DOCTORAL PROGRAMME
IN
CHEMICAL SCIENCES

Director prof. Anna Maria Papini

XLI cycle – academic year 2025/2026

SCIENTIFIC AREA	
ADMINISTRATIVE OFFICE	Department of Chemistry "Ugo Schiff" (DICUS)
WEB	www.dottoratoscienzechimiche.unifi.it
CURRICULA	**1.** Chemistry **2.** Science for the Conservation of Cultural Heritage
	POSITIONS AVAILABLE: 14 Positions with Scholarship: 14 Positions without Scholarship: *not available*
RANKING LIST FOR STANDARD POSITIONS SCHOLARSHIPS AVAILABLE: 2	Funded by Department of Chemistry "Ugo Schiff" (DICUS) Progetto Ministeriale "Dipartimenti Eccellenti 2023-2027" 58503_DIPECC_23_27 C.U.P. B97G22000740001 Dipartimento di eccellenza 2023-2027
RANKING LISTS FOR POSITIONS WITH SPECIFIC RESEARCH TOPICS SCHOLARSHIPS AVAILABLE: 12	**1** - Funded by Department of Chemistry "Ugo Schiff" (DICUS) **Thematic:** "Computational Design of Magnetic Nanographenes by Ab Initio and AI Methods." **Project description:** The PhD scholarships are funded by the Italian Science Fund starting grant 'IPAWNS' (FIS 2 Call). Understanding how to control the magnetic exchange interaction through the application of an electric field in open-shell nanographene-based materials would pave the way for quantum computing based on paramagnetic molecules. The research activity will focus on the development of ab initio methods to model the electronic and magnetic properties of NGS, and on the optimization of high-throughput protocols for the simulation of a large number of molecular systems using quantum chemistry software. The researcher will therefore have to develop methodologies to i) generate new structures and ii) automate the computation of the magnetic properties of interest, in particular the exchange interaction. The integration of post-Hartree Fock (post HF) and density functional theory (DFT) approaches will be required, together with advanced techniques to model spin-electric couplings. Isolated and periodic approximations will be used to derive the spin Hamiltonian parameters, in particular the exchange interactions. The generated database will then be used to train predictive AI models to predict and generate new systems with the desired magnetic properties. The researcher will have the opportunity to participate in all research phases, thus being exposed to an interdisciplinary context. In particular, he/she will be able to participate in the development of predictive deep learning models to rapidly predict the behavior of

	new NGS structures, and in the creation of generative deep learning models to design NGS geometries optimized for maximum spin-electric coupling. **Responsible scientific referent**: Dr. Matteo Briganti Funded by FIS2_2023_BRIGANTI IPAWNS - In Silico Prototypes for Addressable and Scalable Molecular Quantum Gates CUP B53C24009560001 **1** - Cofunded by University of Florence and CSGI Consorzio Interuniversitario per lo Sviluppo dei Sistemi a grande interfase **Thematic:** "Green" surfactants, hydro- and organo- gels and nanogels for the confinement and controlled delivery of chemical compounds and actives." **Project description**: In Cultural Heritage preservation, controlled delivery of chemical compounds onto the surface of works of art is crucial, in particular for the selective and safe removal of soil, aged coatings, and vandalism. Surfactants and gels are the main class of materials to build systems for the controlled delivery of compounds. In particular, the PhD will study novel glycerol-based surfactants and hydro- or organo-gels and nanogels of synthetic or biopolymers, to confine and deliver solvents or aqueous solutions onto the target surfaces (soiled/coated paints, murals, etc.). The work will include the formulation, physico-chemical characterization and application of the new systems, which can impact also on other fields where controlled delivery is essential (detergency, drug-delivery, etc.). **Responsible scientific referent**: Prof. David Chelazzi **1** - Cofunded by University of Florence and CIRMMP Consorzio interuniversitario risonanze magnetiche di metalloproteine paramagnetiche **Thematic:** "Development of new polarizing agents for the Dynamic Nuclear Polarisation applied to solid-state NMR." **Project description**: The DNP (Dynamic Nuclear Polar Polarization) solid-state NMR is one of the most promising NMR techniques emerged in the last decades, enhancing the NMR signal up to a factor 500. This has revolutionized NMR investigation, for example, by enabling the structural determination of molecules present on the material surface. The polarizing agent, a specific paramagnetic radical that enables the transfer of magnetization to nuclei, plays a key role in DNP making possible the signal enhancement. In this project, the student will develop new polarizing agents, combining computational simulations to design new molecules and test them by DNP NMR experiments with applications in the investigation of innovative materials. **Responsible scientific referent**: Prof. Moreno Lelli **9 – Cofunded by University of Florence and Department of Chemistry "Ugo Schiff" (DICUS)** **Thematic 1**: "Computational investigation of magnetic nanographenes adsorbed on surface." **Project description:** The research project, funded by the Italian Science Fund - FIS 2 Call, aims to develop systems based on graphene molecular structures absorbed on the surface that present unpaired electrons (Nanographene Spins) and tunable exchange interactions. These open-shell systems are promising components for quantum logic gates. The aim of the research activity is to rationalize the magnetic coupling as a function of their molecular structure in such a way as to be able to guide the synthesis and development of new structures. It will be necessary to design, consistently with the need for accuracy of the results, different types of multiscale in silico experiments based on the periodic density functional theory. **Responsible scientific referent**: Dr. Matteo Briganti

