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ABSTRACTS

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PLENARY

Insights from single particle spectroscopy of plasmonic nanostructures

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A surface plasmon in a metal nanoparticle is the coherent oscillation of the conduction band electrons leading to both absorption and scattering as well as strong local electromagnetic fields. These fundamental properties have been exploited in many different ways, including surface enhanced spectroscopy and sensing, photothermal cancer therapy, and color display generation. The performance of plasmonic nanoparticles for a desired application not only depends on the particle size and shape, but is tunable through nanoparticle interactions on different length scales that support near- and far-field coupling. Chemical synthesis and assembly of nanostructures are able to tailor plasmonic properties that are, however, typically broadened by ensemble averaging. Single particle spectroscopy together with correlated imaging is capable of removing heterogeneity in size, shape, and assembly geometry and furthermore allows one to separate absorption and scattering contributions. In this talk I will discuss our recent work on understanding the radiative, non-radiative, chiral, electrochemical, and mechanical properties of individual and coupled plasmonic nanostructures including the generation and transfer of hot electrons to semiconductors as well as to liquids, for applications seeking to harvest light energy with hybrid plasmonic materials.

Artificial Intelligence for Materials Science: Transforming Research Paradigms

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Materials science has been facing the problems of high system complexity, low degree of data standardization, and long research chain, which also reveals the limitations of the traditional research paradigm. AI technology is good at handling high-dimensional and multi-scale data, and is able to discover the complex correlation between parameters, which provides a possible solution to the current dilemmas of materials science research.

In this report, we propose three paradigms for materials research and development: the foundation is a Deep Fusion of Data, Models, and Compute; the core methodology is a Symbiotic Drive of Data and Knowledge; and the ultimate goal is End-to-end Materials Development. We believe that AI can equip researchers with cross-disciplinary knowledge and thinking, unleash their innovative potential, and serve as an effective tool covering the entire process from fundamental research to productization in materials science. AI may be able to bring a new future for materials science research that is “without clear understanding” but fast-moving.

Time-resolved SERS study of ultrafast plasmon driven selective excitation of adsorbate vibrational modes

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Plasmon driven photocatalysis on metal particle surface remains a subject of intense current interest. More recently, there have also been reports of plasmon or light enhanced electrocatalysis on metal electrodes, including H_2 generation and CO_2 reduction, suggesting exciting new approaches for solar fuels generation and for dynamic modulation of electrocatalysis. The mechanisms of such processes remain unclear. Many proposed mechanisms assume selective excitation of adsorbate vibrational modes and/or excited states, which leads to non-thermal chemistry by lowering activation barriers and altering reaction pathways. In this talk, I will discuss two recent studies that are aimed at understanding hot carrier induced adsorbate vibrational excitation on metal electrodes and nanoparticles.

In the first study, we use time-resolved vibrational sum frequency generation (TR-VSFG) spectroscopy to directly measure hot electron induced vibrational dynamics of adsorbates on metal electrodes. For CO chemisorbed on Au electrodes, we show that excitation of the Au electrode with visible light leads to the generation of vibrationally excited CO molecules. Detailed analysis of the time-resolved SFG spectra reveals that 1) the formation the excited adsorbates is instrument response time limited (<<100fs) and follows the electronic temperature of the hot electron, indicating the direct coupling of adsorbate vibration modes with hot electrons in the electrodes, likely through selective excitation of the frustrated rotational mode; 2) the extent of adsorbate excitation is dependent on the applied potential, suggesting possible control of hot electron chemistry with applied bias.

In the second study, we use time-resolved surface enhanced Raman spectroscopy (TR-SERS) to investigate selective excitation of adsorbate vibrational modes on metal nanoparticles. For 4-nitrothiolphenol on Au nanoparticles, the excitation of the Au plasmon band lead to selective excitation of the nitro symmetric stretching mode with negligible excitation of other modes, including nitro asymmetric stretching mode. The selective vibrational mode excitation, subsequent intramolecular vibrational energy redistribution (IVR), and photochemistry depend sensitively on the nature of the adsorbate. Ongoing studies are examining the selection rules that govern selective excitation and how the initial nonthermal distribution can compete with IVR to lead to non-thermal photochemistry.

SERS without Field Enhancement
Photons as the Carriers in Electron Transport

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The atomic limit in optical microscopy is attained in ATERS: tip-enhanced Raman scattering (TERS) carried out in the atomistic near-field (ANF), at the prototypical quantum point contact (QPC) of a cryogenic scanning tunneling microscope (STM). As in TERS, the compound optical microscope is replaced with an atomically terminated tapered plasmonic tip that serves as antenna, waveguide, and focusing lens. The paradigm shift in ATERS is that the measurements are conducted at junction gaps where tip and substrate wavefunctions overlap. Generally, the optical signal in the far-field reaches its maximum intensity in contact-mode TERS. Contact clearly precludes optical fields at the junction; coupling to the radiation field must be delegated to the antenna mode outside it. Raman scattering is now strictly driven by the optical current, whereby field enhancement plays no role. The same should hold for a large class of SERS where the molecule is in contact with its plasmonic antenna. The current-coupled tip and molecule is the scaled analog of a radio-wave (RF) antenna and transceiver, where the antenna serves as an impedance transformer that converts free-space photons into electric current, now hard-wired into the molecular electronic circuit. Quantization of transport at the QPC reduces the electric current to the conduction of intracavity (ic) photons, which can be “seen” to be confined on the terminal atom of the tip apex. Accordingly, the second-order Raman scattering reduces to the injection and back-extraction of an ic-photon from the molecular junction. It measures the nonlocal, mode-specific, vibronic conductivity of the molecular circuit along paths traced by the normal modes. In that respect, ATERS serves as the network analyzer of molecular electronics. The reciprocity in the measurements enables a complete characterization of photons in conductive media, leading to the interpretation of the DC tunneling current in STM as first-order scattering (absorption) of an ic-photon. In effect, in the ANF, there is no distinction between electron and photon microscopy. More generally, photons can be identified as the carriers in electron transport, which is, as Maxwell would have it, if we were to recognize the photon in matter as the quantum of electromagnetic displacement. In that regard, it is helpful to note that molecular circuits are inherently photonic.

The above is entirely based on direct observations afforded through ATERS.
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Plasmonic Nanogap-Enhanced Raman Scattering with Nanoparticles

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Synthesizing, functionalizing and controlling targeted metal nanostructures with a superhigh precision are the keys to the reliable and widespread use of plasmonic nanostructures in optics, nanoscience, chemistry, materials science, biotechnology and medicine. Here, I will introduce the design, synthetic strategies and characterization of a variety of different colloidal plasmonic nanogap nanostructures with strong, controllable and quantifiable surface-enhanced Raman scattering (SERS) signals – plasmonic nanogap-enhanced Raman scattering (NERS). I will then show their potential in addressing some of important challenges in plasmonics, biosensing and bioimaging, and discuss how these new plasmonic materials and platforms can lead us to breakthroughs in next-generation nanoscience and nanobiotechnology.

Quantitative SERS at the Single-Molecule Level and Its Prospects Based on Statistical Protocols

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Surface-enhanced Raman scattering (SERS) enables ultrasensitive/ultratrace detection of molecular structural information at nanometer scales, demonstrating significant application value in biological detection, electrochemistry, catalysis, environmental monitoring[1]. However, the physical processes and mechanisms underlying SERS - involving interactions between nanostructures, molecules, and light - present substantial challenges for quantification. As the concentration further drops to the fM, SERS enters the single-molecule spectroscopy measurement regime. Here, the spectral fluctuation characteristics of single molecules render spectral intensity independent of concentration variations. Consequently, traditional intensity-based quantitative approaches lose their physical foundation. By adopting SERS success probability as the observable parameter, we propose a novel physical principle for ultrasensitive SERS quantification (Figure 1). We demonstrate that probability maintains strong concentration responsiveness even at ultralow levels, achieving quantitative detection at 1 fM concentrations with single-molecule resolution[2, 3]. Furthermore, we established a sound physical foundation for the field of statistical quantitative SERS. We revealed the microscopic essence of SERS probability by correlating the measured SERS probability and the average molecule number in a spectrum[3]. The proposal of statistical distribution-based SERS provides a new technical approach for SERS quantification, paving the way for a historic breakthrough in transforming SERS from an ultrasensitive detection method into a quantitative analytical tool.

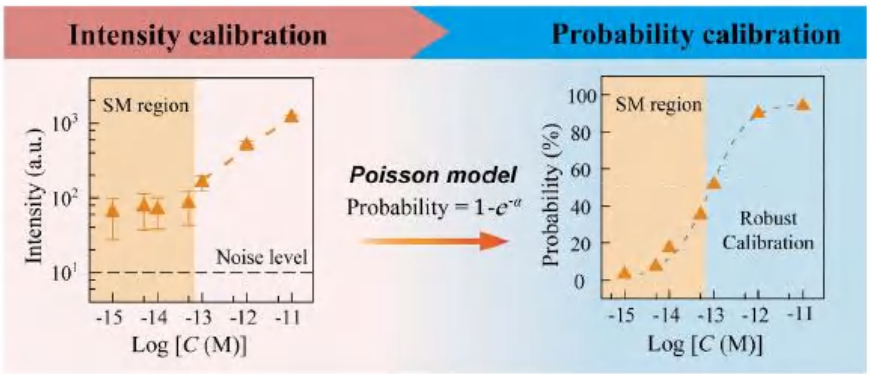

Figure 1: SERS success probability and Poisson statistical model

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KEYNOTE

Background-Free SERS for Biomedical Analysis

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Surface-enhanced Raman spectroscopy (SERS) is considered to be a highly sensitive and specific detection method, and its signal enhancement usually depends on noble metal nanoparticles (such as gold or silver particles). However, the SERS substrates have no selective signal enhancement effect on the surrounding species. Therefore, in biomedical applications, the Raman signals of the organism itself can also be amplified, and the detection signal of targets of interest is submerged in the background signals, resulting in false positives. In this abstract, we propose two background-free SERS detection strategies. By placing the detection signal in the biological Raman-silent region (1800-2800 cm^{-1}) or introducing a stimulus-responsive Raman enhancement strategy, the methods eliminate the interference from background signals, thus achieving biological Raman detection with high signal-to-background ratio. These background-free SERS strategies allow high-fidelity detection of different diseases in vitro or ex vivo, providing a new opportunity for basic biological research and clinical diagnostics.

