



Editorial

# The Context of the *Spectroscopy Journal*—Today and in the Future

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## 1. Introduction

As a scientific discipline at the intersection between physics and chemistry, spectroscopy is historically grounded in curiosity-driven experiments of splitting sunlight into its spectral components. However, it has rapidly expanded from its philosophical beginnings to a discipline of scientific fidelity. Along the way, there have been a series of epoch-determining discoveries and refinements that have enriched our understanding of the natural world. From the early identification of the visible-to-near infrared spectrum to the intricate analysis of atomic and molecular signatures, the evolution of spectroscopy reflects, in large, the broader expansion of humanity's scientific knowledge. The seminal works of Newton, who first dispersed light [1], to the precise measurements of atomic emission and absorption lines by Wollaston, Fraunhofer, Kirchhoff, and Bunsen have laid the groundwork for today's state of the art [2].

Today, spectroscopy moves the frontiers of a multitude of scientific pursuits. It enables chemists to discover new molecules, biologists to probe cellular processes, and astronomers to analyze events in distant galaxies. Beyond that, it is instrumental in industry, contributing to advancements from pharmaceuticals to materials engineering.

It is to be expected that spectroscopic advancements will do their part to propel many fields of science and engineering into the future. With emerging technologies, such as quantum computing and artificial intelligence, alongside ever-improving spectroscopic performance, the future holds unprecedented potential for the refinement of spectroscopic methods.

This editorial aims to showcase the trajectory of spectroscopy as it continues to demystify the unknown and brings clarity to the fascinating world at the interface of light and matter.

## 2. A Short History of Spectroscopy

The nascent phase of spectroscopy can be traced back to the seminal work of Newton in the late 17th century [1]. Newton, through his methodical experimentation with prisms, unveiled the rainbow-colored spectrum inherent to sunlight. His insights may be considered the beginning of any spectroscopy, offering a method through which to analyze the nature of light.

The early 19th century saw the unraveling of more spectral features, most notably with the observations of William Hyde Wollaston [3] and his discernment of dark features within the solar spectrum. Fraunhofer's meticulous cataloging and measurement of over 500 of these lines brought a new systematic approach to spectral line analysis and hinted at the wealth of information locked behind those spectral patterns [4].

In the mid-19th century, the meaning of these spectral lines began to clarify in experimental work. The collaboration between Gustav Kirchhoff and Robert Bunsen revealed that each chemical element emitted and absorbed light of specific wavelengths, manifested as distinctive lines on a spectrum [5]. This discovery of elemental fingerprints transformed curiosity-driven spectroscopy into a systematic scientific method for identifying chemical compositions, whether in a laboratory flame or a distant star. The implications were



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profound, not just for chemistry and physics, but for the emerging field of astrophysics, providing the means to decipher the chemical makeup of stars millions of miles away.

In the second half of the 19th century, James Clerk Maxwell achieved the theoretical unification of electricity, magnetism, and light when he formalized what is now known as Maxwell's electromagnetic theory. His equations describe light as electromagnetic waves, a theoretical foundation that allowed spectroscopy to grow beyond visible-light experiments, foreseeing its expansion into regions from the deep UV to the far IR and beyond.

These pioneers, along with Planck and Einstein in the early 20th century, set the stage for the highly sophisticated spectroscopic techniques that would follow. The rigorous study of spectra became a key that unlocked the structure of molecules, the dynamics of chemical reactions, and the search for life on distant stars. The historical path from Newton's prismatic light to recent attosecond lasers and single molecule experiments reflects an extraordinary expansion of our knowledge of the universe, culminating in a detailed understanding of the quantum mechanical and complex features of matter and light.

### 3. Today's Spectroscopies

Spectroscopy, as it stands today, is a cornerstone in a multitude of scientific inquiries and industrial applications. The adaptability of spectroscopic techniques ensures their status as indispensable tools across a wide spectrum of applications.

In Chemistry, spectroscopy has become synonymous with precision and reliability for the qualitative and quantitative assessment of substances. The ability to identify molecular signatures has revolutionized our approach to chemical analysis, yielding rapid and non-invasive methods to analyze complex mixtures and trace compounds.

Physics has greatly benefited from the capabilities of spectroscopy. Whether used for solid-state physics, galactic nebula or to probe particle-particle interactions, spectroscopy has been used to test theoretical models and basic physical laws.

Biology employs spectroscopy in many forms. For example, magnetic resonance spectroscopy provides a glance into living tissues, enabling the diagnosis and study of diseases without invasive procedures. Infrared (IR) and Raman spectroscopy provide specific signatures of biological molecules, allowing for the study of biological pathways in vivo and molecular relationships critical to the processes of life.

Astronomy uncovers the nature of celestial objects with the help of spectroscopy. Astronomers determine the elemental compositions, temperatures, and densities of stars and galaxies. Such studies have enriched our knowledge of the universe and furthered our understanding of its evolution.

Environmental Science has harnessed the power of spectroscopy to monitor pollutants, greenhouse gases, and atmospheric constituents. Spectroscopic sensors are employed globally to track environmental changes, supporting a sustainable future for our planet's ecosystems.

