Fundamental Field:

Chemical engineering

Habilitation Thesis

Non-Covalent Interactions and Self-Organization in Advanced Materials. From Supramolecular Principles to Functional Nanocomposites

Candidate

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2026

Abstract

The habilitation thesis entitled "Non-Covalent Interactions and Self-Organization in Advanced Materials. From Supramolecular Principles to Functional Nanocomposites" summarizes the candidate's main research directions, professional achievements and scientific contributions, integrating them into a unified perspective on the role of non-covalent interactions in the design, functionalization and understanding of advanced materials.

The first section presents the motivation for elaborating the habilitation thesis and the candidate's main professional and scientific achievements. It highlights the development of his academic and research activity, his participation in scientific projects, the publication of articles in the fields of polymeric materials, nanocomposites, sensors, biodegradation and the valorization of bio-based resources, as well as his contributions through books, scientific communications, conferences, educational activities and science outreach. The professional activity is presented as a progressive development from analytical chemistry and the study of functional compounds towards complex polymeric materials, hybrid systems, carbon nanomaterials and applications relevant to the circular economy and environmental monitoring.

The motivation of the thesis derives from the need to interpret the behaviour of modern materials not only through their chemical composition, but also through the way their components interact at the molecular, supramolecular and interfacial levels. In polymer composites, bio-based materials, elastomeric systems, carbon nanocomposites and active layers for sensors, the final properties are often governed by interfaces. These interfaces act as active zones in which interactions take place through hydrogen bonding, π–π interactions, van der Waals forces, dipole–dipole interactions, electrostatic interactions, hydrophobic effects or adsorption processes. Although these interactions are individually weaker than covalent bonds, their cooperative effect can lead to significant changes in the stability, degradation, morphology, conductivity, moisture sensitivity or mechanical response of materials.

The second section represents the core part of the thesis and builds a scientific narrative based on the author's published works. This section is organized into six chapters that follow the transition from the fundamental concepts of supramolecular chemistry to concrete applications in functional materials.

The first chapter introduces non-covalent interactions as the foundation of supramolecular chemistry, emphasizing the importance of molecular recognition, interfacial organization and host–guest phenomena in understanding complex materials. These principles provide the conceptual framework for interpreting the behaviour of additives, fillers, polymers and nanomaterials in multicomponent systems.

The second chapter discusses self-assembly and self-organization, distinguishing between thermodynamically determined and kinetically controlled processes. In the case of polymers and composites, self-organization occurs not only

at the molecular level, but also at the level of phase domains, filler networks, biomass aggregates or conductive structures formed by nanocarbon. This perspective is relevant for interpreting styrenic block copolymers, in which the polystyrene domains can act as physical junctions, while the elastomeric segments provide the flexibility and processability of the material.

The third chapter analyses the role of non-covalent interactions in the stabilization and degradation of polymers. The candidate's works on oxidation, irradiation, recycling potential and the thermal behaviour of polymers show that degradation is not a process determined exclusively by the covalent structure of the macromolecular chain. It is influenced by molecular architecture, phase organization, the presence of additives, chain mobility and the interactions between components. Additives and fillers can therefore be interpreted as supramolecular modifiers that influence oxidation kinetics, thermal stability and the response to processing or ageing.

The fourth chapter is dedicated to bio-based systems and to the interactions at the bio–polymer interface. Research on polymer composites containing biomass, microalgae, cyanobacteria, cellulose-rich materials or biogenic mineral filler shows that biomass is not a simple inert addition. Owing to its content of proteins, polysaccharides, lipids, pigments and hydroxyl, carboxyl, amine or carbonyl groups, biomass can interact with the polymer matrix and can influence dispersion, stiffness, thermal behaviour, water absorption, biodegradation and the stability of the material. From this perspective, the bio–polymer interface becomes an active zone in which the natural chemistry of biomass is translated into material functionality.

The fifth chapter addresses carbon nanostructured systems and interface chemistry in polymer nanocomposites. Studies on oxidized carbon nanohorns, carbon nano-onions, graphene oxide and their composites with polymers such as PVP or PVA demonstrate that the electrical and sensing properties are governed by the self-organization of conductive networks, by the surface chemistry of the nanocarbon and by interactions with water molecules, alcohols or other analytes. Particularly in the vicinity of the percolation threshold, small changes in the distance between conductive particles can generate large variations in electrical resistance, which explains the efficiency of these materials in resistive sensor applications.

The sixth chapter provides an integrative discussion of supramolecular concepts across different scales, from discrete molecular interactions to interfacial architectures and emergent properties. The thesis emphasizes that the functional properties of advanced materials arise through the cooperation between chemical structure, morphology, interface, component mobility and the external conditions of processing or use. Interfaces are thus presented as functional zones in which chemistry is converted into material property.

In the final part, the Conclusions and future perspectives highlight the fact that non-covalent interactions and self-organization constitute essential principles for the development of advanced materials. Future directions target the design of more sustainable polymer composites, bio-nano-hybrid systems, sensors with improved sensitivity and selectivity, adaptive materials, systems with dynamic response, and integrated assessments of life cycle, safety and ecotoxicological impact. Particular attention is given to the possibility of correlating experimental data obtained through spectroscopy, thermal analysis, microscopy, electrical measurements, mechanical testing, degradation studies and environmental assessments, in order to build predictive models and to accelerate the development of functional materials.

Overall, the habilitation thesis proposes a coherent vision of advanced materials, in which supramolecular chemistry becomes a common language for interpreting stabilization, degradation, compatibilization, dispersion, self-organization and functionality. By integrating the results published in the fields of polymers, bio-based composites, carbon nanomaterials and sensors, the work demonstrates that non-covalent interactions are not merely secondary phenomena, but fundamental mechanisms through which material components organize themselves and generate emergent properties. The thesis thus constitutes both a synthesis of the scientific activity carried out and a platform for the future development of functional, sustainable and intelligent materials.