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Functional Nanoparticles for Ultrasensitive Biodetection and Targeted Delivery

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Nanostructures with size and shape dependent plasmonic, magnetic and enzymatic properties are of tremendous potential across many disciplines spanning chemistry, materials science, photonics, and medicine. The development of plasmonic nanostructures with precisely controlled spectroscopic properties and/or multifunctional characteristics is key to their use in diverse applications. Excited localized surface plasmon resonance (LSPR) dissipates energy of incident light by the combination of Mie scattering and absorption-mediated thermal conversion, making plasmonic nanostructures compelling transducers and photo-absorbers. In particular, tailored LSPR of plasmonic nanostructures allows for spatially confining photons at sub-wavelength scales and controlling light-molecule interactions at specific wavelengths. The extraordinary signal amplification in surface-enhanced Raman scattering and metal-enhanced fluorescence offers the opportunities for sensitive and multiplexing molecular and cellular analysis for disease diagnosis. This presentation summarizes our efforts on developing functional nanostructures and integrated systems for biomarker detection and controlled delivery of therapeutic proteins.

MOF-Enhanced SERS Detection

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We realized site-selective deposition of zeolitic imidazolate framework-8 (ZIF-8) on anisotropic plasmonic metal nanocrystals, including Au nanobipyramids, nanorods, and nanostars [1,2]. ZIF-8 is selectively deposited at the ends and waist and around the entire surface of elongated Au nanobipyramids and nanorods, as well as at the sharp tips of Au nanostars. The nanobipyramid-based nanostructures with end-deposited ZIF-8 exhibit the best surface-enhanced Raman scattering (SERS) performance, implying that molecules can be concentrated by ZIF-8 at the hot spots. In addition, the SERS signal exhibits good selectivity for small molecules because of the molecular sieving effect of ZIF-8. We further introduced ZIF-8 into plasmon-coupled nanogaps [3], which has so far remained experimentally challenging. Ultrasensitive SERS substrates are fabricated through the construction of nanoparticle-on-mirror structures, where Au nanocrystals are encapsulated with a ZIF-8 shell and then coupled to a gold film. The ZIF-8 shell, as a spacer that separates the Au nanocrystal and the Au film, can be adjusted in thickness over a wide range, which allows the electric field enhancement and plasmon resonance wavelength to be varied. By trapping Raman-active molecules within the ZIF-8 shell, we show that our plasmon-coupled structures exhibit a superior SERS detection performance. A range of volatile organic compounds at the concentrations of 10^{-2} mg m^{-3} can be detected sensitively and reliably. Our studies open up a promising route for constructing plasmonic nanostructures with site-selectively deposited metal–organic frameworks, which hold enormous potential for molecular sensing, optical switching, and plasmonic catalysis.

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Nanoarray-Based SERS Rapid Detection of Trace-Level Toxic Pollutants and Drugs

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Highly toxic pollutants and drugs pose serious threats to public health as well as social harmony and stability. On-site, rapid, and highly sensitive detections are crucial for ensuring food safety and combating drug-related crimes. However, conventional techniques such as mass spectrometry are difficult to deploy for rapid field detection. Surface-enhanced Raman spectroscopy (SERS), with its high sensitivity, fingerprint identification capability, and potential for real-time analysis, offers a promising alternative for rapid on-site detection. Still, several practical challenges remain. Clearly, large benchtop Raman spectrometers are unsuitable for field use. Although portable handheld devices are commercially available, their sensitivity is limited, making trace-level detection hard to achieve. The main bottlenecks include the lack of: 1) substrates with high sensitivity and signal uniformity; 2) effective methods for capturing pollutants and extracting drugs from human bodily fluids; and 3) truly portable instruments designed for rapid on-site detection

We have developed a novel approach using ordered porous templates to fabricate nanorod array highly sensitive SERS-substrates, produced a series of such SERS substrates with uniform signal response and high sensitivity, and standardized their preparation process. We have also established standardized procedures for extracting highly toxic pollutants from contaminated food and drugs from the bodily fluids of drug users. Furthermore, a comprehensive database of drugs and toxins has been constructed, and identification software integrated with artificial intelligence algorithms has been developed. These elements—standardized substrates, extraction methods, database, and AI software—have been combined with a handheld Raman spectrometer to create an integrated portable kit. it is capable of identifying hundreds types of drugs and toxins, enabling rapid on-site screening and playing a vital role in investigating food poisoning and drug-related crimes.

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Metal/Alloy Nanoparticle-Based Biosensing and Catalysis

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Surface-enhanced Raman scattering (SERS) is a powerful analytical technique for probing interfacial phenomena with exceptional molecular specificity and sensitivity. This talk highlights our recent advances in two major research directions, biosensing and catalysis, centered on the design and application of metal and alloy nanoparticle systems. We have developed low-cost, portable SERS biosensing platforms based on plasmonic and magnetic nanoprobes integrated with printed fibrous substrates, optimized for the sensitive detection of cancer biomarkers and virus particles [1-2]. These systems leverage antibody bioconjugation and nanoprobe-induced "hot spot" formation to amplify Raman signals. Our studies demonstrate multiplexed SERS detection with excellent selectivity and high sensitivity. We further establish clinical relevance by detecting coronavirus spike and nucleocapsid proteins, along with heat-inactivated and original virus samples. The combination of high-surface-area fibrous substrates and low-volume sample delivery enables a versatile, low-cost platform for diagnostic detection of viruses and protein biomarkers, with strong potential for point-of-care deployment. In parallel, we are advancing SERS-based approaches for probing the surface chemistry and interfacial reactivity of alloy nanoparticle catalysts under operando conditions. Building on our recent studies of binary, ternary, and multimetallic alloy catalysts [3-4], we use preliminary SERS measurements to characterize metal–oxygen interactions, adsorbate species, and structure–reactivity correlations in catalytic and electrocatalytic reaction systems. These efforts are complemented by in-situ/operando high-energy synchrotron X-ray diffraction and environmental TEM techniques, aiming to deliver molecular-level insights into structure–activity–stability relationships critical to alloy nanoparticle catalysis. Together, these two research directions demonstrate how SERS integrated with nanomaterials engineering enables powerful tools for biosensing and catalysis, offering broad opportunities for innovation in diagnostics, sustainable energy, and environmental applications.

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Probing chemical reactions by surface-enhanced Raman scattering using complex plasmonic nanostructures

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One of the most intriguing applications of plasmonic nanoparticles is based on their ability to transform the energy of light into chemical energy. A broad range of chemical transformations have been demonstrated already to be triggered directly by excitation of the nanoparticle's surface plasmon resonance. We have recently established the plasmon-induced transformation of 8-bromoadenine into adenine as a model system, in which the carbon-bromine bond is cleaved by an irreversible transfer of a hot electron from the light-excited nanoparticle to the 8-bromoadenine molecule.[1,2] Very recently, we have studied the control of hot-electron induced reactions by chiral plasmonic nanostructures and using circularly polarized light – a first step towards light-controlled enantioselective synthesis.[3]

Furthermore, we are interested to study chemical transformations in general at a single-molecular level by SERS. DNA origami nanostructures are ideally suited to arrange both plasmonic nanoparticles as well as receptors for analyte molecules with nanometer precision. We have created a dedicated DNA origami nanoantenna,[4] which was also used to detect single proteins.[4-6] Very recently, we have further optimized the plasmonic nanoantennas by comparing the SERS performance of dimers of different nanoparticle species from spherical Au and Ag nanoparticles to anisotropic gold nanoflowers and combinations thereof.[7]

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In-situ Terahertz Spectroscopic Observation of Electrical Double Layers using Surface-enhanced Raman Scattering

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Surface-enhanced Raman spectroscopy (SERS) is widely used to study electrochemical interfaces. This method is mostly operated in the frequency range of 400 – 1600 cm^{-1}, which corresponds to the mid-infrared (MIR) region or the so-called molecular fingerprint region where intramolecular vibrations are found. On the other hand, SERS is rarely used to observe collective intermolecular vibrations lying in the frequency range below 300 cm^{-1}. Because such low-frequency vibrations in the terahertz (THz) region can provide the information about picosecond dynamics of chemical species, in-situ SERS observation of electrical double layers in the THz region would be useful for deeper understanding of electrochemical processes. Owing to the recent advancement in manufacturing of optical notch filters, the detection of low-frequency Raman signals is now not so hard. Nevertheless, there remained an essential issue for low-frequency SERS; vibrational information in THz region is nearly concealed by a huge background continuum in SERS spectra [1]. Recently, we have identified that the background continuum in SERS is dominantly caused by plasmon-enhanced electronic Raman scattering. This finding allowed us to develop an analytical method of SERS spectrum in the entire frequency range covering 10 – 4000 cm^{-1} [2-5]. In this talk, we will demonstrate in-situ THz and MIR observation of electrical double layers at various electrochemical interfaces with hydrogen-bond networks using SERS [6-8].

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An optical nano-coulometer approach for measuring the contact resistance between nanoparticle and electrode

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Conventional potentiostat often uses amperemeter to report on the electrode current as a function of applied potential. Although powerful, it lacks spatial resolution and sensitivity to directly measure the reaction current of single nanoparticles. In recent years, we have developed a methodology to determine the redox current of single nanoparticles by watching the oxidation and reduction kinetics of single nanoparticles with optical microscopy. Taking Prussian blue, a classic electrochromic material, as an example, the reduction of single Prussian Blue nanoparticles formed Prussian White, which was accompanied with significant drop in the optical intensity. Because the optical intensity was quantitatively dependent on the redox state, and thus the state-of-charge of the nanoparticle, derivative of the optical intensity trajectory resulted in the electron transfer rate, i.e., current, of single nanoparticles. In other words, each single nanoparticle serves as an optical nano-coulometer to report on its own charge quantity, and the redox current of single nanoparticles can be quantitatively resolved from its derivative. By using this strategy, we were able to 1) uncover the significant impact of nanoparticle-substrate contacts on the apparent reactivity among different individuals, 2) determine on the intrinsic chemical diffusion coefficient of ions. and 3) reach a current detection sensitivity as low as 20 aA (10^-18 Ampere) to reveal the tunneling nature between Prussian blue and electrode sustrate.

