

Training School

Exploring Confined Environments with Polymers, Ionic Liquids, and Deep Eutectic Solvents: Predicting Emerging Applications through Modeling and Advanced Experiments

DAY 1 - Thursday, 8 May 2025

- ◆ 08:30 – 09:00 | Registration and Welcome Coffee
- ◆ 09:00 – 09:15 | School Opening
- ◆ 09:15 – 10:15 | **Lecture: Introduction to ionic liquids**
 - Aatto Laaksonen, Stockholm University, Sweden
- ◆ 10:15 – 11:15 | **Lecture: QM/MD and NMR characterization of ionic liquids**
 - Kestutis Aidias, Institute of Chemical Physics
Vilnius University, Lithuania
- ◆ 11:15 – 11:45 | Coffee break
- ◆ 11:45 – 12:45 | **Lecture: Force field parameters and challenges in ionic liquids simulations**
 - Francesca Mocci, Cagliari University, Italy
- ◆ 12:45 – 14:30 | Lunch break
- ◆ 14:30 – 15:30 | **Lecture: Theoretical and experimental characterization of nanoparticle enhanced ionic liquids for heat exchange applications**
 - Alina Minea, Gheorghe Asachi Technical University of Iasi
- ◆ 15:30 – 16:30 | Coffee break / Poster session
- ◆ 16:30 – 18:30 | **Practical training: Calculation of NMR parameters of ionic liquids by QM/MM**
 - Kestutis Aidias, Institute of Chemical Physics
Vilnius University, Lithuania





DAY 2 - Friday, 9 May 2025

- ◆ 09:00 – 10:00 | **Lecture: Theoretical modelling and/or experimental characterization of IL/DES and confinement effects**
 - *XiaoYan Ji*, Lulea University, Sweden
- ◆ 10:00 – 11:00 | **Lecture: Harnessing Polymer Science for Effective Gene Therapy Solutions**
 - *Dragoş Peptanariu*, Petru Poni Institute of Macromolecular Chemistry, Iasi, Romania
- ◆ 11:00 – 11:30 | Coffee break
- ◆ 11:30 – 12:30 | **Lecture: Medical applications of ionic liquids**
 - *Lenuța Profire*, Grigore T. Popa University of Medicine and Pharmacy, Iasi, Romania
- ◆ 12:30 – 14:00 | Lunch break
- ◆ 14:00 – 15:00 | **Lecture: Development of force field parameters for the simulation of ionic liquids**
 - *Sonja Grubisic*, Institute of Chemistry, Technology and Metallurgy, University of Belgrade, Serbia
- ◆ 15:00 – 15:15 | Coffee break
- ◆ 15:15 – 17:00 | **Practical training: Ionic liquids simulations**
 - *Francesca Mocchi*, Cagliari University, Italy
 - *Tudor Vasiliu*, Petru Poni Institute of Macromolecular Chemistry, Iasi, Romania
- ◆ 17:00 – 18:30 | Coffee break / Poster session
- ◆ 18:30 – 19:00 | Award for best poster and Closing remarks

