

Scheda di Programma

Per l'attivazione nell'ambito del Corso di Dottorato di ricerca in SCIENZE CHIMICHE del seguente Programma di ricerca, a valere sulle risorse di cui al DM n. 351/2022, relativamente alla seguente Misura:

M4C1- Inv. 3.4 "Didattica e competenze universitarie avanzate" → **Dottorati dedicati alle transizioni digitali e ambientali.**

M4C1- Inv. 4.1 "Estensione del numero di dottorati di ricerca e dottorati innovativi per la pubblica amministrazione e il patrimonio culturale". In particolare:

Dottorati PNRR

Dottorati per la Pubblica Amministrazione

(selezionare l'area/le aree CUN di riferimento del programma tra quelle di seguito indicate)

- Area 09 – Ingegneria industriale e dell'informazione
- Area 11 – Scienze storiche, filosofiche, pedagogiche e psicologiche
- Area 12 – Scienze giuridiche
- Area 13 – Scienze economiche e statistiche
- Area 14 – Scienze politiche e sociali

Dottorati per il patrimonio culturale

(selezionare l'area/le aree disciplinare/i e la tematica del programma tra quelle di seguito indicate)

- Area 01 – Scienze matematiche e informatiche **Tematica** – Informatica, patrimonio e beni culturali
- Area 02 – Scienze Fisiche **Tematica** – Fisica applicata al patrimonio culturale e ai beni culturali
- Area 03 – Scienze chimiche **Tematica** – Chimica, ambiente, patrimonio e beni culturali
- Area 04 Scienze della Terra **Tematica** – Georisorse minerarie per l'ambiente, il patrimonio e i beni culturali
- Area 05 Scienze Biologiche **Tematica** - Ecologia, patrimonio e beni culturali
- Area 08 – Ingegneria civile e Architettura **Tematiche** 1) Architettura, ambiente antropizzato, patrimonio e beni culturali 2) Architettura e paesaggio 3) storia dell'architettura; 4) Restauro; 5) Pianificazione e progettazione dell'ambiente antropizzato; 6) Design e progettazione tecnologica dell'architettura
- Area 10 Scienze dell'antichità, filologico-letterarie e storico -artistiche **Tematiche** 1) Archeologia; 2) Storia dell'arte; 3) Media, patrimonio e beni culturali
- Area 11 – Scienze storiche, filosofiche, pedagogiche, psicologiche **Tematiche** 1) Biblioteconomia; 2) Archivistica; 3) Storia del patrimonio e dei beni culturali 4) Paleografia; 5) Estetica; 6) Didattica dell'arte; 7) pedagogia dell'Arte
- Area 12 - Scienze giuridiche **Tematica** Diritto del patrimonio culturale
- Area 13 - Scienze Economiche e statistiche **Tematiche** 1) Economia della cultura e dell'arte 2) Economia e gestione delle imprese artistiche e culturali; 3) Statistica e Data Analytics per i beni culturali
- Area 14 Scienze Politiche e sociali **Tematiche** 1) Sociologia dei beni culturali 2) sociologia dell'ambiente e del territorio

❖ **Titolo del Programma di ricerca:** Novel halogen-free hybrid molecules as flame retardants for composite materials.

❖ **Descrizione** (MAX 5000 CARATTERI SPAZI ESCLUSI):

The flammability of polymeric materials limits their application in numerous fields, such as transportation, construction, electric and electronic sectors, where the risk of fire (probability of ignition) and its level of danger (consequences that it may have) are of particular relevance. It is not possible to develop a completely non-combustible organic material able to maintain the features of ease of processing, low specific weight and low cost, typical of polymeric materials. However, the addition of flame retardants (FRs) to the polymeric materials, can reduce the ease of ignition and/or the speed of combustion propagation, in order to increase the time lapse needed to extinguish fire. FRs are chemical compounds that are added or incorporated to a wide range of materials, even for industrial use, to reduce their flammability. They are often used in cables, wires, construction products, insulation materials, fabrics, automotive and interior components, paints and coatings and in general, in plastics. About half of the currently developed polymeric materials must have a basic level of fire protection hazard. Among the different additives for polymers, FRs represent the highest economic value and are subject to constant research development, due to the continuous increase in the severity of rules governing the use of materials in applications where fires can occur. In addition to the more traditional flame retardant additives, newer additives and others still under development are continuously designed taking into account their potential advantages and possible defects, not only in relation to their ability to improve the flame retardant behavior of polymers, but also for other issues such as, for example, their interaction with the environment, the ease of recovery and cost.

