Gap-controlled infrared method enables analysis of molecular interfaces

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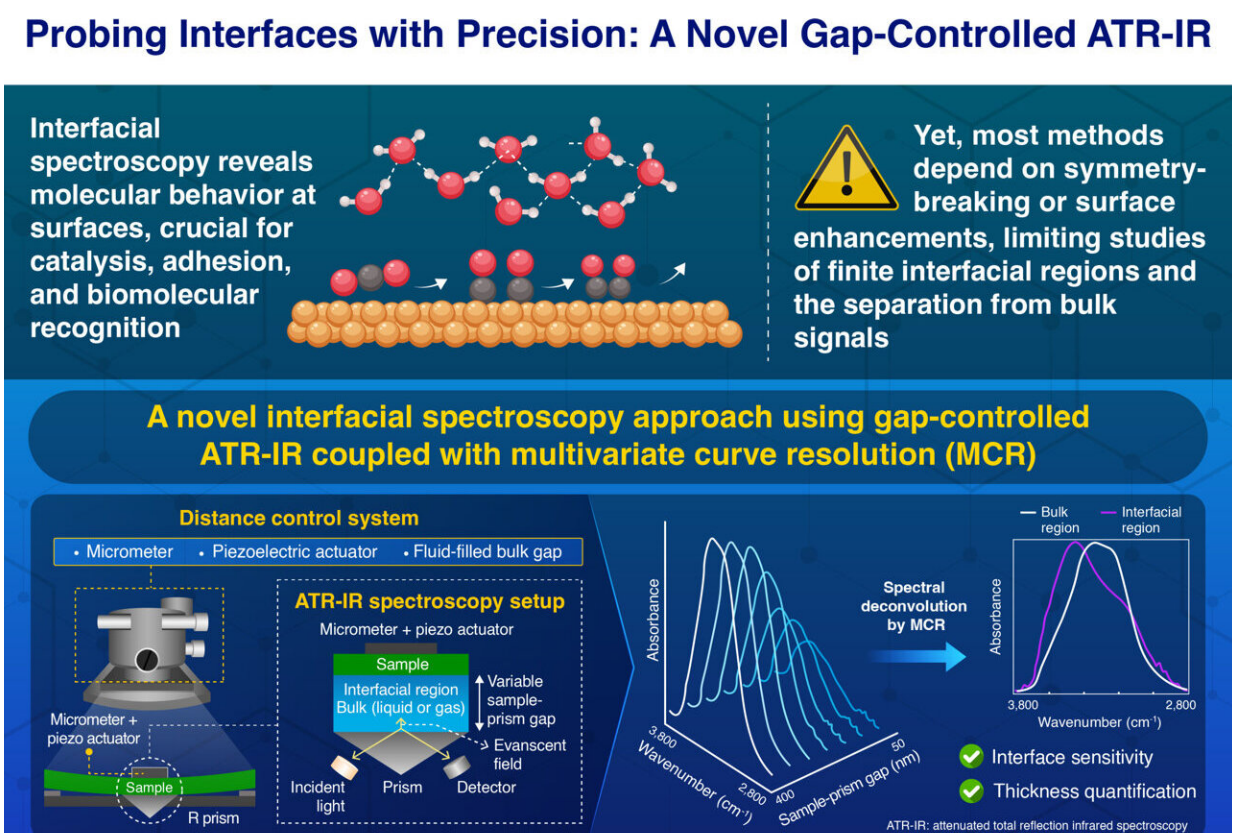

Researchers have developed a low-cost method for the analysis of interfacial molecules by combining ATR-IR with precise gap-control and multi-variate data analysis. Credit: Institute of Science Tokyo

A novel spectroscopic method developed at Institute of Science Tokyo, Japan, enables highly sensitive analysis of molecules at material interfaces, using a combination of conventional ATR-IR, precise gap-control and advanced data processing. The technique offers a low-cost alternative to conventional interfacial spectroscopy and has potential applications in material sciences, nanotechnology, and biological sciences.