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Plasmonic Pathway to Hybrid Nanomaterials through Energy Transfer

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Plasmon-induced resonance energy transfer (PIRET) is a promising approach for plasmonic photocatalysis and energy conversion, but challenges include elucidating the mechanism and maximizing its efficiency, both of which are hampered by competing processes. Another challenge is demonstrating that PIRET can photoinitiate reactions that follow efficient pathways compared to bulk processes. We report a plasmon-induced route to plasmonic-polymer hybrid nanomaterials using *in-operando* single-particle spectroelectrochemistry. An energy transfer efficiency of 40% is achievable when the spectral overlap between the gold nanorod scattering and monomer absorption is maximized. We also show that PIRET-initiated polymerization proceeds through a different mechanism than bulk polymerization, supported by spectroscopic evidence and density functional theory calculations, highlighting efficient energy cascade from photon to plasmon to exciton and finally, to new light-initiated chemistry. [1]

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Single-Molecule Raman Detection via Synergic Electromagnetic and Chemical Enhancement Enabled by Coulomb-Attraction Driven Spontaneous Molecule-Hotspot Pairing

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Raman spectroscopy offers a great power to detect, analyze and identify molecules, and monitor their temporal dynamics and evolution when combined with single-molecule surface-enhanced Raman scattering (SM-SERS) substrates [1,2]. In this talk we present a SM-SERS scheme that involves simultaneously giant chemical enhancement (CME) from WS_2 2D materials, giant electromagnetic enhancement (EME) from plasmonic nanogap hot spot, and inhibition of molecular fluorescence influence under near-infrared laser illumination [3-6]. We show that Coulomb attraction between analyte and gold nanoparticle can drive spontaneous formation of molecule-hotspot pairing with high precision, stability and robustness. The scheme has enabled realization of universal, robust, fast, and large-scale uniform SM-SERS detection for three Raman molecules of rhodamine B (RhB), rhodamine 6G (R6G), and crystal violet (CV) with a very low detection limit of 10^{-16} M and at a very fast spectrum acquisition time of 50 ms. Moreover, for a dilute mixture of RhB, R6G, and CV at concentrations of as low as 10^{-16} M, this SM-SERS substrate enables the sighting, counting, identification, and distinction of individual molecules with high efficiency, stability, and robustness. We expect that this EME-CME synergy SM-SERS strategy can offer a powerful capability of optically probing and monitoring the spatial-temporal evolution of the physical, chemical, and biological properties of molecules, which would open up a new frontier of molecular science.

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Quantum Tunnelling Induced Nonlinear Optics in Plasmonic Nanocavities

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In this talk, I will discuss several nonlinear optical phenomena in symmetry-broken plasmonic nanocavities. These include: 1) light-induced electromagnetic asymmetry for enhancing the surface second-harmonic generation (SHG) of noble metals by three orders of magnitude compared to conventional strategies [1]; 2) electron-tunnelling-induced second-order nonlinearity in conductive molecular nanojunctions [2]; 3) Lorentz-driven SHG output at the plasmon-induced magnetic dipolar resonance in an inversion-symmetry-broken plasmonic nanocavity [3]; and 4) plasmon-mediated, inelastic-electron-hopping-driven phonon pumping, leading to strong Raman nonlinearity at light intensities almost three orders of magnitude lower than in the conventional opto-mechanical systems [4].

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Tip-Enhanced Raman Spectroscopy for Chemical Imaging at the Nanometer Scale

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Tip-enhanced Raman Spectroscopy (TERS), introduced in the year 2000, is a nanoscale chemical analysis and imaging method with a spatial resolution down to a few nm, even at ambient conditions [1]. TERS relies on the enhancement of the local electromagnetic field by a plasmonic metal nanostructure that is scanned over the sample by means of a scanning probe microscope, using either AFM or STM feedback. Analogous to SERS, the local electromagnetic field of Raman scattered light is enhanced by many orders of magnitude in TERS. In this fashion, TERS is a variant of scanning probe microscopy that provides localized chemical information.

The working principle, experimental realization, and capabilities of TERS will be introduced [1], with special emphasis on how to avoid artifacts and how to best define the spatial resolution [2].

We will then discuss recent applications of TERS to the spatially resolved chemical analysis and imaging of molecular systems. Examples from recent TERS studies in our laboratory will be chosen, focusing on catalysis [3], biological membranes [4], and the nanostructure of photovoltaic cells [5].

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Polarized excitation, angular scattering and directional effects in tip-enhanced Raman spectroscopy

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Tip-enhanced Raman spectroscopy (TERS) enables vibrational spectroscopy down to the sub-nanometer scale, driven by a strongly enhanced local electromagnetic field at a metallic probe tip in close proximity to the sample surface. While there are extensive studies on the excitation mechanism, enhancement factors, and the tip-sample geometries, much less is known about the spatial characteristics of far-field TERS emission and how it relates to the chemical or molecular structures under investigation in the gap. In particular, angular scattering and directional effects in the far-field play a crucial role for quantitative analysis, reproducibility, and cross-comparison of TERS results across different laboratories.

In my talk I will discuss recent advances on angularly resolved TERS emission and polarization-dependent effects, linking experimental observations with theoretical insights [1, 2]. I will address issues such as how the directionality of tip-enhanced far-field emission depends critically on tip-geometry, tip-sample coupling, excitation polarization, and far-field collection schemes. Particular emphasis will be given to back-focal plane imaging, which allows mapping of angular emission patterns, and on how mode-specific vibrational polarizability tensors influence the visibility and spreading of Raman intensities in the far-field.

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Shell-isolated nanoparticle-enhanced Raman spectroscopy (SHINERS): Example applications and synthesis of nanomaterials

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Analyzing surfaces of various materials is crucial from both a scientific and economic perspective. Surface analysis is particularly challenging in the case of so-called buried interfaces (e.g., the surface of a solid sample immersed in a liquid or in a gas at high pressure). One of the tools that can be used for investigations of buried interfaces is developed by J.-F. Li *et al.* shell-isolated nanoparticle-enhanced Raman spectroscopy – SHINERS [1]. In this method, the surface under study is covered with a layer of surface-protected plasmonic P@D nanoparticles (where P denotes a plasmonic metal as Ag or Au, and D denotes a transparent dielectric, e.g., SiO_2, Al_2O_3, MnO_2, TiO_2 or ZrO_2), and then the Raman spectrum is recorded. The plasmonic cores of the deposited nanoparticles act as electromagnetic resonators, significantly enhancing the electric field of the incident electromagnetic radiation, which leads to a very large increase in the intensity of the generated Raman signal (the increase in Raman scattering efficiency is approximately proportional to the fourth power of the field enhancement [2]). The ultrathin protecting coating does not significantly damp the enhancement of the electric field generated by the plasmonic cores, but it does separate the metallic plasmonic cores from direct contact with the analyzed material (the analyzed sample can significantly change its structure during direct interaction with metals, therefore, covering the plasmonic cores with a protective layer allows for obtaining information about a much less disturbed sample) and prevents agglomeration of nanoparticles. SHINERS spectroscopy has found numerous practical applications, for example in the study of electrochemical processes (including battery research), heterogeneous catalysis, and the study of living organisms [3].

This contribution will present various methods of synthesis of SHINERS nanoresonators (various plasmonic materials, various shapes of plasmonic cores, and various materials used to protect the plasmonic cores). Example applications of SHINERS (e.g., electrochemistry, heterogeneous catalysis, and studies of living organisms) will be also presented. The synthesizing of SHINERS nanoresonators with magnetic properties will be also discussed.

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INVITED



Dual-fingerprint Raman measurement technologies for multi-targeted bio analysis

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The researcher's work integrates various Raman measurement techniques such as Raman scattering (RS), surface-enhanced Raman scattering (SERS), and stimulated Raman scattering (SRS). Focusing on the design and synthesis of novel molecular/nanomaterials, the researcher introduces a new concept of "Dual fingerprint" Raman detection, revolutionizing Raman measurement technology and developing specialized instruments. This has led to a series of innovative achievements in multi-factor rapid analysis and imaging analysis. The presentation will cover the following aspects [1-10]: (1) Exploring the synthesis mechanism of multi-dimensional noble metal nanostructures, proposing the construction of micro-area surfaces with "hot spots" such as tips or intra-particle gaps and interstices, which are uniformly arranged in 2D/3D, enhancing the sensitivity and reproducibility of direct SERS detection. (2) Optimizing SERS labels and applying them to indirect SERS detection of biological macromolecules and organic small molecules/ions in complex biological fluids, as well as multi-factor targeted imaging at the "cell-tissue-body" levels. (3) Synthesizing a variety of labelled/responsive molecules, polymer monomers, and organometallic coordination polymers with "narrow-band single-peak" Raman scattering characteristics in the biological silent region (1800-2800 cm-1), creating a series of Raman encoding technologies such as "click-SERS" that can be used for multi-factor liquid biopsy and biological imaging.

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Coherent Raman Spectroscopic Imaging of Biological and Medical Systems using Supercontinuum Light Source

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Coherent anti-Stokes Raman scattering (CARS) microscopy provides label-free, non-invasive visualization of molecular dynamics in living cells [1]. To incorporate spectroscopic analysis based on molecular fingerprints, we developed an ultrabroadband CARS spectroscopic imaging system using a supercontinuum light source and demonstrated label-free fingerprint imaging of living cells [2]. Through visualization of cellular senescence, we found the peak of the nucleolar amide I band shifted to a higher wavenumber in binuclear senescent cells, which reflects changes in the protein secondary structure from predominant α-helices to β-sheets originating from amyloid-like aggregates [3]. Furthermore, comprehensive mapping of molecular distributions in the developing mouse brain revealed region-specific ceramide accumulation associated with axonal myelination (Fig. 1) [4]. These results highlight the potential of CARS spectroscopic imaging as a powerful tool for probing intracellular biochemical processes and for medical diagnostics of pathological changes.

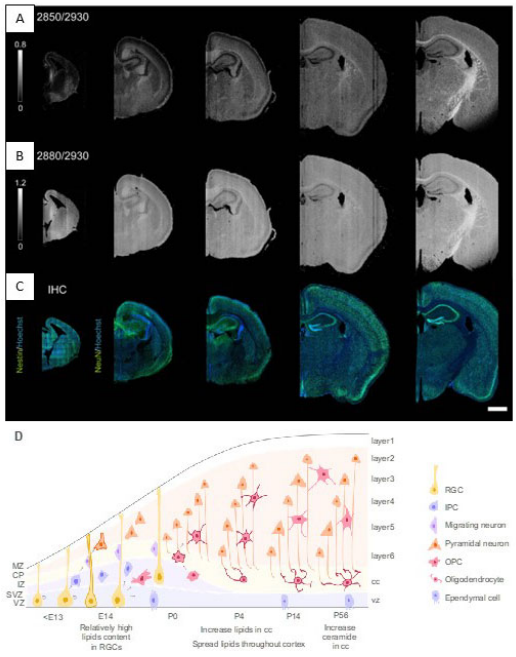

Figure 1. CARS spectroscopic imaging of the developing mouse brain (A,B) Wide-field ratio images (2850/2930, 2880/2930 cm^{-1}) of the left hemispheres at E14.5, P0, P4, P14, and P56. (C) corresponding immunohistochemistry (IHC) images. Scale bar: 1 mm. (D) Schematics of cell-type distribution during development. Abbreviations: MZ, marginal zone; CP, cortical plate; IZ, intermediate zone; SVZ, subventricular zone; VZ, ventricular zone; IPC, intermediate progenitor cell; RGC, radial glial cell; OPC, oligodendrocyte precursor cell.

