



UNIVERSITATEA BABES-BOLYAI  
BABES-BOLYAI TUDOMÁNYEGYETEM  
BABES-BOLYAI UNIVERSITAT  
BABES-BOLYAI UNIVERSITY  
TRADITIO ET EXCELLENTIA



Tradiție și Excelență prin  
Cultură - Știință - Inovație din 1581

# Quantum Chemistry of Excited States

## QCES-2025

29.09-3.10

### Day 1, 29.09

9.00 - 9.15 Opening

9.15-12.00 Overview of modern Quantum Chemistry (VV+KP)

12.00-13.00 Lunch

13.00-17.00 Set up of the lab. Hartree-Fock (VV). Basis Sets (VV)

17.00-18.00 Discussion

### Day 2, 30.09

9.00-12.00 DFT and TDDFT (FP)

12.00-13.00 Lunch

13.00-17.00 Single reference methods. Response theory (KP)

17.00-18.00 Poster session

### Day 3, 1.10

9.00-12.00 Electron correlation (LDV+GLM)

12.00-13.00 Lunch

13.00-16.00 Classification and analysis of excited states (FP)

16.00-19.00 Excursion

### Day 4, 2.10

9.00-12.00 New development in multiconfigurational theory (LDV, GLM)

12.00-13.00 Lunch

13.00-17.00 Multistate CASPT2 and alternative PT2 (LDV, GLM)

17.00-18.00 Discussion

19.00 - Dinner

### Day 5, 3.10

9.00-12.00 Spectroscopy. Theory and experiment (RSD)

12.00-13.00 Lunch

13.00-16.00 Environmental effects (VV)

16.00 - Conclusion and departure