

Timetable of the COST Training School 2023

"Multiscale modeling of the properties of compounds: From isolated molecules to 3D materials relevant for industrial and astrophysical applications"

19th – 22nd September 2023, Belgrade, Serbia

TUE, Sep 19	
9:30-10:15	Registration
10:15-10:30	Opening and school presentation (Sonja Grubišić and Jiří Vaníček)
10:30-11:30	María Pilar de Lara-Castells (Spain) <i>"On the computational modelling of atomic metal clusters: soft-deposition, stabilization, aggregation, oxidation, and photo-absorption"</i>
11:30-12:00	Coffee break
12:00-13:30	Majdi Hochlaf (France) <i>"Capture of carbon dioxide on functionalized gold clusters and surfaces"</i>
13:30-15:00	Lunch
15:00-16:30	Cristina Puzzarini (Italy) <i>"Quantum-chemical composite schemes in gas phase: Accurate molecular structures, spectroscopic properties and energetics"</i>
16:30-17:00	Coffee break
17:00-18:00	Vladimir Srećković (Serbia) <i>"Molecular data for confined molecular systems and astrochemical modelling"</i>
18:00-18:30	Practice (program installation)

WED, Sep 20	
9:30-10:30	Cristina Puzzarini (contd.) <i>"Quantum-chemical composite scheme in gas phase: Application to astrochemistry"</i>
10:30-11:30	Aatto Laaksonen (Sweden) <i>"Introduction to modern molecular modelling and simulations"</i>
11:30-12:00	Coffee break

12:00-12:30	Aatto Laaksonen (contd.) <i>"Introduction to modern molecular modelling and simulations "</i>
12:30-14:00	Francesca Mocci (Italy) <i>"Molecular dynamics and coarse-grained models for Bio & Soft Matters "</i>
14:00-15:30	Lunch
15:30-16:30	Sonja Grubišić (Serbia) <i>"Grand canonical Monte Carlo simulations of gas adsorption in metal-organic frameworks"</i>
16:30-17:00	Coffee break
17:00-18:30	Practice (Francesca Mocci)

THU, Sep 21	
9:30-11:00	Martin Quack (Switzerland) <i>"Molecules in motion: symmetries and primary processes between less than yoctoseconds and more than days"</i>
11:00-11:30	Coffee break
11:30-13:00	Andrei Neamtu (Romania) <i>"Sampling strategies for complex systems: enhanced-sampling simulations for the study of biomolecules"</i>
13:30-15:00	Lunch
15:00-16:30	Practice (Andrei Neamtu)
16:30-17:00	Coffee break
17:00-18:30	Miljan Dašić (Czech Republic) <i>"Computer-aided drug design"</i>

FRI, Sep 22	
9:30-11:00	Jiří Vaníček (Switzerland) <i>"Semiclassical dynamics and electronic spectroscopy"</i>
11:00-11:30	Coffee break
11:30-13:00	Practice (Miljan Dašić)
13:30-15:00	Lunch
15:00-17:00	*Poster session and cocktail
17:00	Closing addresses
17:00-20:00	Free afternoon
20:00-	Social dinner

All lectures will take place in the Lecture Hall "Belgrade panorama" of Palace Hotel (6th floor).

*Poster session will be held in the Banquet Hall, 1st floor (Hotel Palace)