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On-bead microspectroscopy for SERS biosensing

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This study will explore the design of microbead sensing carriers and their combination with SERS microspectroscopy for biosensing and coding. Three biosensing strategies based on the on-bead microspectroscopy will be presented here. (1) Selective detection of small molecules in complex systems using SERS-active hydrogel microbeads. SERS-active hydrogel microbeads are prepared by loading plasmonic nanoparticles into hydrogel microspheres using a microfluidic chip. The pores of the hydrogel can shield biological macromolecules and allow the diffusion of small molecule targets, enabling the detection of small molecules in complex sample systems [1, 2]. (2) Detection technology for genetically modified crops using magnetic polymer microspheres based on size and Raman coding[3]. The CRISPR/dCas9/sgRNA complex is assembled on the microbeads to recognize genetically modified nucleic acid sequences. It can simultaneously detect 6 genetically modified corn events while maintaining good specificity. (3) CHA/HCR-SERRS detection of genetically modified crops enhanced by the spatial confinement effect on the surface of magnetic microbeads (MBs). A magnetic-plasmonic composite microsphere probe is prepared, which can be activated by a small amount of target RNA to initiate catalytic hairpin assembly (CHA). The spatial confinement effect on the microsphere surface can significantly improve the efficiency of CHA. The resulting CHA products serve as a bridge for the subsequent hybridization chain reaction (HCR), forming repeated dsDNA on the microspheres that allows a high loading of DNA dyes. This CHA/HCR-SERRS platform combined with on-bead microspectroscopy has high specificity for the CaMV35s promoter binding site and its downstream RNA fragments in genetically modified crops[4].

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Ice–Water Interfacial SERS Reveals Novel Icing Inhibition Dynamics

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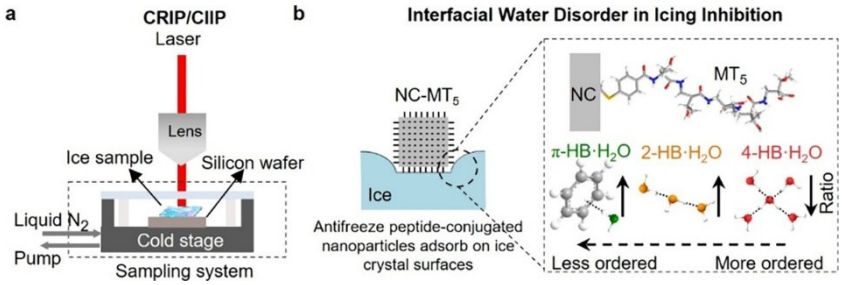
Ice formation and growth are pervasive phenomena with profound implications for global climate dynamics, geological process, and biological systems. The fact has been recognized that interfacial water is the most important player in heterogeneous ice nucleation and ice recrystallization inhibition (IRI), but its molecule-level understanding remains a well-known challenge because of complex water structure, composition, and intricate interfacial interaction with materials. The dual role of water as reactants and solvents further hinders the decrypting of interfacial water, particularly when regulating the potential dependence of IRI activity on different materials. Existing spectroscopy techniques, such as sum-frequency generation spectroscopy and terahertz spectroscopy, have provided valuable insights into antifreeze protein (AFP)-mediated ice inhibition. However, these techniques are either unable to distinguish the OH-stretch region or typically focus on probing the existence of ordered water molecules at the AFP surface, which clearly limits our understanding of ice growth and regulation at molecular levels. To bridge this gap, we developed a Cryo-Raman/Infrared interaction profiling (CRIP/CIIP) technique (Scheme 1) combined with molecular dynamics (MD) simulations for investigating the structure and dynamic change process of interfacial water at the ice–water interface. Plasmonic electric field enhancement at the ice–water interface enables sensitive tracking of interfacial water changes during ice recrystallization. MD simulation and spectral regions support the synergetic IRI activity of benzene rings via π-HB·H2O. Through π-HB·H2O tuning strategies in the vicinity of the ice–water interface, disordered water structure can effectively suppress long-range ice lattice ordering within a confined interfacial region. CRIP also reveals allostery-driven benzene conformational changes upon peptide–ice binding, offering label-free IRI activity discrimination. This platform provides a general strategy for designing next-generation cryoprotectants via interfacial water engineering and allosteric recognition.



Scheme 1. (a) Illustration on Raman/Infrared Microscopy Combining Cold Stage. (b) Interfacial Water Disorder and Transition in Presence of Antifreeze Materials.

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2D SERS nanomaterials for biosensing

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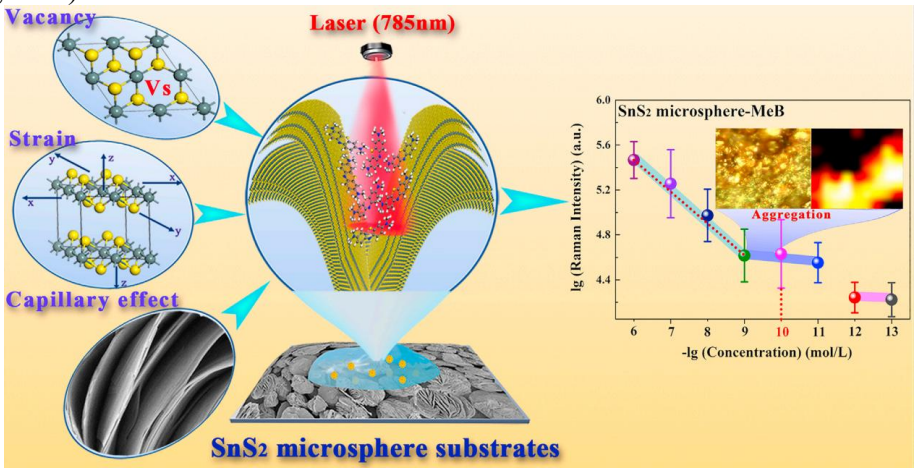
The SERS detection limit of most reported pure semiconductor substrates is still generally lower than the detection level of 10^{-10} M, which is difficult to meet the sensitivity requirement of SERS sensors for biological molecules in actual detection. Recently, our research group has developed some novel highly sensitive two-dimensional sulfide SnS_2 SERS active substrates. Firstly, the static Raman spectra and HOMO/LUMO energy distribution of 8 common sulfides and selenides were calculated by DFT, and the SnS_2 material with better SERS activity was selected. Then, the growth driving force of SnS_2 nanosheets was controlled by adjusting the concentration of the reactor, and SnS_2 nanosheets with different morphologies were generated: Hexagonal stacked nano-sheets, micron spheres and micron flowers, which all showed excellent SERS performance. Among them, the EF of SnS_2 microspheres with nanosheet hierarchical structure to MeB was as high as 3.0×10^8, and the LOD was as low as 10^{-13} M, which is one of the highest sensitivities among the reported pure semiconductor-based SERS substrates. On the one hand, due to the unique nano "canyon" morphology on the surface of SnS_2 microspheres, capillary effect was generated on the surface of microspheres, which further enriched probe molecules and improved SERS detection sensitivity. On the other hand, due to the lattice strain and sulfur vacancy of SnS_2 nanosheets composed of micronspheres, the bandgap of SnS_2 can be adjusted to promote charge transfer, thus improving the chemical enhancement effect (Figure 1).



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A Question of Attribution: What exactly is Pt-OH when electrosorbed at Pt{hkl}?

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Abstract

The lecture will examine the electrosorption of Pt-OH, particularly at potentials negative of the so-called "oxide formation" region using recent SHINERS results (amongst others) to argue the case for two types of PtOH being present at platinum electrodes. The first type of PtOH corresponds to a truly chemisorbed moiety that readily gives rise to a surface-Raman signal and is associated with either i) intermediates formed during the oxygen reduction reaction or ii) as a precursor during electrochemical oxide formation. The second type is proposed to be a specifically adsorbed hydroxide anion which remains SERS-silent at all potentials but whose presence may be inferred from both AC voltammetry [1] and Nafion™ adsorption [2]. An attempt is made to quantify the amount of the latter type of "PtOH" formed on Pt{311} by utilising an approach first pioneered in [3] to deduce the potential of zero total charge (pztc).

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CATALYTIC PERFORMANCE OF PLASMONIC METAL NANOSTRUCTURES

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Abstract: Based on the unique properties of plasmonic metal nanostructures, we have designed and constructed metal nanoparticle structures. We further revealed the interfacial and coupling effects between metal nanoparticles and explored their applications in energy, environmental catalysis and so on. By combining the "top-down" ink direct-writing 3D printing technology with the "bottom-up" nanosynthesis assembly technology, the multi-scale (nano-micro-macro) ordered structure of surface plasmon nanomaterials was constructed. Based on the enhanced effect of surface plasmons, the influence of catalytic reactions in energy and environmental catalytic systems was further studied, which laid a theoretical and experimental foundation for the practical application of surface plasmon nanostructures.

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Towards Polaritonic Electrochemistry

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We have investigated the preparation and characterization of molecular polariton systems, uncovering resonant enhancements of molecular at electrified interfaces through exotic electronic excitation processes (Fig. 1). Detailed vibrational analyses revealed new ways to construct electronic excitation modes using plasmonic nanostructures, leading to novel interactions between molecules and optical cavity modes from single to ensemble scales. We found that plasmonic surface lattices and Fabry–Perot mirrors enable strong coupling between electronic and vibrational modes. Remarkably, these molecule–polariton systems exhibit distinct properties even without photo-illumination, allowing modulation of molecular physicochemical properties under strong electromagnetic confinement.

We further apply this concept to enhance electron transfer at electrode–electrolyte interfaces. Within Gerischer's framework, strong cavity coupling introduces an additional electron-transfer channel via virtual photon excitation (Fig. 2), effectively turning a single-electron process into a quasi-two-particle reaction. This quantum pathway dominates when the mode volume is small and many molecules reside in the vacuum field, offering a route to improved electrochemical energy conversion.