Due to their distribution, these chemicals are persistent pollutants and can pollute water, soil, food or become airborne and thus can bioaccumulate in humans. In particular, halogenated FRs, which occupy an important part of the world market, are known to exert serious effects on human health (e.g. dioxin) by causing thyroid disorders, cancer and neurological dysfunctions.

Therefore, there is an increasingly urgent need to develop new halogen-free molecules, able to produce a powerful flame retardant effect at low loading concentrations in the polymer matrix with the ideal characteristic of simultaneously inhibiting the combustion process, both in the condensed phase and in the phase gaseous and without altering the mechanical properties of the polymer. This research project aims to give new solutions, by developing hybrid molecules, able of synergistically retard the flame, both in gaseous phase and/or in condensed phase, highly versatile in terms of structural modifications and with tunable chemical and physical properties such as hydrophobicity, thermal properties and stability, in order to respond to specific requests for different types of materials and to the industrial demand. Efficient synthetic methods will be developed for the preparation of new hybrid compounds containing organophosphoric systems coupled to triazole systems able, to release nitrogen, after pyrolysis processes, and/or sulfenamide systems characterized by a bond between a divalent sulfur atom and a trivalent nitrogen atom which, by homolytic cleavage, can generate aminyl and thiyl radicals able to provide excellent FR properties to the polymeric substrate. The project proposal therefore plans to perform the following realization objectives: - Synthesis and characterization of new hybrid molecules with flame retardant activity; - Incorporation of the synthesized molecules and/or the suitable formulations with additives in the polymer matrices and chemical, physical and mechanical characterization of the composite materials. Consequently, the synthetic methodologies that will be developed primarily plan to start from low-cost and easily available compounds and, above all, the use of solvents with low environmental impact or green solvents, such as deep eutectic solvents (DESS) that can also guarantee the recovery of intermediates and final reaction products for simple filtration. Another goal is the optimization of effective synergistic formulations based on hybrid molecules/inorganic additives. The polymeric matrices used for the project are polypropylene and polyethylene which represent the most used materials in the world, but unfortunately also the polymers that burn more easily. The obtainment of ideal FR that can be used in composites based on PP and PE without modifying their mechanical properties and that can receive certification according to the ASTM D 3801 standard, represents one of the most important results in terms of project realization for application in industrial field. The research carried out within the project will be reported in scientific publications and communications at conferences that will ensure the dissemination in the international scientific community of the most significant results for the advancement of knowledge; A further planned result of the project is represented by the training of young researchers (PhD students) with knowledge in fields ranging from synthetic chemistry to the study of the chemical-physical properties of composite materials, namely a typically professional profile of great interest for academic research, as well as for the manufacturing and fine chemicals industries.

❖ **PERIODO IN IMPRESA – CENTRI DI RICERCA – P.A.:**

Il Programma di ricerca sarà svolto in collaborazione con il seguente soggetto:

Ragione sociale: _____
Sede legale: _____
Rappresentante legale: _____

L'ente sopra citato ospiterà il dottorando beneficiario della borsa finanziata sulle risorse del DM 351/2022 per n. _____ mesi (**min 6 max 12**) nel corso del dottorato.

❖ **PERIODO ALL'ESTERO:**

Il Programma di ricerca prevede un periodo all'estero di n. 6 mesi (**min 6 max 18**) presso la seguente istituzione:

Departamento de Química Orgánica, Universidad de Córdoba (Spain)

dichiara inoltre che il presente programma è conforme al principio "di non arrecare un danno significativo" (DHS) ai sensi dell'art. 17 del regolamento (UE) 2020/852 in coerenza con gli orientamenti tecnici predisposti dalla Commissione Europea (Comunicazione della Commissione Europea 2021/C58/01) e garantisce il rispetto dei principi orizzontali del PNRR (contributo all'obiettivo climatico e digitale c.d. tagging, il principio della parità di genere e l'obbligo di protezione e valorizzazione dei giovani).