For Materials Science, spectroscopy has been pivotal in characterizing the structure and composition of novel materials and aiding in the understanding of surfaces, e.g., in the field of nanotechnology. Spectroscopy is pivotal in studying the properties of semiconductors, dielectrics, superconductors, and plasmonic materials. New spectroscopic developments may well be the driver for future industries.

Even currently known spectroscopic techniques have expanded well beyond those used decades ago. Mass spectroscopy (MS) has evolved into tandem and time-of-flight configurations. NMR spectroscopy now operates at ultra-high fields, providing high resolutions of complex molecular structures. IR spectroscopy has grown and evolved into Fourier-transform infrared (FT-IR) techniques that capture detailed vibrational information of molecules much faster and with increased sensitivity. X-ray spectroscopy is becoming more nuanced with synchrotron radiation, as well as table-top sources. Raman spectroscopy has seen great advancements in sensitivity and spatial resolution through surface-enhanced Raman scattering (SERS), revolutionizing the detection of single molecules. Coherent

anti-stokes-shifted Raman spectroscopy (CARS) has been deployed in chemical biology with remarkable successes [6].

The current state of spectroscopy reflects a dynamically evolving field, integral to both academics and practice. With each technological advancement and methodological refinement, spectroscopy continues to extend its reach, affirming its central role in uncovering ever more materials, as well as insights into our natural and technical world.

#### 4. Future Spectroscopy

What does the future of spectroscopy hold? Spectroscopy continues to experience improvements, especially in robustness, range, and speed. Such improvements are triggered by advancements that have mainly occurred in two directions: technology and computation.

The pursuit of high-resolution spectroscopy will continue unabated, with emerging technologies enabling researchers to capture the most subtle of spectral nuances. Concurrently, autonomous high-throughput spectroscopy will transform quantitative analysis, allowing vast sample numbers to be analyzed with unparalleled speed and robustness. This dual advancement will be critical in areas such as pharmaceuticals, where rapid, detailed compound screening is essential.

The trend in miniaturizing spectroscopy will continue, with portable and handheld devices becoming more ubiquitous. This trend in spectroscopy will enable deployment to remote areas, in field settings without access to a power grid, and in rural healthcare diagnostics.

Combining spectroscopy with other techniques, such as chromatography, microscopy, and mass spectrometry, will enable scientists to derive multifaceted insights from a single investigation, correlating compositional, structural, and dynamic information.

Space exploration will reach beyond the identification of elements and minerals on celestial bodies. It will be pivotal in the search for extraterrestrial life, deciphering biosignatures on other planets and moons. On earth, the application of spectroscopies in satellites and drones will enhance our ability to monitor environmental health, track climate change, and manage our limited resources.

The intersection of spectroscopy with artificial intelligence (AI) and machine learning (ML) is perhaps among the most transformative prospects. AI algorithms will process complex spectral data at speeds beyond human capability, detecting patterns and making predictive models with a degree of precision and efficiency previously unimaginable.

As concerns computational spectroscopy, quantum phenomena will increasingly become a part of spectroscopic analysis, and this will lead to the predictive modeling of the spectral properties of materials and biologics. Machine learning, on the other hand, will provide the necessary capabilities in interpreting the large datasets that modern spectroscopy generates, thereby transforming data into actionable insights.

One can anticipate a transformative period where fundamental and technological advancements will allow for new synergies in the scientific discovery process. Hopefully, spectroscopy will not only deepen our fundamental understanding of nature but will also guide humanity toward a more responsible and sustainable way of life on earth.

#### 5. Summary and an Invitation to Contribute to the *Spectroscopy Journal*

The improvements of spectroscopic methods have not merely kept pace with the broader currents of scientific progress but have frequently acted as the catalyst, pushing the frontiers of what is observable, measurable, and, ultimately, doable.

Current spectroscopy use spans from the atomic to the astronomical, providing insights with a spatiotemporal reach over many orders of magnitude to an extent that would have been unimaginable just a few decades ago.

Miniaturization, computational power, and cross-disciplinary integration have expanded the horizons of spectroscopy beyond traditional laboratory settings. Now, equipped with portable spectrometers, scientists venture into the field, exploring environments from the deepest oceans to the outer reaches of our atmosphere and beyond, to the surfaces of other planets. This mobility has brought with it a level of accessibility to spectroscopy,

allowing for real-time decision-making in environmental science, quality control in manufacturing, and diagnostics in personalized medicine.

Spectroscopy, in its ever-evolving form, will continue to decode nature's secrets. The evolution of spectroscopy mirrors humanity's intellectual ascent as we continue to push the boundaries of scientific achievement. In this context, this journal entirely dedicated to the field of spectroscopy is more pertinent than ever. The MDPI *Spectroscopy Journal* stands as a resource to publish ongoing and forthcoming scientific explorations, discoveries, and innovations that diverse research groups in the realm of Spectroscopy will report. As such, please encourage your scientific colleagues to contribute to the *Spectroscopy Journal*.

**Conflicts of Interest:** The author declares no conflicts of interest.

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