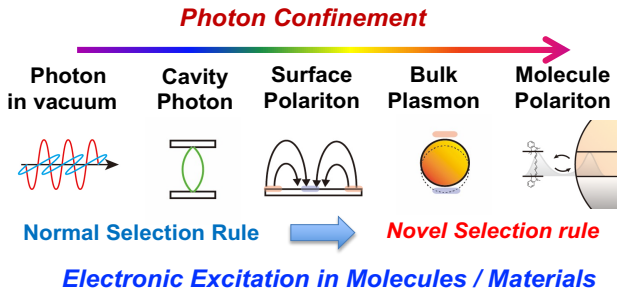

Figure 1. Schematic illustration of the concepts for the photon confinement from (left) the light to (right) the molecular polariton states, leading to the modification of the electronic excitation process.

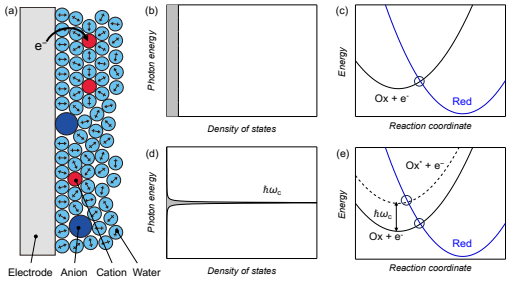

Figure 2. Schematic illustration of the electrode–electrolyte interface at which electron transfer reactions are considered under strong electromagnetic confinement.

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Combining *in situ* SERS and IR spectroscopy to study thiol molecules on Au surfaces

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In this talk, we present a combined *in situ* surface-enhanced Raman spectroscopy (SERS) and IR spectroscopy to probe the structure, configuration, and orientation of thiol monolayers on gold surfaces. To achieve this, we fabricated templated TiO_2 substrates decorated with arrays of Au nanoparticles (NPs) [1]. The SERS technique was used to monitor the photocatalytic degradation of 4-nitrothiophenol (4NTP) on Au NPs. Furthermore, we employed polarization modulation infrared reflection absorption spectroscopy (PM-IRRAS) and density functional theory (DFT) calculations to elucidate how the molecular tilt angle of 4NTP on Au(111) evolves under an applied electrode potential. This integrated approach provides a comprehensive mechanistic understanding of the experimentally observed intensity changes. The SERS and IR studies of β-thioglucose self-assembled monolayer on Au NPs will also be presented [2]. The SERS and IR spectra collected in the double layer region suggest the β-thioglucose monolayer is well hydrated and hence can be used for hydrophilic modifications of a gold surface.

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Effect of Subradiant Plasmon Resonance on Surface-Enhanced Raman Scattering Signal

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From the moment of its discovery, surface-enhanced Raman scattering (SERS) [1–3] has been the subject of mechanistic studies, i.e. both electromagnetic (EM) and chemical enhancement [4], for approximately five decades. A key factor in EM enhancement is the plasmon resonance of SERS substrates [5]. While the radiant plasmon modes involved in SERS have been well investigated through both quantitative experiments and theoretical calculations, the effects of nonradiant plasmon mode or subradiant one for SERS are not clearly identified [6].

In this talk, I will introduce the effect of subradiant plasmon resonance to SERS EM enhancement [6]. Spectral uncorrelation between SERS and Rayleigh (or extinction) spectra is mainly due to subradiant (or nonradiant) plasmon resonances; therefore, clarifying these resonances is essential for analysis of SERS. For the direct evaluation of subradiant plasmon resonance in plasmonic systems, the importance of absorption spectroscopy will be also introduced.

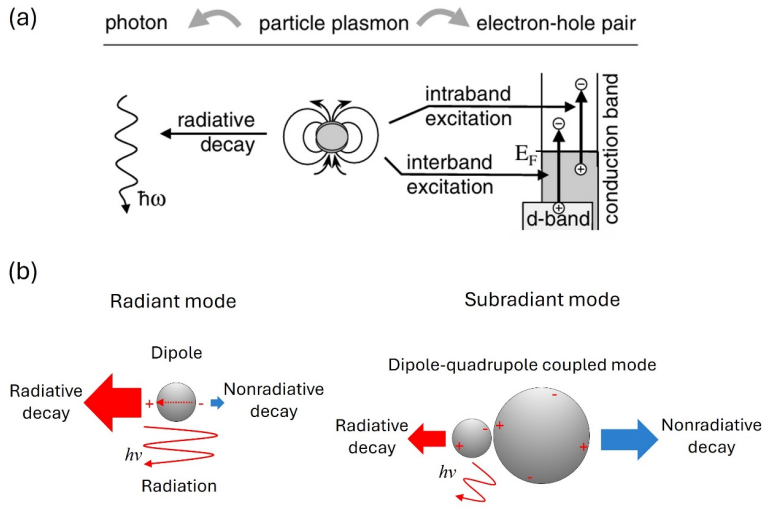

Figure 1. (a) Schematics of radiative (left) and nonradiative (right) decay of localized surface plasmon induced by metal nanoparticle. Reprinted with permission from Ref. X: Copyright 2002 American Physical Society. (b) Schematics of radiant and subradiant plasmonic modes.

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Updated Mechanism of Salt-Induced Aggregation-Based Single-Molecule Surface-Enhanced Raman Spectroscopy

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Since the first discovery of the surface-enhanced Raman scattering (SERS) effect in 1974, particularly the great breakthroughs in the single-molecule SERS (SM-SERS) in 1997, the interest of the scientific community in SERS had been rekindled immediately owing to this powerful combination of single-molecule sensitivity and spectroscopic fingerprinting in many fields. In the last three decades, the basic scientific question regarding the interaction between light and nanostructures has been investigated intensively. Along with the prosperity of nanotechnology, an immense amount of plasmonic nanostructures used as SERS substrates have been exploited. However, up to now, all seems to imply that it is still very difficult to reach a stable detection using diverse nano-structural SERS substrates to an ultra-low limit of detection (LOD), e.g. ~10^{-14} M, relying only on the electromagnetic hot spot effect.

In our recent studies, a salt-gradient model was proposed to deeply investigate the physical nature and update insights into the morphological, structural, and component evolution processes of Ag NPs. A gradient interface has been observed and an ultra-high sensitivity approaching single molecule level, e.g. ~10^{-16} M with stable signal for CV molecule, has been achieved in Ag colloidal system. Unlike Au NPs, the morphological, structural, and component evolution processes in Ag NPs have been observed. An unusual dissolution of Ag, the release of Ag^+ ions from Ag NPs, and final precipitation of AgCl can be evidenced. Based on these observations, we figured out a concept, which we name confined-enhanced Raman spectroscopy, in which the overall Raman properties can be remarkably improved with in situ-formed active nanoshell on the surface of silver or gold nanoparticles. The nanoshell can confine and anchor molecules onto the surface of plasmonic nanoparticles, and avoid desorption from hot spots so that "on and off" blinking effect can be eliminated.

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Nanogap-confined Optical Cavities for High-Sensitivity Detection of Surface-Bound Molecules

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Plasmonic nanostructures enable sensitive detection of reaction pathways by confining optical fields near catalytically active surfaces.[1] However, achieving precise physical control and high-sensitivity observation of surface-bound molecules remains a key challenge for advancing their practical applications.

In this presentation, I will discuss the dynamic behavior of highly polarizable molecules within the NPoM nanogaps. The NPoM architecture enables strong field confinement, allowing the observation of unusual surface-enhanced Raman scattering (SERS) responses from highly symmetric and polarizable molecules—features that are typically inaccessible in ensemble measurements.

In addition, I will introduce plasmonic nanostructures with varying shapes and dimensions used to construct cavities originated from single nanogap for probing the photodynamics of surface-bound species. The crucial influence of surface conditions on the optical cavity formation and their impact on molecular spectroscopy will be addressed.

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A Simple View of the (Rather Complex) Stark Effect in SERS

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The vibrational Stark effect refers to how an applied electric field shifts the molecular frequencies, being controlled by the electrode potential in standard electrochemical SERS experiments. The expected behavior is that the potential should tune the frequencies in a more or less linear manner, but this is not always so simple. Nitrile groups are often used because their vibrational modes are well-defined and sensitive to the electric field, making them excellent probes. Figure 1 shows the dependence of the cyanide frequencies on the applied potential corresponding to several results compiled by Billman and Otto [1] where three sharp differentiated regions can be seen. Region B shows the expected linear dependence, but Region A seems to be flat.

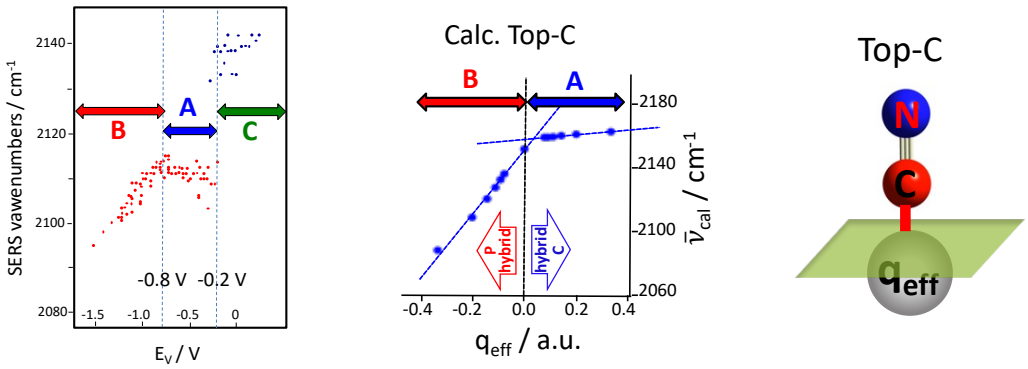

Figure 1. SERS frequencies of cyanide recorded on a silver electrode [1] and calculated values for Ag_n^{qeff}-CN^- linear complexes with different densities of charge where cyanide always maintains an on-top coordination bonded to the metal through carbon (Top-C) [2].

DFT calculations of Top-C Ag^{qeff}-CN^- complexes with different densities of charge (q_{eff}) predict that the frequencies should be very dependent at negative densities of charge (Region B, P-Hybrid) but almost insensitive to applied bias at positive charges of the metal (Region A, C-Hybrid). Therefore, Regions A and B correlate with two different electronic structures of the same Top-C complex [2].

