

Download: [Program Summer School 2023 \(.pdf\)](#)

### SUNDAY 24/9

12:00 - 13:30 Registration  
13:30 - 14:00 Welcome  
14:00 - 15:30 **Introduction to Computational Chemistry** (Dimitrios Pantazis)  
15:30 - 16:00 Coffee Break  
16:00 - 18:30 **Introduction to ORCA** (Frank Wennmohs) & **ORCA practical**  
18:30 - 21:00 Dinner and welcome reception

### MONDAY 25/9

09:00 - 10:30 **Ligand Field Theory** (Serena DeBeer)  
10:30 - 11:00 Coffee break  
11:00 - 12:30 **Optical Spectroscopy** (Frank Neese)  
12:30 - 14:00 Lunch  
14:00 - 16:30 **Practical: Optical spectroscopy & LFT** (Dimitrios Manganas)  
16:30 - 17:00 Coffee break  
17:00 - 18:00 **Spin Hamiltonians** (Frank Neese)  
18:30 - 19:30 Dinner

### TUESDAY 26/9

09:00 - 10:30 **Magnetochemistry** (Thorsten Glaser)  
10:30 - 11:00 Coffee break  
11:00 - 12:30 **EPR Spectroscopy** (George Cutsail)  
12:30 - 14:00 Lunch  
14:00 - 14:45 **Advanced EPR Techniques** (Alexander Schnegg)  
15:00 - 17:00 **Practical: Magnetochemistry** (Daniel SantaLucia)  
17:00 - 19:00 **Practical: Simulation of EPR spectra** (Alexander Schnegg & George Cutsail)  
19:00 - 21:00 Dinner and **Poster Session**

### WEDNESDAY 27/9

09:00 - 10:30 **Vibrational Spectroscopy** (Maurice van Gastel)  
10:30 - 11:00 Coffee break  
11:00 - 12:30 **X-ray Spectroscopy** (Serena DeBeer)  
12:30 - 14:00 Lunch  
14:00 - 16:00 **Practical: Vibrational spectroscopy** (Maurice van Gastel)  
16:30 - 18:30 **Practical: X-ray Spectroscopy** (Serena DeBeer)  
18:30 - 19:30 Dinner

### THURSDAY 28/9

09:00 - 10:30 **Reactivity** (Sergio Jannuzzi)  
10:30 - 11:00 Coffee break  
11:00 - 12:30 **Mössbauer Spectroscopy & Practical** (Daniel SantaLucia & Derya Demirbas)  
12:30 - 14:00 Lunch  
14:00 - 16:00 **Practical: EPR calculations** (Dimitrios Pantazis)  
16:30 - 18:30 **Practical: Reactivity** (Sergio Jannuzzi)  
18:30 - 19:30 Dinner

### FRIDAY 29/9

09:00 - 10:00 **Magnetic Circular Dichroism** (Frank Neese)  
10:00 - 11:00 **Resonant inelastic X-ray Scattering** (Derek Rice)  
11:00 - 11:45 **Modeling Solids** (Dimitrios Manganas)  
11:45 - 12:30 **Modeling Metalloproteins** (Maria Drosou)  
12:30 - 13:30 Lunch  
13:30 - 14:30 **Excited States** (Benjamin Helmich-Paris)  
14:30 - 15:30 **Spectroelectrochemistry** (Olaf Rüdiger)  
15:30 - 16:30 **QM/MM with ORCA** (Sinjini Bhattacharjee)  
16:30 - 17:00 Coffee break  
17:00 - 18:00 **Closing Keynote Lecture: Ivana Ivanović-Burmazović**  
18:00 - 21:00 Farewell dinner / BBQ

## Topics

Introduction to Computational Chemistry  
Introduction to the ORCA Program System  
Ligand Field Theory  
Optical Spectroscopy  
Vibrational Spectroscopy  
Magnetochemistry  
Electron Paramagnetic Resonance Spectroscopy  
X-ray Spectroscopy  
Magnetic Circular Dichroism Spectroscopy  
Mössbauer Spectroscopy  
Reactivity

A series of Special Interest Lecture will also be offered on advanced topics of experimental techniques and computational methods.