Molecular interfaces—such as those found on solid surfaces, thin films, and liquid boundaries—are central to countless processes in materials science, chemistry, and biology. These interfaces influence everything from the potential field of electrochemistry to the molecular interactions in proteins and cell membranes.

But despite their importance, the study of these interfaces has remained a longstanding challenge. While some methods exist, conventional spectroscopic techniques usually fail, as the strong signals from the bulk material often overpower the subtle signals from the interface.

To address this limitation, a team of researchers from Institute of Science Tokyo (Science Tokyo), Japan, led by Associate Professor Tomohiro Hayashi from Department of Materials Science and Engineering, School of Materials and Chemical Technology, Science Tokyo, along with Graduate Student Shoichi Maeda and Team Leader Takuo Tanaka of RIKEN, developed a novel yet accessible technique called "Gap-Controlled Infrared Absorption Spectroscopy" to analyze molecular interfaces. The findings of the study were published in the journal *Analytical Chemistry* on September 13, 2025.

The approach is based on a widely used spectroscopic method called attenuated total reflection infrared (ATR-IR) spectroscopy. In ATR-IR spectroscopy, a sample is brought into contact with an infrared-transparent crystal to generate a weak "evanescent wave", which is an electromagnetic wave that selectively probes molecules at or near the surface.

However, in conventional ATR-IR, isolating the surface-specific information is often difficult due to background signals from the bulk material. To overcome this, the team introduced a distance-control mechanism to precisely control a nanometer-scale distance between the infrared crystal and the sample.

"The nanometer-scale gap allows us to vary the contribution of interfacial molecules to the spectrum," explains Hayashi.

The researchers then applied multivariate curve resolution (MCR) to the resulting series of spectral data. MCR is a sophisticated data analysis approach that mathematically separates and extracts the spectra of pure components and their concentration changes from a mixed dataset of overlapping signals. In this way, the developed method effectively filters out the background "noise" coming from the bulk material and isolates the signals of the molecular interface.

"The strength of this approach lies in its simplicity," says Hayashi. "By building on ATR-IR, which is already widely available, we eliminate the need for expensive instruments or specialized techniques to study interfacial molecules."

Furthermore, to demonstrate the scope of their method, the researchers applied the developed approach to a diverse range of systems. These included the analysis of water molecules at the surfaces of self-assembled monolayers, quartz surfaces under different pH conditions, and even polystyrene, a material widely used in cell culture dishes.

The results showed excellent agreement with two highly specialized and expensive interfacial techniques: sum frequency generation (SFG) spectroscopy and surface-enhanced infrared absorption spectroscopy (SEIRAS). This confirms that the developed gap-controlled method was not only reliable but also practical for a wide range of applications.

The implications of the research carry broad significance across multiple domains. As interfacial phenomena are central to many technologies ranging from material coatings to biomaterials and nanodevices, the accessibility of this gap-controlled ATR-IR technique could drive breakthroughs in these technologies. Additionally, since it does not rely on rare equipment or costly enhancements, it offers an affordable and attractive tool for many laboratories.

"We believe that our technique will accelerate both fundamental research and industrial applications in surface science, nanotechnology, and materials engineering," concludes Hayashi.

Looking ahead, the researchers plan to refine this technique for real-time monitoring of dynamic interfacial processes. With its unique combination of sensitivity, simplicity, and scalability, this technique offers a promising tool for researchers, opening new avenues in the hidden world of molecular interfaces.

More information: Shoichi Maeda et al, Gap-Controlled Infrared Absorption Spectroscopy: A Unique Interface-Sensitive Spectroscopy Based on the Combination of Linear Spectroscopy and Multivariate Curve Resolution, *Analytical Chemistry* (2025). DOI: 10.1021/acs.analchem.5c02765

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