



# From Vibrational Dynamics to Functional Materials: The Scientific Legacy of Giuseppe Zerbi

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As a recently established forum dedicated to the broad and interdisciplinary fields of photochemistry and spectroscopy, *Photochemistry and Spectroscopy* seeks not only to disseminate cutting-edge research but also to recognize the scientists whose vision and achievements have shaped these disciplines over the decades. Scientific progress is built upon the contributions of pioneering researchers whose ideas, methods, and discoveries continue to influence contemporary investigations. For this reason, the journal is committed to highlighting the work and legacy of outstanding figures whose contributions have had a lasting impact on the development of spectroscopy, photochemistry, and related areas of molecular science.

The present volume constitutes the second part of a collection of invited contributions celebrating the scientific achievements of Professor Giuseppe Zerbi, one of the most influential spectroscopists of his generation. Throughout a career spanning more than six decades, Professor Zerbi has made seminal contributions to vibrational spectroscopy, theoretical and computational spectroscopy, polymer science, conjugated materials, nonlinear optics, carbon-based materials, and numerous other areas where spectroscopy serves as a powerful tool for understanding molecular structure and properties. His work has profoundly influenced both the theoretical foundations and practical applications of modern spectroscopic methods, and many of the concepts and approaches introduced by him remain central to current research.

The articles gathered in this collection reflect the breadth of Professor Zerbi's scientific interests and the remarkable influence he has exerted on several generations of researchers. They bring together contributions from colleagues, collaborators, former students, and scientists whose own work has been inspired, directly or indirectly, by his ideas and achievements. Taken together, these papers illustrate not only the diversity of fields touched by his research but also the vitality and continuing relevance of the scientific questions that he helped to formulate.

We first became aware of Professor Zerbi's work during our undergraduate studies, long before we had the opportunity to interact with other scientists associated with his school of spectroscopy. Even at that time, his name was already synonymous with scientific rigor, intellectual creativity, and a profound understanding of molecular spectroscopy. Over the years, our admiration for the breadth and depth of his contributions has only grown. What is perhaps even more remarkable is that, after such an extraordinarily productive career, Professor Zerbi continues to follow scientific developments with enthusiasm and intellectual curiosity, remaining an active and inspiring presence within the spectroscopic community. His enduring commitment to science serves as a powerful example for both established researchers and younger generations entering the field.

Giuseppe Zerbi was a pioneer in molecular spectroscopy, particularly infrared and Raman spectroscopy, ranging from the development of theoretical models for spectral interpretation to applications in materials science. His scientific career at the Politecnico di Milano began in the 1960s, when the discoveries of Nobel Laureate Giulio Natta sparked intensive research into the structure of semicrystalline polymers at the Institute of Industrial Chemistry. From that time onward, polymer spectroscopy played a central role in Zerbi's research. In close



collaboration with his wife, Mariangela Gussoni, who developed the theoretical and computational aspects of this work, and with a team of young physicists and chemists, he made fundamental contributions to the study of the vibrational dynamics of crystalline polymers. He laid the foundations for interpreting spectroscopic signals associated with crystallinity and conformational defects, providing evidence of intermolecular interactions in crystals, chain folding at the surface of crystalline lamellae, and conformational disorder in pre-melting and melting phases. The basic concepts developed by Zerbi continue to underpin the use of vibrational spectroscopy for the structural analysis of polymers.

At the beginning of his career, modeling in vibrational spectroscopy was focused primarily on the development of empirical force fields and the study of vibrational normal modes. Zerbi contributed extensively to these areas, particularly through studies of small organic molecules and phonons in the crystalline phases of various polymers. In contrast, the investigation of infrared absorption and Raman scattering intensities was pursued by only a few research groups worldwide. In this field, in 1980, Zerbi established a research program devoted to the study of electronic charge distribution in molecules and polymers through the construction of empirical electro-optical parameters derived from measurements of IR and Raman band intensities.

In the study of polymer spectra, he also promoted investigations of anharmonic phenomena, such as Fermi resonance, highlighting their fundamental impact on intensity patterns.

It was precisely the study of spectroscopic intensities that, from the mid-1980s onward, convinced Zerbi of the necessity of introducing theoretical and computational chemistry among the tools employed by the theorists in his group. Quantum-chemical calculations, particularly those based on Density Functional Theory (DFT), still provide the theoretical framework and interpretative support for spectroscopists trained within his school.

His early experience, during a period of relatively limited computational resources that constrained the accuracy of theoretical simulations, taught him the importance of comparing theoretical predictions with spectroscopic observables. In particular, he recognized that trends in key parameters across structurally related classes of molecules and materials constituted a powerful means of validating theoretical models.

Giuseppe Zerbi was always attentive to and curious about the most innovative developments in organic materials. He possessed the ability to foresee how vibrational spectroscopy could be used to reveal and explain the distinctive properties of new materials. This vision is reflected in his numerous contributions to the study of conducting polymers, a field in which he consistently sought to bridge molecular-level approaches and solid-state physics. Particularly emblematic was his introduction of the Effective Conjugation Coordinate (ECC) in the study of polyenes and conjugated systems. The development of ECC Theory established a connection with the Amplitude Mode Theory developed by theoretical physicists to explain the spectroscopic response of doped polyacetylene.

As soon as the first studies on molecules exhibiting nonlinear optical properties appeared, Zerbi realized that, as in conducting polymers, the presence of conjugated  $\pi$ -electrons would impart distinctive features to their vibrational spectra. Experimental and theoretical investigations of these systems, carried out in collaboration with groups synthesizing novel nonlinear optical materials, led to the establishment of relationships between nonlinear optical response and IR and Raman activity. These studies paved the way for predicting nonlinear optical properties from vibrational spectroscopic measurements. In parallel, Zerbi worked extensively on photochromic organic materials, establishing a highly productive collaboration with the Brera Astronomical Observatory. Together, they conceived and developed applications of photochromic materials for astronomical instrumentation.

His experience in Raman spectroscopy of conjugated systems also enabled Zerbi to make original contributions to the study of graphene, carbon nanotubes, and graphene molecules.

On the experimental side, he introduced Surface-Enhanced Raman Scattering (SERS) techniques into his laboratory and contributed to the development of methods for producing and testing nanostructures functioning as SERS-active substrates, as well as to the interpretation of the spectral differences between SERS and normal Raman.

While pursuing rigorous theoretical research and promoting computational studies of advanced materials, Zerbi never ceased to cultivate spectroscopic applications in emerging areas of materials science. In particular, he devoted significant effort to the diagnosis of material aging and degradation and to conservation issues in the field of cultural heritage. For several years, he organized a specialized school at the Politecnico di Milano that contributed significantly to disseminating the use of innovative characterization methods within this field.

It is therefore a privilege for *Photochemistry and Spectroscopy* to dedicate this collection of papers to Professor Giuseppe Zerbi. We hope that the contributions assembled here and in the previous issue of the journal (first part of the full collection of articles dedicated to Giuseppe Zerbi) will not only honor his remarkable scientific legacy but also inspire future advances in the fields to which he has devoted his career.

This collection represents only a small, yet thoroughly deserved, tribute to his long, fruitful, and highly influential career as a scientist, spectroscopist, and academic.

#### **Conflicts of Interest**

The authors declare no conflict of interest.

#### **Use of AI and AI-Assisted Technologies**

No AI tools were utilized for this paper.