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Enhanced Raman Spectroscopy in optical and acoustic traps for the detection of small microplastics and nanoplastics

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Microplastics pollution (particles < 5 mm, MPs) has emerged as a critical global challenge, posing substantial risks to ecosystems' stability, biodiversity conservation and public health protection. While microRaman spectroscopy is routinely used for the determination of the number, size, shape and chemical nature of MPs after filtration of the liquid solutions, technical limitations persist in detecting and analysing MPs directly in watery media, in complex liquid matrices (e.g. organic tissues digestates) and in continuous fluid streams. MPs smaller than 10 µm (small MPs), in particular, are subject to Brownian motion, which hinders the detection of sparse particles in liquid by standard microRaman analysis due to limited interrogation time. The detection of nanoplastics (particles < 1 µm, NPs) is even more challenging because of the much smaller cross section. This makes even the simple assessment of the presence of sparse small MPs and NPs in a liquid cell or stream, a challenge [1]. Techniques to enhance the Raman signal are, therefore, crucial to increase the sensitivity of Raman-based sensors and detect NPs as small as few tens of nm. Recently, SERS has emerged as a new route to enhance the Raman signal via plasmonic particles and substrates on which plastics are deposited or adsorbed after dissolution in suitable solvents, with all the known inconveniences [2]. Here we propose a different approach that employs Raman spectroscopy in optical and acoustic traps, also in combination with thermoplasmonic particles, to concentrate micro/nanoplastics particles directly in liquid, thereby enhancing the Raman signal by several orders of magnitude. We present example of using optical and thermophoretic forces within Raman tweezers setups to detect 25 nm polystyrene (PS) particles in water [3]. Subsequently we show the detection of 2 µm to 50 nm PS particles in liquid droplets levitated in air by Raman acoustic tweezers. This latter is a container-less and contact-less technique which results in background-free signals [4]. The role of plasmonic particles addition to plastics solutions in fostering and speeding up the aggregation processes is discussed. We acknowledge the projects NextGenEU PNRR-SAMOTHRACE (ECS00000022), ECOSISTER-PURE (ECS00000033), PE0000023-NQSTI, and PRIN2022-PLASTACTS (202293AX2L), FLASH2D (2022FWB2HE), SEMPER (20227ZXT4Z) for financial support.

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Sensitive metal-free SERS substrates

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Metal-free SERS substrates exploiting the chemical enhancement mechanism have recently been developed. These systems arise from the resonance Raman effect of charge-transfer complexes formed between the analyte and the substrate. Such metal-free SERS substrates generally demonstrate superior signal uniformity and durability, as the chemical mechanism operates across the entire surface of the substrate rather than at nanoscale electromagnetic fields generated by plasmon resonance, which often induce photothermal degradation. Nonetheless, their sensitivity remains suboptimal. To address this limitation, heteroatom doping has been extensively explored as a strategy to enhance sensitivity. Here, we introduce simple methodologies for the improvement of the sensitivity of various types of metal-free SERS substrates: carbon-based materials, conducting polymers, and Prussian blue analogues (PBAs) [1–3].

In the carbon-based SERS substrates, nitrogen (N) atoms are doped via carbonization of electrospun polyacrylonitrile nanomesh at varying temperatures [1]. At carbonization temperatures of 1000–1200 °C, graphitic-N structures are introduced into the conjugated π-electron system. Consequently, carbon substrates containing graphitic-N structures exhibit markedly superior SERS sensitivity compared to graphite obtained through carbonization at higher temperatures.

For the fabrication of conducting polymer SERS substrates, various monomers were electropolymerized [2]. Among these, poly-3,4-ethylenedioxythiophene (PEDOT) possesses the highest occupied molecular orbital (HOMO) energy level close to the lowest unoccupied molecular orbital (LUMO) of rhodamine 6G (R6G). As a result, R6G molecules on PEDOT, which form charge-transfer complexes, yield substantially stronger SERS signals compared to those on the carbonized polymer and other conducting polymers.

To dope different metals into PBAs, they were chemically synthesized by mixing aqueous potassium ferrocyanide solutions with various metal ions [3], generating crystal defects within the PBAs. Since the SERS performance varies depending on the type of incorporated metal, it can be systematically tuned through deliberate control over the formation of crystal defects. Indeed, the Cu-doped PBA markedly enhances SERS activity compared to pristine Prussian blue and other PBAs.

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Detecting Collective Molecular Vibrations with Surface-Enhanced Raman Spectroscopy

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In surface-enhanced Raman scattering (SERS) vibrations of molecules couple with optical modes of a plasmonic nanocavity via a molecular optomechanical interaction. This effect is typically assumed to occur at individual molecules neglecting intermolecular vibrational coupling. Here, we show instead how collective vibrations are observed in SERS through two different mechanisms: 1. Molecules can couple into collective vibrations through direct infrared (IR) dipole coupling, which is usually observed with IR spectroscopy. We show that cooperative frequency shifts from these collective IR vibrations can be also detected with SERS [1]. These collective states can be tuned with mixed self-assembled monolayers and allow us to monitor photochemical reactions. 2. Molecules can also form collective vibrations through the coupling of induced Raman dipoles when driven with intense laser pulses [2]. We show how such collective Raman vibrations enhance the optomechanical coupling with plasmonic nanocavities and reduce the onset of vibrational nonlinearities.

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Plasmon enhanced Luminescence of RE^{3+} doped nanoparticle

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Rare earth doped luminescence has many properties of narrow band and multicolor, which has been widely used in energy-saving lighting, special light sources, biomedical imaging, optoelectronic information. Due to 4f electronic shielding and f-f forbidden transition effect, the fluorescence lifetime of rare earth ions is long and the quantum yield is low, which is hard to meet the high-frequency control requirements of the next generation optical interconnect and quantum communication. Here, the luminescent properties of rare earth doped nanomaterials are improved by using plasmon near-field enhancement, localized and thermal effects. By constructing a plasmonic tilted nanocavity, the fluorescence properties of rare earth doped nanoparticles have been improved in frequency and time domain, and the luminescence lifetime is compressed to the nanosecond level.[1-2] In addition, micro/nanocrystal structure can be in-situ and rapidly optimized by plasmonic photothermal effects, which is used to develop an application on all-optical storage.[3-4]

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Meta-tricks: Making SERS quantitative with built-in optical interferometry

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Surface-enhanced Raman scattering (SERS) has long been recognized for its extraordinary potential in enabling ultrasensitive molecular detection, down to the single-molecule level. Despite this promise, the translation of SERS into a truly quantitative and analytically robust technique remains a major challenge, largely due to poor reproducibility and difficulties in controlling enhancement factors across different substrates. In this context, all-dielectric SERS-active substrates are emerging as a compelling alternative to plasmonic platforms, offering superior reproducibility and long-term stability [1-3]. Beyond their role in Raman signal amplification, all-dielectric substrates also hold promise as versatile multimodal platforms, capable of integration with complementary analytical methods such as mass spectrometry, optical spectroscopy, and infrared spectroscopy [4,5]. In this work, we highlight how diverse types of SERS-active substrates can be endowed with built-in optical interferometry, thereby providing a self-referenced, all-in-one approach that enables quantitative SERS measurements. This strategy opens the way toward establishing SERS as a reliable tool for both fundamental research and real-world analytical applications.

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ORAL

Machine Learning-Aided label-free SERS Sensing for Early Detection of Lung Cancer

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Lung cancer (LC) is the leading cause of cancer-related mortality worldwide, underscoring an urgent need for strategies that enable early detection and phenotypic classification. Here, we report a label-free surface-enhanced Raman spectroscopic (SERS) analysis of serum exosomes from 643 participants to elucidate the biochemical deregulation associated with LC progression and the unique phenotypes of different LC subtypes.[1] Iodide-modified silver nanofilms were prepared to rapidly acquire SERS spectra with a high signal-to-noise ratio using 0.5 μL of patient exosomes. We performed interpretable and automated machine learning (ML) analysis of differential SERS features of serum exosomes to build LC diagnostic models, which achieved accuracies of 100% and 81% for stage I lung adenocarcinoma and its preneoplasia, respectively. In addition, the ML-derived exosomal SERS models effectively recognized different LC subtypes and disease stages to guide precision treatment. Our findings demonstrate that spectral fingerprinting of circulating exosomes holds promise for decoding the clinical status of LC, thus aiding in improving the clinical management of patients.

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Studying Stress Response Process of Cell during Electrical Stimulation Through Spectra Techniques

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Electrical stimulation (ES) is treated as a promising physical means for the diagnosis and treatment of diseases, which can regulate cell proliferation, differentiation and cell death. Thus, it is widely used in the biomedical field. Recently, we found that electrical stimulation can controllable and rapidly trigger cancer cell pyroptosis.We find that the ES-induced cancer-cell pyroptosis is through the activated caspase-3 (pathway) cleavage of gasdermin E (GSDME) to form a N-terminal fragment (GSDME-N), and observe nuclear shrinkage, reduction of the number of nucleoli and expression level of nucleolin depressing during pyroptosis. Simultaneously, the endoplasmic reticulum stress was examined during cell pyroptosis. The results demonstrated that expression levels of calcium ions, calreticulin and calcium adhesin subtypes were obviously changed. Interestingly, weak electrical stimulation could effectively inhibit the migration of cancer cells. Importantly, we found that the number of exosomes released by cancer cells was significantly higher than that of normal cells, and the miRNA content released by cancer cells was significantly higher than that of normal cells. These studies provide reliable methods and potential clinical application value for the diagnosis and treatment of electrical stimulation cancer and monitoring the changes of key factors in the process of diagnosis and treatment.

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DNA Secondary Conformations Studied by Surface-Enhanced Raman Spectroscopy

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Besides B-type antiparallel DNA double strands (DSs), DNA sequences can form varieties of secondary conformations, including parallel double helixes, triplexes, G-quadruplexes (G4s) and i-motifs etc. Each individual secondary DNA structure not only gives specific biological function, but also can be used to construct biosensor and functional nanomaterials. However, the accurate prediction of DNA conformations based on their sequences has remained great challenge due the conformational complexity and variety. Recently, we use silver nanoparticles modified by aluminium ion and iodine ion (Ag IMNP-AI^{3+}) as substrate for the SERS detection of secondary DNA conformations, a series of featured bands have been identified corresponding to the formations of G-quartet in G4s, C•C^{+} base pairs in i-motifs, showing the potential of SERS towards DNA secondary conformational studies [1-2]. Meanwhile, using bromine ion and magnesium ion modified gold nanoparticles (Au MMNPs-Mg^{2+}) as the substrate, weak interactions presented in A•A base pairs and parallel DNA helixes formed in acidic conditions were identified [3]. Employing machine learning, the best combinations of cation and anion that modified Ag and Au nanoparticles for DNA conformational studies were selected, which are able to provide more DNA structural details [4]. Furthermore, fast and accurate classification of DNA conformations were achieved by the combination of machine learning and SERS fingerprint spectra [5]. A new SERS platform for secondary DNA conformational studies will be reported in this presentation.

