

SolvATE2024

7th meeting of the SolvATE network November 25-26, 2024, Dijon

Monday, November 25, 2024

08:30-10:00	Welcome
10:00-11:00	Olga Russina (University of Rome Sapienza) "Structural solvation features in novel solvent media"
11:00-11:30	Coffee break
11:30-12:00	Mohammad Nadim Kamar (University of Rennes) "Deep eutectic solvents: properties induced by nanometric confinement"
12:00-12:30	Stella Christodoulou (University of Toulouse) "Efficient machine learning-based new tools to design eutectic mixtures and predict their viscosity"
12:30-14:00	Lunch
14:00-15:00	Judith Peters (Université Grenoble Alpes) "The many ways of biosystems for coping with extreme conditions"
15:00-15:30	Jean-Baptiste Chagnoleau (Université Côte d'Azur) "Extraction of natural compounds using sustainable solvents"
15:30-16:00	Mélissa Justin (L'Institut Agro Dijon) "Impact of scCO2 on C-phycocyanin stability in presence of polyethylene glycol"
16:00-16:30	Coffee break
16:30-17:00	Nacer Idrissi (University of Lille) "Local structure of supercritical fluids near the Widom line"
17:00-17:30	Antoine Carof (Université de Lorraine) "Fast calculation of solvation structure and thermodynamics in supercritical CO2"
17:30-18:00	Artem Shagurin (University of Lille) "Molecular dynamics analysis of interfacial properties of curcumin and supercritical fluids"
18:00-18:30	Rodolphe Pollet (Université Paris-Saclay) "Chemistry in aqueous solutions as described by ab initio molecular dynamics: case of a green catalyst under "in-water" and "on-water" conditions"



18:30-19:15

19:15-21:30

Posters

Dinner











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Tuesday, November 26, 2024

08:30-09:00	Welcome
09:00-10:00	Ellen Backus (University of Vienna) "Structure and dynamics of water at photocatalytic interfaces"
10:00-10:30	Mohammed Bin Jassar (ENS, PSL & Sorbonne Universities) "On the chemistry at oxide/water interfaces: the role of interfacial water"
10:30-11:00	Stephan Steinmann (ENS de Lyon) "Investigating organic molecules at the water-platinum interface: from single-crystal surfaces to nanoparticles via density functional tight binding"
11:00-11:30	Coffee break
11:30-12:00	Pierre Illien (Sorbonne University) "Stochastic density functional theory for ions in a polar solvent"
12:00-12:30	Florent Calvo (Université Grenoble Alpes) "Concurrent processes in the time-resolved solvation of alkali ions in helium nanodroplets"
12:30-14:00	Lunch
14:00-15:00	Alexander Lyubartsev (Stockholm University) "Multiscale modelling of biomolecules at inorganic surfaces"
15:00-15:30	Emeline Boyer (Université Paris-Saclay) "Structure of flexible chiral molecules and unconventional solvents by vibrational circular dichroism spectroscopy"
15:30-16:00	Jean-Thomas Pouzens (University of Burgundy) "SNAr reactivity of thiophene derivatives investigated using conceptual DFT"
16:00-16:15	Meeting closing









