



### Monday, November 6, 2023

10:00-11:00	M.F. Ruiz-López : <i>hommage</i>
Iñaki Tuñón	Chemical Catalysis and Motion. Role of the Environment
11-11:30	Coffee Break
11:30-11:55	Dielectric response of interfacial and confined water
Daniel Borgis	
11:55-12:20	How the acidity of aqueous droplets and films is controlled by the air-water interface
Miguel De La Puente	
12:30-14:00	Lunch
14:00-14:45	Anti-Correlated Hydrogen-Bonds of D2O evidenced by 2D-IR spectroscopy
Johannes Hunger	
14:45- 15:10	Topological graphs and algorithmic graph theory in molecular dynamics simulations
Marie-Pierre Gaigeot	
15:10-15:35	Liquid-liquid Extraction of Strontium(II) by a Crown Ether: the effects of Acidity and Concentration on Interface Crossing investigated by PMF Simulations
Alain Chaumont	
15:35-16:00	Second harmonic scattering of highly concentrated electrolyte: measurement of the screening length
Julien Duboisset	
16:00-16:30	Coffee Break
16:30-16:55	Simulating divalent ions-rich systems: challenges and hopes
Élise Duboué-Dijon	
16:55-17:20	On analytical theories for conductivity and self-diffusion in concentrated electrolytes
Pierre Illien	
17:20-17:45	Electrochemistry at the interface formed between two immiscible aqueous electrolyte solutions
Gregoire Herzog	
17:40-19:00	Posters
19:00-22:00	Dinner

### Tuesday, November 7, 2023

9:30-10:15	Molecular level characterization of multiphase processes relevant to the atmosphere
Céline Toubin	
10:15-10:40	Kinetic and mechanistic study of the reactions of NO <sub>3</sub> radical with two unsaturated aldehydes: 2- and 3-methyl-2-butenals
Jean-Claude Rayez	
10:40-11:10	Coffee Break
11:10-11:35	Determination of Total Vapor Pressure and Surface Tension of Deep Eutectic Solvents (DES) and conventional green solvents
Sophie Fourmentin	
11:35-12:00	Solvent influence on the ortho-metallation of s-tetrazine
Paul Fleurat-Lessard	
12:00-12:30	GDR Meeting
12:30-14:00	Lunch
14:00-14:25	Molecular dynamics investigation of the influence of surfactants with differently charged headgroups on the surface propensity of bromide
Rawan Abouhaidar	
14:25-14:50	Exploring the Interactive Mechanisms of Bioglasses through an Advanced Multiscale Technique during the Initial Immersion Stages
Amira Ghneim	
14:50-15:15	Self-assembling Of Biomolecules For The Development Of Emergent Biomaterials
Sara Catalini	
15:15-15:45	Closing word