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SERS detection of biomaterials using plasmonic nanoarrays

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Surface-enhanced Raman scattering (SERS) offers ultrahigh sensitivity for molecular detection, yet conventional substrates suffer from heterogeneous hotspot distributions, limiting the SERS sensitivity for biosensing applications. To address these challenges, we developed a precisely engineered plasmonic nanoarray composed of A-B-A trimers with sub-2 nm gaps. In this design, a central trap nanoparticle (B) is flanked by two plasmonic nanoparticles (A), ensuring spatial alignment of target molecules with intense electromagnetic hotspots. The practical utility is demonstrated in bioenvironments: (1) Early biomarkers for lung cancers were detected with single-molecule sensitivity in fresh tissue samples, and (2) integration with hydrogel yields a wearable membrane for metabolite analysis in sweat.

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Single-Cell Raman Spectroscopy Combined with Metabolomics Reveals Distinct Metabolic Profiles in Medulloblastoma Subtypes

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Tumor heterogeneity poses a major challenge to the precision treatment of medulloblastoma (MB). Rapid and accurate subtyping tools are urgently needed for informed clinical decision-making. Herein, we demonstrate the utility of Raman spectroscopy (RS) as a label-free, noninvasive approach for molecular characterization and subtype discrimination of MB at the single-cell level. Five representative MB cell lines from group 3 and sonic hedgehog (SHH) subtypes, along with microglial controls, were profiled by RS and validated using mass spectrometry-based metabolomics. RS-derived single-cell metabolic fingerprints revealed subtype-specific variations in nucleic acids, amino acids, lipids, and proteins. Group 3 cells, exemplified by metastatic D283, exhibited elevated levels of unsaturated lipids compared with most SHH cells. Notably, Daoy cells from the SHH subtype displayed unsaturation levels comparable to D283, reflecting intragroup heterogeneity and membrane remodeling in MB. Machine learning classifiers achieved high diagnostic performance, with an average area under the curve of 0.994 and a Matthews correlation coefficient of 0.935. Furthermore, cisplatin-treated D283 cells showed increased unsaturated lipid content relative to Daoy cells, revealing subtype-dependent metabolic shifts in drug response. These findings underscore the metabolic diversity of MB subtypes and the role of lipid metabolism in tumor progression and therapy. Collectively, our results exemplify the power of RS combined with metabolomics for molecule-resolved, label-free MB subtyping and therapeutic stratification.

SERS-based chiral detection strategies and their applications in detecting cancer-associated salivary biomarkers of D-amino acids

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Many biomolecules and pharmaceuticals are chiral, existing as L- and D-form enantiomers with identical chemical compositions but often exhibiting distinct biological and pharmacological activities. Chiral preference is a signature of life. Living organisms typically utilize one given enantiomeric form to sustain normal biological functions, while the opposite enantiomer may contribute to diverse diseases [1]. Therefore, accurate discrimination between enantiomers is highly significant yet challenging.

Although surface-enhanced Raman scattering (SERS) offers high sensitivity in molecular detection, it generally lacks chiral specificity because the Raman spectra of enantiomers are identical. To enable enantiomeric discrimination *via* SERS, chiral recognition strategies have been developed [2]. These can be implemented by either endowing metallic nanostructures with chirality or applying enantioselective pretreatment to samples for selective capture of target chiral molecules. Based on these approaches, we have constructed several types of chiral SERS substrates, ranging from intrinsically chiral ligand-free gold nanoparticles (NPs) to substrates functionalized with chiral molecules or gold nanoclusters [3-5]. These chiral substrates interacted enantioselectively with amino acid enantiomers, inducing detectable differences in their SERS signals and thereby enabling enantiomeric discrimination.

Furthermore, using D-amino acid oxidase (DAAO) as a chiral selector [6], we achieved enantioselective deamination of D-amino acids (e.g., D-alanine, D-proline) to generate H_2O_2. This product oxidized the Raman reporter 3-MPBA, allowing SERS-based detection of D-AAs on a gold NPs-assembled film substrate. This strategy was successfully applied to detect salivary D-AAs, distinguishing gastric cancer patients from healthy individuals by monitoring elevated D-Ala levels. It demonstrates promising potential for non-invasive diagnosis of gastric cancer, offering an alternative to traditional invasive methods such as forceps biopsies and endoscopic examinations. The above research expands the application of SERS in chiral discrimination and the detection of chiral biomarkers.

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From single particle spectroscopy to shape-controlled plasmonic metamolecules

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Top-down lithographic patterning produces polygonal nanoparticles (NPs) with precise sizes, shapes, and compositions unachievable through wet-chemical methods. Template-assisted assembly uses capillary forces to organize these NPs into metamolecule structures, where NP and template properties control coordination numbers, interparticle gaps, and defect locations. For gold polygonal NPs, plasmonic resonances correlate structure with optical properties. Close-packed assemblies with center NPs enable collective interactions that alter magnetic optical modes and multipolar interactions in Fano resonances. Reduced interparticle distances strengthen plasmonic coupling, while structural symmetries determine orientation-dependent scattering. Single-particle studies reveal that gold nanorod photoluminescence results from Purcell effect-enhanced hot carrier radiative recombination, with hot carrier temperatures exceeding 1000K under continuous wave excitation—far above lattice temperatures. Copper nanocubes exhibit interband transition-dominated absorption and emission. These insights into plasmonic architecture and hot carrier processes have significant implications for photocatalysis and optoelectronic applications.

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Abstract Title Clinical translations of silent-region SERS theranostics for simultaneous monitoring and promotion of bacterial wound healing

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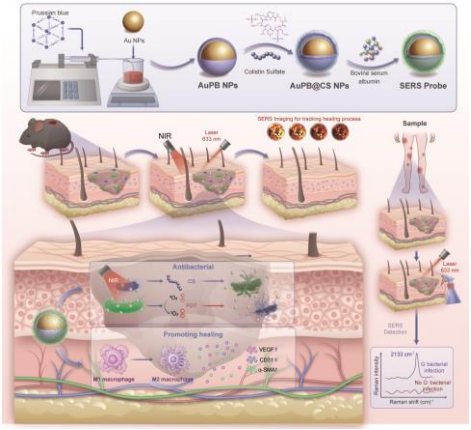

Bacterial wound infections, particularly those caused by *Escherichia coli* and *Pseudomonas aeruginosa*, are difficult to treat due to biofilm formation, multidrug resistance, and chronic inflammation. Here, we report a multifunctional nanoplatform based on a surface-enhanced Raman scattering (SERS) probe that enables simultaneous photodynamic therapy, antibiotic delivery, and real-time infection monitoring. The probe comprises gold nanoparticles coated with Prussian blue, which acts both as a near-infrared photosensitizer and a Raman reporter in the spectroscopically silent region, further loaded with colistin sulfate and stabilized with bovine serum albumin. Upon irradiation with a 650 nm laser, the probe produces reactive oxygen species, and, in combination with antibiotic release, achieves synergistic eradication of Gram-negative bacteria (>90% reduction) using a significantly reduced antibiotic dose. The SERS signal in the silent region enables background-free, *in situ* discrimination and quantification of bacterial load during treatment. In both normal and diabetic mouse wound models, the probe accelerates bacterial clearance, facilitates M2 macrophage polarization, and promotes angiogenesis and collagen deposition, thereby resulting in improved wound healing. Analysis of 36 clinical wound samples demonstrates sensitive and specific Gram-positive and Gram-negative bacterial identification (AUC = 0.94). This approach establishes a clinically translatable strategy for precise infection management, real-time monitoring, and enhanced wound repair.

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V-Shaped Heterostructure Nanocavities Array with CM and EM Coupled Enhancement for Ultra-Sensitive SERS Substrate

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Abstract

The field of semiconductor surface-enhanced Raman scattering (SERS) substrates has experienced significant advancements, leading to a wide range of applications in several fields. However, the quest for new ultra-sensitive semiconductor SERS materials is still of utmost importance. In this regard, an efficient and novel substrate, F4TCNQ/MoS_2 heterostructure is introduced, assisted by V-shaped aluminum anodic oxide (AAO) nanocavities with different depths. Utilizing the efficient charge transfer of organic/inorganic semiconducting heterostructure and the photoconfinement capability of the nanocavity structure of the AAO nanotemplate, excellent stability, fast sensing, enhanced Raman, and photodegradation activities are achieved. Due to its unique 3D structure, the optimized F4TCNQ/MoS_2/AAO with 1500 nm depth achieves ultra-high sensitivity detection of 9.0×10^{-16} M for conventional probe molecules. Furthermore, precise detection of water contaminants is observed for the first time with a V-shaped heterostructure due to combined organic/inorganic features that differ significantly from conventional MoS_2 structures or other metal/inorganic or inorganic/inorganic semiconductors. This research presents a novel and versatile strategy for SERS and demonstrates its diverse potential performance in practical applications.

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Design and applications of ECL/SERS sensing platform based on spherical nucleic acids enzyme

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The concept of Spherical Nucleic Acids Enzyme (SNAzyme) has been introduced based on spherical nucleic acids (SNA), comprising a dense monolayer of G-quadruplex DNAzyme (G4-DNAzyme) assembled on a gold nanoparticle core. This configuration exhibits catalytic efficiency that is approximately two orders of magnitude greater than that of free G4-DNAzyme, alongside markedly enhanced stability in whole blood compared to unbound DNA. The architecture effectively integrates the high catalytic activity characteristic of DNAzymes with the biological stability and facile separability afforded by nanoparticle platforms. Building upon the SNAzyme framework, we have developed various forms including self-growing SNAzymes, covalently linked SNAzymes, and non-covalently modified SNAzymes, which have been employed to construct a series of electrochemiluminescence and chemiluminescence sensors. These sensors facilitate rapid and highly sensitive detection of microRNAs (miRNAs) within complex biological matrices such as serum, cellular extracts, and exosomes. Notably, the system enables detection of miR-499 at concentrations as low as 10 attomolar in the serum of patients with acute myocardial infarction within 30 minutes. Moreover, endogenous miR-499 was successfully quantified in patient serum samples, allowing effective discrimination between individuals with acute myocardial infarction and healthy controls. Recent investigations have further demonstrated the exceptional performance of SNAzymes in surface-enhanced Raman scattering (SERS) detection, particularly with histidine-rich sequence-enhanced SNAzymes, which can detect hydrogen peroxide under diverse physiological conditions with a detection limit below 10 micromolar. This finding holds significant potential for the monitoring and diagnosis of diseases such as diabetes and inflammatory disorders.

