

SUMMER SCHOOL 2024
**SPECTROSCOPY AND ELECTRONIC STRUCTURE
OF TRANSITION METAL COMPLEXES**

SUNDAY 22/9

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 23/9

09:00 - 10:00 **Group Theory** (Serena DeBeer)
10:00 - 10:30 Coffee break
10:30 - 12:00 **Ligand Field Theory** (Serena DeBeer)
12:00 - 13:30 Lunch (KoFo)
13:30 - 15:00 **Optical Spectroscopy** (Frank Neese)
15:00 - 15:30 Coffee break
15:30 - 17:30 **X-ray Spectroscopy** (Serena DeBeer)
18:00 - 19:30 Dinner & **Poster Session** (CEC)

TUESDAY 24/9

09:00 - 10:30 **Vibrational Spectroscopy** (Maurice van Gastel)
10:30 - 11:00 Coffee break (**Group Photo?**)
11:00 - 12:30 **Practical: Vibrational Spectroscopy** (Maurice van Gastel)
12:30 - 14:00 Lunch (KoFo)
14:00 - 15:30 **Facility Tours in Small Groups: 1) Raman, 2) UV-Vis
RFQ/Stopped Flow, and 3)/4) Both X-ray Labs**
15:30 - 18:30 **Practical: Excited State Spectroscopy** (Dimitrios
Manganas)
18:30 - 20:30 Dinner & **Poster Session** (CEC)

WEDNESDAY 25/9

09:00 - 10:30 **Spin Hamiltonians** (Frank Neese)
10:30 - 11:00 Coffee break
11:00 - 12:30 **Magnetochemistry** (Daniel SantaLucia)
12:30 - 14:00 Lunch
14:00 - 15:30 **EPR Spectroscopy** (Alexander Schnegg)
15:30 - 16:00 Coffee break
16:00 - 18:00 **Practical: Magnetochemistry** (Daniel SantaLucia)
18:00 - 19:30 Dinner

THURSDAY 26/9

09:00 - 10:30 **Practical: Simulation of EPR spectra**
(Alexander Schnegg & George Cutsail)
10:30 - 11:00 Coffee break
11:00 - 12:30 **Practical: EPR calculations** (Dimitrios Pantazis)
12:30 - 14:00 Lunch
14:00 - 15:00 **MCD Spectroscopy** (Frank Neese)
15:00 - 15:15 Coffee break
15:15 - 16:15 **Mössbauer Spectroscopy** (Daniel SantaLucia)
16:15 - 16:30 Coffee break
16:30 - 18:30 **Practical: Mössbauer Spectroscopy** (Daniel SantaLucia)
18:30 - 19:30 Dinner

FRIDAY 27/9

09:00 - 11:30 **Facility Tours in Small Groups: 1) SQUID/MCD, 2)
Mössbauer, and 3)/4) Both EPR Labs**
11:30 - 12:30 Open Q & A Session
12:30 - 13:00 Survey
13:00 - 14:30 Lunch
15:00 Start of the Eckhard Bill Symposium