

PhD in CHIMICA INDUSTRIALE E INGEGNERIA CHIMICA / INDUSTRIAL CHEMISTRY AND CHEMICAL ENGINEERING - 39th cycle

PNRR 118 PNRR Research Field: HYDROPHILIC AND HYDROPHOBIC EUTECTIC SOLVENTS AND EUTECTOGELS FOR SUSTAINABLE CHEMISTRY

Monthly net income of PhDscholarship (max 36 months)

€ 1400.0

In case of a change of the welfare rates during the three-year period, the amount could be modified.

Context of the research activity

Motivation and objectives of the research in this field

The need for cleaner and sustainable chemical processes is constantly stimulating the research of alternative solvents - neoteric solvents - with sustainable environmental profiles, especially as far as the release of volatile organic compounds (VOC) in the atmosphere is concerned. Deep eutectic solvents (DES) stand out as an emerging class of compounds fulfilling these requirements. DES are binary mixtures of an H-bond donor (HBD) and a H-bond acceptor (HBA) leading to a non-ideal system characterized by a depression of the melting point larger than predicted by solution thermodynamics. The network of interaction at the base of the local structuration of DES and the technology related to DES are emerging topics of interest, according to the exponential growth of related scientific publications. Firstgeneration DES are typically composed of a salt - choline chloride is the archetypical example – and a molecular Hbond donor, e.g. urea, diols, etc. More recently, the socalled Type V DES, binary systems of two molecular components mainly hydrophobic, stood out as disruptive systems for extraction of added value chemicals from complex matrixes, vehiculation of chemicals and environmental remediation. Finally, in the last few years, the easy formation of supramolecular eutectogels composed of DES and low molecular weight gelators was demonstrated and it is being systematically investigated.



	The ease of preparation, the benign sustainability profile and the virtually infinite technological applications of those systems call for a deeper knowledge of their intermolecular interactions, solvation and transport properties. This is even more important in light of possible technology transfer in hot sectors such as drug delivery, biomass valorization, environmental remediation, solvometallurgic recovery of critical raw materials from spent electronic devices, etc. The PhD programme here proposed starts from the consolidated experience and scientific background of the proponents in the field. The main goals are to explore new DES from natural components (NADES), from pharmacologically active ingredients (Therapeutic DES of THERADES), the obtainment of a variety of eutectogels, the characterization of the systems in terms of intermolecular interactions, rheology, solvation properties, extraction and release capability. The research will be carried out with an interdisciplinary approach and with international
	collaborations.
Methods and techniques that will be developed and used to carry out the research	The experimental section will be made of a) preparation of the DES and eutectogel; b) structural and dynamic characterization of the systems, c) applications to drug delivery and extraction. The techniques and facilities will be: organic chemistry lab, advanced NMR methods, vibrational spectroscopies, scattering methods (SAXS and SANS), thermal methods and rheology, release kinetics. In the course of the project, according to the possible successful applications, LCA and green metrics will be applied. The PhD candidate will be in contact with experienced researchers in those fields outside the expertise of the proponent research group within some national and international collaborations.
Educational objectives	1 Acquire the state-of-the-art of the DES research international panorama 2 Get used to preparation and testing of DES and eutectogels 3 Acquire a good level of confidence in physical methods of characterization, mainly state-of-the-art NMR spectroscopy

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	4 Design suitable applications and testing of the most promising systems5 Learn a multidisciplinary way of doing research
Job opportunities	The technology of DES is rapidly spreading out also due to the low costs associated to their preparation, use and recycle, and the performance highlighted so far. This allows one to foresee a growing interest of the industries to this technology, especially in the accomplishment of the green transition. Additionally, the applications covered in this PhD programme - from drug delivery to extraction of reusable products from waste - are of strategic interest in the current economic scenario.
Composition of the research group	1 Full Professors 1 Associated Professors 2 Assistant Professors 1 PhD Students
Name of the research directors	Prof. Andrea Mele

Contacts

Additional support - Financial aid per PhD student per year (gross amount)	
Housing - Foreign Students	
Housing - Out-of-town residents (more than 80Km out of Milano)	

Scholarship Increase for a period abroad		
Amount monthly	700.0 €	
By number of months	0	

National Operational Program for Research and Innovation	
Company where the candidate will attend the stage (name and brief description)	
By number of months at the company	0
Institution or company where the candidate will spend the period abroad (name and brief description)	University of Burgos - ICCRAM Universidad de Burgos, Centro de I+D+I. Plaza Misael Bañuelos s/n 09001 Burgos (Burgos) Spain https://www.ubu.es/english-version
By number of months abroad	6

Additional information: educational activity, teaching assistantship, computer availability, desk availability, any other information

Individual budget for research (5.700 euro): 1st year: 1.900 euro; 2nd year: 1.900 euro; 3rd year: 1.900 euro

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Teaching assistantship (availability of funding in recognition of supporting teaching activities by the PhD student): there are various forms of financial for activities of support to the teaching practice. The PhD student is encouraged to take part in these activities within the limits allowed by the regulation.