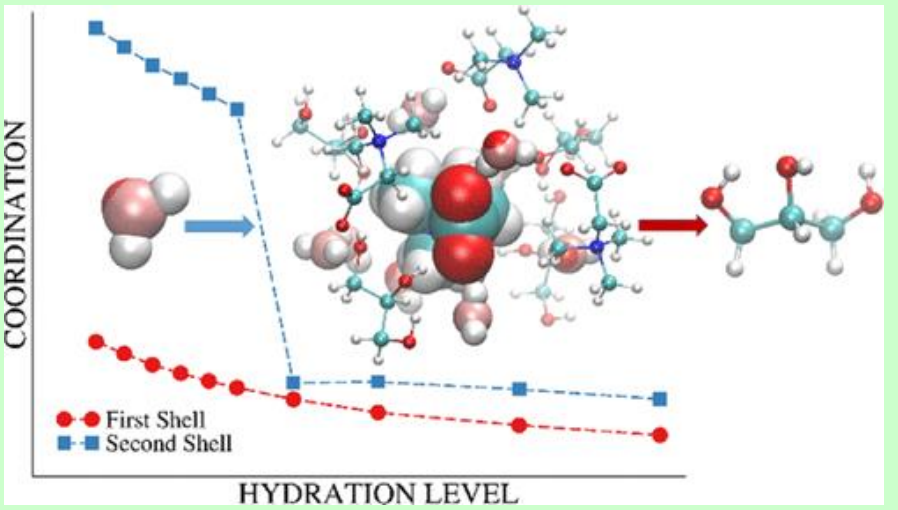
NEWSLETTER

JANUARY - OCTOBER 2022

Ongoing work - Structure and Dynamic Properties of a Glycerol–Betaine Deep Eutectic Solvent: When Does a DES Become an Aqueous Solution?

Deep eutectic solvents (DESs) are an emerging class of green solvents, with a wide spectrum of potential applications, whose properties may be further tailored through the addition of water. In this work, the authors studied, through molecular dynamics, the influence of water on the properties of a betaine–glycerol–water (B:G:W) DES (1:2:ζ; ζ = 0 to 100), aiming at getting insight into the structural and dynamic crossover between a DES and an aqueous solution. The density, shear viscosity, and diffusion coefficients are found to exhibit a non-linear dependence of ζ, similar to that observed for the solvation layers' composition. Each Gly and Bet are replaced, respectively, by ∼3 and ∼5 water molecules, with the highest rates of depletion being found for Gly around Bet and Gly around Gly. Above ζ = 7 (70 mol %; 29.5 wt %), a major structural transformation occurs, with the complete disruption of the second Bet-Gly solvation layer and the formation of a new second layer at a shorter distance, accompanied by a sudden change in the rate of increase of the components' diffusion. Nonetheless, opposite to other DES, the results indicate a smooth crossover between a DES and an aqueous solution.



Structure and Dynamic Properties of a Glycerol–Betaine Deep Eutectic Solvent: When Does a DES Become an Aqueous Solution? Hugo Monteiro, Alexandre Paiva, Ana Rita C. Duarte, and Nuno Galamba. ACS Sustainable Chem. Eng. 2022, 10, 11, 3501–3512.

CryoDES wins ERC Proof of Concept grant

The CryoDES project, which aims to use natural eutectic systems for cryopreservation, received, recently, the green light from the European Research Council (ERC), which approved a 18-month Proof of Concept grant. The aim is to complete the development and commercialization of a new cryoprotectant based on the use of natural deep eutectic systems, which is cheaper, safer, and less toxic than the current and widely used cryoprotectant (DMSO). The applications can go from research purposes to medicine and cell therapies, enabling a completely disruptive approach to cryopreservation methodologies.

Participation in conferences

- 14th ENQO & 7th ENQT - 14th National Organic Chemistry Meeting and 7th National Medicinal Chemistry Meeting
- ISGC 2022 - International Symposium on Green Chemistry
- 5th ASPIC – 5th Portuguese Association for Cancer Research International Congress
- 2nd Chem&Biochem – 2nd Chem & Biochem Students Meeting
- IMRC 2022 - XXX International Materials Research Congress
- EuChemS 2022 - 8th EuChemS Chemistry Congress
- BTP 2022 - Biosystems in Toxicology and Pharmacology – Current challenges
- ESAT 2022 – 32nd European Symposium on Applied Thermodynamics 2022
- 9th ICGC – 9th IUPAC International Conference on Green Chemistry

Publications

- "Structure and Dynamic Properties of a Glycerol–Betaine Deep Eutectic Solvent: When Does a DES Become an Aqueous Solution?" – *ACS Sustainable Chem. Eng.*
- "DES as phase change materials in solar thermal power plants: Energy and Exergy analyses" - *Molecules*
- "Extraction of bioactive compounds from cannabis sativa L. flowers and/or leaves using deep eutectic solvents" - *Front. Nutr., Sec. Nutrition and Food Science Technology*
- "Use of natural DES as new cryoprotectant agents in the vitrification of mammalian cells" - *Scientific Reports*
- "Extraction of Biocompatible Collagen From Blue Shark Skins Through the Conventional Extraction Process Intensification Using NADES" - *Front. Chem., Sec. Green and Sustainable Chemistry*
- "Investigation of carbon dioxide solubility in various families of DES by the PC-SAFT EoS" – *Front. Chem.*
- "Fractionated extraction of polyphenols from mate tea leaves using a combination of hydrophobic/ hydrophilic NADES" – *Curr. Res. Nutr. Food Sci.*
- "Selective terpene based THEDES against colorectal cancer" - *Eur J Pharm Biopharm*
- "Current methodologies for the assessment of DES toxicology: challenges and perspectives" - *J. Mol. Liq.*
- "Assessment of deep eutectic solvents toxicity in zebrafish (Danio rerio)" – *Chemosphere*
- "Assessing the influence of betaine-based natural Deep Eutectic Systems on Horseradish peroxidase systems" - *ACS sustainable Chem. Eng.*

1st DES.Solve PhD student

Filipa Santos was the first student to finish PhD in DES.Solve group. The defense took place on the 8th of July and the thesis was entitled "Exploring anti-tuberculosis drugs through green solvents for effective treatment of tuberculosis".

Outreach

DES.Solve group continues to receive students from several ages, countries, academic degrees and institutions. One of the major outreach events was "EXPO FCT NOVA", to encourage high school students to follow the areas of science and engineering. FCT NOVA received more than 5000 students, that had access to more than 160 activities. DES.solve was present with the activity "The sugar that wanted to be a liquid".

NOVA Sustainability Week

This event brings together several Schools of NOVA University, and Prof. Ana Rita Duarte, as representative of the start up Des Solutio, was invited to participate in the discussion panel "Innovation and Community", to discuss the sustainability as a factor of competitiveness in innovation.

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