	Cofunded by FIS2_2023_BRIGANTI IPAWNS - In Silico Prototypes for Addressable and Scalable Molecular Quantum Gates CUP B53C24009560001 **Thematic 2**: "Sustainability, electrodeposition and metal recovery in Made in Italy and for the production and use of hydrogen." **Project description:** Sustainability in Electroplating processes that reduce the quantities of metal used are a rapidly evolving, multidisciplinary subject of study that involves various sectors of Chemistry and beyond. Research includes theoretical simulations, study of electrodeposition processes with innovative techniques with the simultaneous use of analytical techniques for the evaluation of corrosion resistance and compositional, morphological and structural variation of the deposits. Research in the field of metal recovery from any production waste or from any waste will be central and strategic for the circularity of the industrial processes studied but also for the supply of metals and their use in the energy field. **Responsible scientific referent**: Prof. Massimo Innocenti Cofunded by INNOCENTIAMPERE - INNOCENTI-ITALFIMET21 - INNOCENTI-3M **Thematic 3**: "Multivalent and biocompatible scaffolds for the presentation or recognition of tumor antigens." **Project description:** Development of multivalent scaffolds, including pre-organized scaffolds, which will be functionalized with antigens, including saccharidic antigens or their mimetic. The bioconjugates so obtained will be characterized and studied as immunostimulants and for their binding properties vs. specific lectins. **Responsible scientific referent**: Prof. Cristina Nativi Cofunded by DM737_BANDO_SENIOR_MERMAID_CRISTINANATIVI CUP B55F21007810001 - NATIVI_AIRC_IG2021_ID25762 CUP B99J21025210007 - CRISTINANATIVIPRIN2015 CUP B96J15002080001 **Thematic 4**: "Development of multilayered hybrid molecular architectures for optical devices." **Project description:** The proposed activity will focus on the development and the chemical and physical investigation of molecular and inorganic multilayered thin films using advanced methods, including both wet-chemistry approaches and physical vapor deposition techniques. These properties will be studied through advanced microscopy and photoemission spectroscopy. A key activity will be optimizing the deposits for realizing optical cavities functioning as lasing units, within the framework of the APACE, HORIZON-EIC PATHFINDER CHALLENGES 2023. The project adopts a bio-inspired approach to develop a novel sunlight-pumped laser, leveraging biological principles. This involves the deposition of biomolecular and dye-based systems as active media, along with metal thin films serving as cavity mirrors. **Responsible scientific referent**: Prof. Matteo Mannini Cofunded by CELARDOAPACE24 project APACE — HORIZON-EIC-2023-PATHFINDERCHALLENGES-01 CUP B93C24000830006 at Dipartimento di Fisica e Astronomia **Thematic 5:** "Chirality-induced spin selectivity in nanostructured molecular systems." **Project description:** The research activity will be framed in the ERC Synergy Grant CASTLe (www.castle.unifi.it) and will involve the design, realization, and characterization of nanostructured molecular systems to investigate the phenomenon of Chirality-Induced Spin Selectivity. Preparation methods will include self-assembly on surface from solution, as well as thermal deposition and electro-spray. The characterization will be performed by using transport and magnetotransport

