



UNIONE EUROPEA
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TABLE 3 – PhD Programme MATHEMATICAL AND PHYSICAL SCIENCES

THE PhD PROGRAMME	
Administrative location	University of Udine - Department of Mathematics, Computer Science and Physics (DMIF) – via delle Scienze 206, 33100 Udine, Italy (+39 0432 558400).
Associated location	-
Location for training, teaching and research activity	Teaching and other training activities will take place primarily at the administrative programme location or in other locations of the University of Udine. The research program will be mainly developed, with reference to the assigned scholarship, at one of these locations: administrative location, enterprise
Coordinator	Prof. Alberto Giulio Marcone (alberto.marcone@uniud.it)
Programme duration	3 years
Curriculum	-
Programme website	https://www.dmif.uniud.it/dottorato/smf

ADMISSION REQUIREMENTS	
Required degree	Italian Laurea (before DM 509/99) or Italian Laurea Specialistica/Magistrale (ex DM 509/1999 and Decree DM 270/04). Foreign degrees and titles: refer to art. 3 and 4 of the Call.
Knowledge of the following foreign language	English

DOCUMENTS AND TITLES TO BE ATTACHED TO THE APPLICATION FOR ADMISSION	
Compulsory documents (Art. 5 of the Call)	<ol style="list-style-type: none"> 1. Certification or self-certification (refer to art. 5 paragraph 5 of the Call) of the academic title needed for admission to the PhD programme (with candidate's grade and highest possible grade) and certified list of the exams (with candidate's grades, average grade, highest possible grade) passed during the Italian first level (bachelor) and the Laurea Specialistica/Magistrale programmes or during the Italian programmes ante D.M. 509/99 or during the foreign academic programmes; 2. Curriculum vitae et studiorum, dated and signed; 3. Copy of a valid identity document (citizens of countries not belonging to the European Union a copy of a valid passport, comprehensive of the pages containing the holder's photo, personal details, passport number, date and place of issue, date of expiry); 4. Master thesis ("Tesi di Laurea") associated to the degree/title providing access to the PhD programme. Applicants who are not graduated on the expiration date of this Call can submit an extended abstract in place of the complete thesis, in Italian or English language, signed by the thesis Supervisor (between 15,000 and 25,000 characters, spaces included); 5. A research project, dated and signed, developed in accordance with the description of the research topic (Thermodynamic characterization and software development for the prediction of the interaction between organic groups and green solvents), which highlights the contribution that the applicant can offer to the development of it (approximate limit 10,000 characters, spaces included, in English language); 6. Motivation letter from the applicant explaining the reasons for admission to the PhD programme, dated and signed (between 1,500 and 2,500 characters, spaces included).
Optional documents (Art. 5 of the Call)	<ol style="list-style-type: none"> 1. Publications (max 3); 2. Letters of reference (max 2) written by university professors, scientific researchers or other experts in the field (art. 6 of the Call).
All documents must be presented exclusively in PDF format, dated and signed by the candidate.	

SELECTION COMMITTEE	
Appointed Members	Federico Fogolari – Associate Professor – University of Udine Paolo Giannozzi – Associate Professor – University of Udine Lorenzo Gianni Santi – Associate Professor – University of Udine
Alternate Members	Alessandra Corazza – Associate Professor – University of Udine

ADMISSION

GENERAL COMPETITION (art. 8 of the Call for Applications)

Positions available: 1



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Detailed description	N.	Funding	Annual gross amount	Period abroad	Period in enterprise (identified by the Univ. of Udine)	Research topic
Positions WITH SCHOLARSHIP: 1	1	National Operational Program (PON) Research and Innovation 2014-2020 "Education and research for recovery – REACT-EU" (M.D. 1061/2021) and University of Udine	€ 15.343,28	max 6 months optional	min 6 - max 12 months mandatory	1.1 Green Topic "Thermodynamic characterization and software development for the prediction of the interaction between organic groups and green solvents" (PON RI 2014/2020 Axis IV Action IV.5)

Competition procedure and test schedule

Evaluation of qualifications and oral examination.

For the evaluation of applicants' attitude for scientific research and their knowledge to develop the topic of interest, the Selection Committee can attribute up to 100 points to each applicant: max 30 points to the titles and max 70 points to the oral examination. The applicant is admitted to the interview if his/her qualifications receive at least 15 points. The oral examination is passed with at least 49 points. The applicant is eligible for the PhD programme if he/she passes the oral examination. Only for eligible applicants, the points attained in the oral examination will be added to the points of the qualifications.

Scholarships are assigned according to the provisions of art. 10 of the Call.

DATE FOR THE PUBLICATION OF THE ADMITTED APPLICANTS TO THE INTERVIEW: within November 2, 2021

DATE FOR THE PUBLICATION OF THE FINAL RANKING LIST: within November 11, 2021

Foreign language that can be used for examination	Italian or English	
Evaluation Criteria of qualifications <i>During the preliminary meeting the Selection Committee may establish sub-criteria for the evaluation</i>	Curriculum vitae et studiorum and Scientific publications	10
	Title and average grade of exams and Thesis/Abstract	10
	Research project and Applicant's letters (Motivation letter + Letters of reference)	10
Oral examination	Interview about titles, previous career and research project also aimed at understanding the applicant's knowledge about fundamental topics in computer science, mathematics and/or physics. Reading and understanding a short scientific text in English.	
Calendar of the oral examination	Date	November 3, 2021
	Time	4:30 pm
	How to conduct the examination	The oral examination will be held online (MS Teams)
	Based on the number of applicants, the oral examination may take more than one day. Applicants must exhibit a valid ID.	

Research Topics Description

Research topic 1.1: Thermodynamic characterization and software development for the prediction of the interaction between organic groups and green solvents

The use of solvents in industrial chemical reactions is massive and the search for "green" solvents with less impact on the environment is a research area in continuous development. The understanding at the molecular level of the thermodynamics of the solvation of different chemical groups in these solvents is still little developed due to the difficulty of the problem characterized by an enormous number of degrees of freedom, with extensive correlations and indistinguishable molecules.

The characterization of the thermodynamics and the development of software for the prediction of the interaction of organic groups with green solvents will provide essential tools for reasoning about the reactivity in these solvents.

The project will have impact on:

- Innovative production processes with high efficiency and for industrial sustainability;
- Innovative and environmentally friendly materials;
- Technologies for biomaterials and biobased products and Biorefineries.

The goal is to provide the same tools commonly available for molecules in aqueous solvent. The expected results are the understanding and the ability to predict the effect of green solvents on the chemical-physical properties, such as solubility,



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ionization equilibria and the effects on the entropy of solutes. These properties determine the possibility of using a given solvent for chemical reactions or even to separate and purify solutes. The methodologies are those of molecular simulation and free energy calculations. Through the comparison with the experimental data the models will be refined and specific simulation and analysis protocols will be developed. Understanding the solvation of different molecules in different solvents of interest for green chemistry will lead to the development of predictive software.

Research activities to be carried out in the company and degree of involvement of the same in the definition of the training path:

Development of simulation and analysis protocols on high-performance computing systems (HPC) in which the company is an international leader. Development of software packages dedicated to the prediction of physico-chemical properties for green solvents.

Expected results and repercussions of the research activity for the enhancement of the PhD student's skills with reference to the sector of intervention:

The PhD student will learn how to set up research in the simulation field and will acquire the theoretical and practical tools necessary for the development of software for the prediction and simulation of reactions in various green solvents, such as water, ionic solvents, supercritical fluids and solvents of biological origin.