



## 4<sup>èmes</sup> Journées Plénières du GDR SolvATE en partenariat avec le GDR Hydrates de gaz

Le 9 et 10 décembre 2021 – Amphi de l'Institut Chevreul -Lille

### 09/12/2021 08h30- 12h10 : Solvation and Interfaces/surface, nanoconfined media

08h30-08h50: Welcome

08h50-09h20 Pal Jedlovszky, [Eszterházy Károly University, Eger, Hungary](#)

*Contribution of the different molecules and moieties to the surface tension in aqueous surfactant solutions*

09h20-09h40 Denis Morineau, [IPR, Université de Rennes 1, France](#)

*Confining deep eutectic solvents in nanopores: insight into thermodynamics and chemical activity*

09h40-10h00 Richard Asamoah Opoku, [PhLAM, Université de Lille, France](#)

*Relativistic quantum embedding calculations of halogenated species adsorbed at the air-ice/liquid interface and bulk layer*

10h00-10h20 Ari Paavo Seitsonen, [ENS Paris, France](#)

*Simulation into the solvation and spectroscopic characterisation of 3-hydroxyflavone in various solvents*

10h20-10h50 Posters + Coffee Break

10h50-11h10 Florent Real, [PhLAM, Université de Lille, France](#)

*Nuclear recycling process: the new extracting molecules bring new challenges for molecular modelling*

11h10-11h30 Kamalesh Damodaran, [CEA Marcoule, France](#)

*Deciphering the non-linear impact of Al on chemical durability of silicate glass*

11h30-11h50 Porwal Vishal Kumar, [LPCT, Université de Lorraine, France](#)

*Vibrational properties of organic and biological molecules nanoconfined within layered double hydroxides*

11h50-12h10 Alekos Segalina, [LPCT, Université de Lorraine, France](#)

*Modeling the effect of ionic additives on the energetics of p-type DSSC: the case of Dye-sensitized NiO interface*

**09/12/2021 14h00-17h30 : Solvents in Chemistry towards a sustainable future**

**14h00-14h30** [Yaocihuatl Medina-Gonzalez](#), LOF, Université de Bordeaux, France  
*Solvent Engineering for chemical processes engineering (Video Conference)*

**14h30-14h50** [Emilie Bertrand](#), IETN, Université de Rennes 1, France  
*Caractérisation des Solvants Eutectiques Profonds (Deep Eutectic Solvent ou DES) en spectrométrie de masse en mode d'ionisation Cold-Spray (CSI)*

**14h50-15h10** [Corinne Lagrost](#), ISCR, Université de Rennes 1, France  
*Polyphenols in Deep Eutectic Solvents. Towards modulation of their antioxidant capacity and long-term stability*

**15h10-15h30** [Agilio Padua](#), ENS Lyon, France  
*Solvation in ionic liquids and DES using polarizable simulations*

**15h30-16h00** Posters + Coffee Break

**16h00-16h30** [Margarida Costa Gomes](#), ENS Lyon, France  
*Reactive separations using porous ionic liquids*

**16h30-16h50** [Carine Michel](#), ENS Lyon, France  
*Surface state of heterogenous Ru catalysts in liquid water under gas phase environments*

**16h50-17h10** [Daniel Borgis](#), ENS Paris, France  
*Ion-induced long-range orientational correlations in diluted aqueous electrolytes: What do second harmonic scattering experiment measure?*

**17h10-17h30** [Adriaan van den Bruinhorst](#), ENS Lyon, France  
*Thermodynamics of Mixing for Eutectic Solvents: Choline Chloride + Water/Diol*

**17h30-18h30** Réunion du bureau du GDR

**10/12/2021 8h30-11h50 : Solvation in systems with interest in the biological and pharmaceutical field and for food processing**

**08h30-9h00** [Damien Laage](#), ENS, Paris, France  
*Aqueous interfaces: dynamics, dielectric properties, and chemical reactivity*

**09h00-09h20** [Emeline Dudognon](#), UMET, Université de Lille, France  
*Investigation by Dielectric Relaxation Spectroscopy and Molecular Dynamics simulations of the influence on amorphous Terfenadine dynamics of strongly Hydrogen-bonded water molecules*

**09h20-09h40** [Marie Plazenet](#), LIPhy, Université Grenoble Alpes, France  
*Heterogeneous Microscopic Dynamics of Intruded Water in a Superhydrophobic Nanoconfinement: Neutron Scattering and Molecular Modeling*

**09h40-10h00** [Akos Gyorgy Juhasz](#), LASIRe, Université de Lille, France  
*Creating three dimensional biopolymer matrices for biomedical purposes*

**10h00-10h30** Posters + Coffee Break

**10h30-10h50** [François-Xavier Legrand](#), [Université Paris-Saclay, France](#)

*Solvants eutectiques profonds pour le traitement topique de maladies infectieuses : toxicité et perspectives*

**10h50-11h10** [Pierre Fouilloux](#), [AgroSup Dijon, Université Bourgogne Franche-Comté, France](#)

Using low-field NMR relaxometry to reveal slow dynamics and structure in polygalacturoate hydrogels

**11h10-11h30** [Luisa Roca Paixao](#), [UMET, Université de Lille, France](#)

*When residual water influences the cocrystallization output: the carbamazepine and tartaric acid case*

**11h30-11h50** [Salma Soussi](#), [ICM, Université Bourgogne Franche-Comté, France](#)

*Molecular Modeling for Pyrrolidine: Using Computational Chemistry Techniques Associated with Experimental study*

## **10/12/2021 14H00- 16H20 : Recent advances in Gas Hydrates : fundamentals to applications**

**14h00-14h20** [A. Desmedt](#), [ISM, Université de Bordeaux, France](#)

*Hydrates de gaz: des recherches allant du génie des procédés à l'astrophysique et aux géosciences en passant par les sciences moléculaires (Video conference)*

**14h20-14h50** [C. Cuadrado-Collados](#), [LMA, University of Alicante, Spain](#)

*Methane hydrate formation in the confined space of porous materials for gas storage (Video Conference)*

**14h50-15h20** [M. Ciulla](#), [University G. d'Annunzio of Chieti-Pescara, Chieti, Italy](#)

*Some recent advances on technological applications of gas hydrates*

**15h20-15h40** [S. Zafar](#), [PhLAM, Université de Lille, France](#)

*CO<sub>2</sub> hydrates as an alternative solution to water desalination and greenhouse gas mitigation*

**15h40-16h00** [B. Chazallon](#), [PhLAM, Université de Lille, France](#)

*Gas hydrates: characterization and properties probed by micro-Raman spectroscopy*

**16h00-16h20** [D. Broseta](#), [LFC, Université de Pau et Pays de l'Adour, France](#)

*Microscopic observations of gas hydrate growth processes (Video conference)*

**16h20** Discussion sur les interactions entre les deux GdR et clôture des Journées