	experiments on different scales (microscopic devices, nanojunctions, scanning probe microscopies) combined with spectroscopic techniques of different types (optical, photoelectron, and magnetic resonance spectroscopies). **Responsible scientific referent**: Prof. Roberta Sessoli Cofunded by SESSOLI_ERC-2022-SYG_CASTLE - Chirality and spin selectivity in electron transfer processes: from quantum detection to quantum enabled technologies CUP B97G21000120006 Progetto UE Horizon Europe **Thematic 6:** "Study of the mechanism of action of metal compounds with pharmacological activity by multi-omics approaches." **Project description:** Metal compounds with pharmacological activity are generally characterized by complex mechanisms of action involving multiple biomolecular targets. To characterize the mode of action of such substances at the cellular level, it is necessary to integrate sophisticated and information-rich methods of analysis, such as some well-established omics methods. This research project will be based on the analysis of transcriptomic, proteomic and metabolomic data related to the treatment of cancer cells with cytotoxic metal compounds and will aim at their interpretation in mechanistic terms using advanced bioinformatic methodologies. The hypotheses formulated will then be validated by specific cellular and molecular assays. **Responsible scientific referent**: Prof. Luigi Messori Cofunded by MESSORI_AIRC_IG2021_ID26169 CUP B99J21023960007 **Thematic 7:** "Synthesis of glycomimetics as antibacterials and in the treatment of protein misfolding diseases." **Project description:** The project involves the study of stereoselective reactions for the synthesis of nitrogenated glycomimetics (amino and/or iminosugars) starting from sugars and other natural compounds. The study will focus on the synthesis of mono- and bicyclic structures containing a β-lactam functionality or lipophilic chains for the selective interaction with lysosomal enzymes. The first compounds will be tested as antibacterial or antifungal agents, while the second ones will be evaluated in particular as chaperones and/or activators of glucocerebrosidase, an enzyme involved in Gaucher and Parkinson's diseases. For both applications, derivatives decorated with photosensitive units will also be developed to trigger the biological activity when needed. **Responsible scientific referent**: Prof. Prof. Francesca Cardona Cofunded by: GOTI PRIN 2010L9SH3K_006 CUP B11J12002450001 CARDONACRF20180942 CUP B94I18007230008 – CARDONABANDOSALUTE2020 CUP G14I18000270002 TELETHON_GSA22P001_Clemente CUP B97G22000780007 PRIN2022_CARDONA CUP B53D23015580006 EROGAZIONE_liberaleAIG_Clemente and MORRONEAMMEC2019 CUP B54I19004090007 at Department NEUROFARBA **Thematic 8:** "Responsive nanoparticles embedded into gels: novel tools for the analysis of artworks." **Project description:** The study of complex substrates in cultural heritage and forensic field, requires robust and validated solutions, to identify minor components, degradation products, bio-contaminants, also contributing to solve issues about provenance, falsification and security of art objects. Novel hybrid NPs@gel composites designed to selectively interact with substances to be analysed will be used as sponges for the sampling of analytes and/or for the delivery of active sensing molecules, such as plasmonic or fluorescent units, or active biomolecules such as enzymes. After the adsorption of the analytes, the material can be stably stored without losing or

	damaging it. Both hydro- and organo-gels will be considered as interacting matrix. **Responsible scientific referent**: Prof. Rodorico Giorgi Cofunded by PRIN2022_GIORGI CUP B53D23013630006 and by CSGI Consorzio Interuniversitario per lo Sviluppo dei Sistemi a grande interfase. **Thematic 9:** "Proteins as targets for metal-based anticancer drugs: from molecular interactions toward therapeutic applications." **Project description:** The multidisciplinary project aims to elucidate the role of the molecular interactions between target proteins and cytotoxic metal-based drugs with anticancer activity, i.e. Pt(II)-, Au(I)- and Au(III)-based compounds, commercial or synthetized in this study. The combination of mass spectrometry, circular dichroism, and resonance Raman and UV-vis absorption spectroscopies, allows one to study the drug complexes with i) cytochrome c and its physiological complex with cardiolipin, directly involved in the cellular apoptotic process; ii) serum albumin, abundant in blood plasma, as a model drug-carrier. The evaluation of the biological activity of the protein/drug complexes selected according to the most promising results, discloses a potential opportunity for new therapeutic applications. **Responsible scientific referent**: Dr. Federico Sebastiani Cofunded by BECUELIL13 - BECUCCICDR17 - MESSORI_AIRC_IG2021_ID26169 CUP B99J21023960007
STUDY/RESEARCH PERIODS ABROAD	6 months
DOCUMENTS REQUIRED FOR THE ADMISSION (under penalty of exclusion)	● Copy of the Identification Document ● Self-certification for qualifications obtained in Italy (laurea triennale, specialistica o magistrale o ciclo unico) with list of exams taken, credits and related grade, title of the thesis and graduation mark (using this **template** or similar forms containing the required information) ● Qualifications obtained abroad (Bachelor's and Master Degrees or combined cycle Degree) with a list of all exams taken, credits and related grade, rating scale, title of the thesis and graduation mark *The same documentation except for the final mark must be submitted by those who will graduate within the 31/10/2025*
DOCUMENTS REQUIRED FOR THE EVALUATION	**MANDATORY** ● Curriculum vitae et studiorum including a typewritten self-declaration for each qualification obtained (bachelor and master, or combined cycle degree) reporting the date of first enrollment, exams passed with number of credits, weighted and arithmetic average of the marks ● One Research project for EACH fellowship the candidate shall compete (each one shall be congruent to each specific thematic (up to 13 projects) ● Title and extended abstract of the M.Sc. thesis (maximum five A4 sheets) **OPTIONAL** ● List of scientific publications ● List of qualification documents including periods spent abroad for study or research mobilities ● Up to a maximum of two reference letters

<table>
<tr><td>RESEARCH PROJECTS</td><td>Each research project shall be written in English in no more than 12,000 characters including spaces, including abstract (no more than 500 characters including spaces), introduction and references, in order to assess the applicant’s aptitude to research.
The candidate can apply for several rankings by submitting a specific research project for each ranking (clearly state the reference to the chosen thematic).</td></tr>
<tr><td>INTERVIEW MODE</td><td>In person
(In the application form candidates may ask to conduct the interview remotely)

The interview can be conducted in the English language.
If it is presented in Italian, the interview shall include an assessment of English language proficiency.</td></tr>
<tr><td>EVALUATION MARKS</td><td>
<table>
<tr><th>parameter</th><th>minimum score</th><th>maximum score</th></tr>
<tr><td>Curriculum vitae et studiorum, research project, publications, other qualification documents</td><td>40/120</td><td>60/120</td></tr>
<tr><td colspan="3">Applicants who obtain a mark of at least 40/120 in the evaluation of the above parameters will be admitted to the interview</td></tr>
<tr><td>Interview: discussion of the research project, publications and qualification documents</td><td>40/120</td><td>60/120</td></tr>
<tr><td colspan="3">Eligibility is achieved with a minimum score of 80/120</td></tr>
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</td></tr>
<tr><td>FURTHER INFORMATION ON THE EXAMINATION</td><td>The interview will be focused on each research project. The discussion with the committee members will be based on the scientific background of the candidate also in the field of the research performed for the Bachelor and Master thesis or for equivalent titles. Each research project must be presented by maximum 8 slides. Moreover, the candidate can present 1 slide to introduce the CV.</td></tr>
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EXAMINATION SCHEDULE			
	DATE	**TIME**	**PLACE**
INTERVIEW	July 16th 2025	08:30 a.m.	Biblioteca “Parrini” Via della Lastruccia, 13 Sesto Fiorentino (Florence)
The list of the candidates admitted to the interview and the final ranking will be published at the page **PhD courses**			