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Research on the mechanism of electric-modulation in SERS

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Electric-modulation SERS is a technique that uses an electric field to precisely control Raman signals, which is achieved by manipulating the electro-physical and chemical properties of metal or two-dimensional material substrates to enhance SERS signal output. This enhancement can occur through charge transfer processes and the modulation of plasmon resonance. Based on experimental and theoretical studies, we achieved a 70-fold enhancement of SERS signals on a rigid substrate (Ag NPs/graphene/$BaTiO_3$) and reduced the limit of detection (LOD) by three orders of magnitude to 10^{-14} M after applying a thermoelectric field. This enhancement stems from the thermoelectric field generated by the substrate, which drives charge transfer between the SERS substrate and molecules, significantly improving SERS performance.[1] To further adapt to practical application scenarios, we present a flexible SERS substrate consisting of Ag film/$BaFe_{12}O_{19}$/$BaTiO_3$/polydimethylsiloxane, and introduce the flexoelectric effect as a strategy to overcome challenges. When the SERS substrate undergoes bending or deformation, a tunable polarization field is generated, which can amplify the SERS signals by up to ten times and reduce the limit of detection by four orders of magnitude. Theoretical and experimental findings indicate that the flexoelectric field can effectively modulate the electron density of Ag, thereby synchronously enhancing the electromagnetic field intensity and improving the charge transfer efficiency. Moreover, the applicability of the flexoelectric SERS substrate is further verified through the in-situ detection of pityrosporum, borax, and gibberellin in multiple scenarios. We contend that this research can deepen the understanding of SERS mechanisms and expedite the application process of SERS.

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Interface microenvironment regulation electrocatalytic deuteration using D_2O

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The high Faradaic efficiency (FE) of the electrocatalytic deuteration of organics with D_2O at a large current density is significant for developing a feasible and promising room-temperature deuteration strategy.[1-4] However, the FE and current density are the two ends of a seesaw because of the severe D_2 evolution side reaction at nearly industrial current densities. Herein, we report a combined scenario of a nanotip-enhanced electric field and surfactant-modified interface microenvironment to enable electrocatalytic deuteration of arylacetonitrile in D_2O with an 80% FE at -100 mA cm^{-2}, which are both the best records for current electrocatalytic deuteration reactions.[5] The increased concentration with low activation energy of arylacetonitrile due to the large electric field along the tips and the accelerated arylacetonitrile transfer and suppressed D_2 evolution by the surfactant-created deuterophobic microenvironment contribute to breaking the trade-off between a high FE and large current density. Furthermore, the application of our strategy in other deuteration reactions with improved FE at -100 mA cm^{-2} rationalizes the design concept.

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SERS XMU-2025 | ICSERS - 2025
3rd International Conference on Surface Enhanced Raman Spectroscopy
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Investigation of the Interfacial Growth Mechanism of SURMOFs by Surface Infrared Reflection-Absorption Spectroscopy

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Metal–organic frameworks (MOFs) serve as an ideal platform for studying the controllable self-assembly of functional crystalline materials. We used surface self-assembled monolayers (SAMs) as directing groups and employed liquid-phase epitaxial stepwise growth (LPE) to achieve controlled interfacial self-assembly of MOF thin films (SURMOFs).[1] Importantly, we have developed a surface infrared reflection-absorption spectroscopy (IRRAS) technique to study the growth mechanism of SURMOFs at SAM modified substrates. By correlating IRRAS peak positions and intensities with XRD and SEM data, we established a "first-layer order–temperature–crystal orientation" phase diagram for SURMOFs. [2,3] This study demonstrates the unique advantages of IRRAS in elucidating the mechanisms of interfacial nucleation, ligand exchange, and defect evolution in SURMOFs, providing universal criteria for the controlled fabrication of highly oriented MOF thin films.

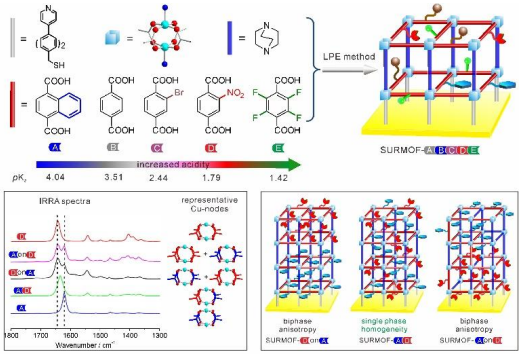

Figure 1. Scheme of growth of SURMOFs with mixed linkers and IRRAS spectra under heterogeneous and homogeneous assembly

Keywords：SURMOFs; IRRAS; self-assembled monolayers; oriented growht

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Surface-enhanced Raman nanostructure design and in situ analysis of high temperature processes

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High-temperature reactions are among the most widely used fundamental reactions in the modern chemical engineering and energy sectors. Real-time monitoring and on-site analysis of high-temperature reaction processes using in-situ techniques are of great significance for deciphering reaction mechanisms, guiding material design, and improving operational efficiency. Surface Enhanced Raman Scattering (SERS) technology leverages the plasmon resonance effect of gold and silver nanostructures to amplify Raman scattering signals. It not only retains the advantages of conventional Raman spectroscopy—such as non-destructive detection, no requirement for a vacuum environment, and resistance to thermal radiation and water peak interference—but also possesses trace analysis capability and sensitive response performance that conventional Raman spectroscopy lacks. This makes it particularly suitable for in-situ detection and tracking of trace key species and microstructural evolution at reaction interfaces, endowing it with excellent application potential in the in-situ study in high-temperature reactions, including catalysis and solid oxide cells, etc. This work will present the progress and existing challenges of SERS in the fields of in-situ research on high-temperature reactions and solid oxide cells, as well as the research work conducted by our team on the design of Raman-enhanced nanostructures and high-temperature in-situ analysis by SERS.

Development and Mechanism Study of Transition Metal Sulfide-Based Laccase-Mimicking and SERS Bifunctional Substrates

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Laccases, key redox enzymes in fungi and plants, efficiently catalyze phenolic compound oxidation without cofactors, making them a research focus. Recently, nanomaterials with dual nanozyme and SERS activity have attracted wide interest for building multifunctional[1−3]. Utilizing the unique unfilled 3d orbitals of Ni, this study synthesized $NiCo_2S_4$ nanosheets hydrothermally. By optimizing sulfur source conditions, the material achieved excellent morphology and remarkable nanozyme-SERS bifunctionality, reaching a detection limit of 10^{-7} M for crystal violet (Figure 1a). Furthermore, the electronic state characteristics of Ni enable strong adsorption with oxygen molecules, providing abundant active sites to promote the activation and conversion of reactants, thereby enhancing catalytic efficiency. As shown in Figure 1b, the laccase-mimicking activity was evaluated using a typical chromogenic reaction involving laccase substrates 2,4-dichlorophenol (2,4-DP) and 4-aminoantipyrine (4-AP), monitored by UV-Vis spectroscopy. The antioxidant properties of various tea polyphenols were compared, revealing that the number of hydroxyl groups significantly influenced the reaction rate of $NiCo_2S_4$ nanosheets catalyzing polyphenols. This two-dimensional metal sulfide-based laccase-mimicking nanomaterial holds significant application potential in analytical detection, antibacterial performance, and environmental pollutant degradation.

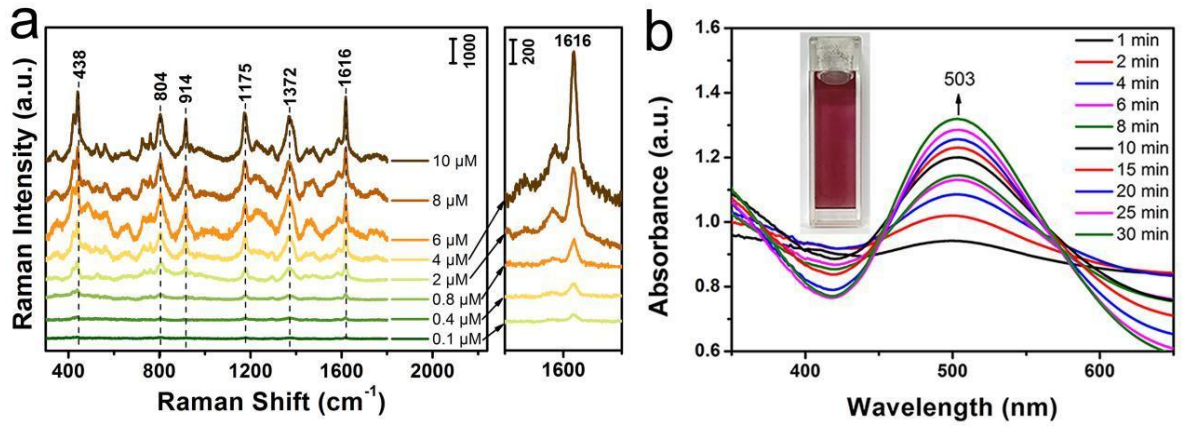

Figure 1: (a) SERS spectra of crystal violet on $NiCo_2S_4$.
(b) UV-Vis monitoring of the laccase-mimicking activity of $NiCo_2S_4$ nanosheets.

Keywords: Nanozyme; Surface-Enhanced Raman Spectroscopy; Transition Metal Sulfide; Tea Polyphenols

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Versatile Plasmonic Coupling Islands for Ultrasensitive SERS Sensing and Photodegradation

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Plasmonic nanostructures with micro-scale offering powerful platforms for plasmon-based catalysis and enhanced sensing have remained a major challenge in plasmon-mediated chemical reactions (PMCRs) and SERS sensing. Herein, by operating microsphere lithography on a hydrophilic surface, a plasmonic coupling strategy implemented under ambient conditions was developed through self-assembling gold nanoparticles at the site of microsphere shade. [1,2]

To confirm the coupling performance, an in-situ growth of gold nanowires (AuNWs) in the micrometre islands was operated under the induction of 4-mercaptobenzoic acid (pMBA). In the confined islands, the AuNWs showed anisotropic growth and formed interconnected 3D networks with high-density plasmonic hotspots, which generated strong localized surface plasmon resonance (LSPR) coupling, enhanced electromagnetic fields (Fig. 1). Such 3D plasmonic platform first displays ultrasensitive sensing of trace biogenic amine gases (BAs) with a detection limit as low as 10^{-14} M in spoiled seafood through integrating into food packaging. [3]

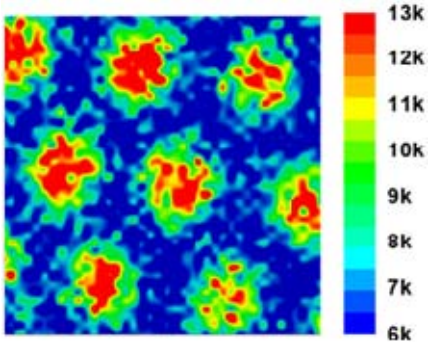
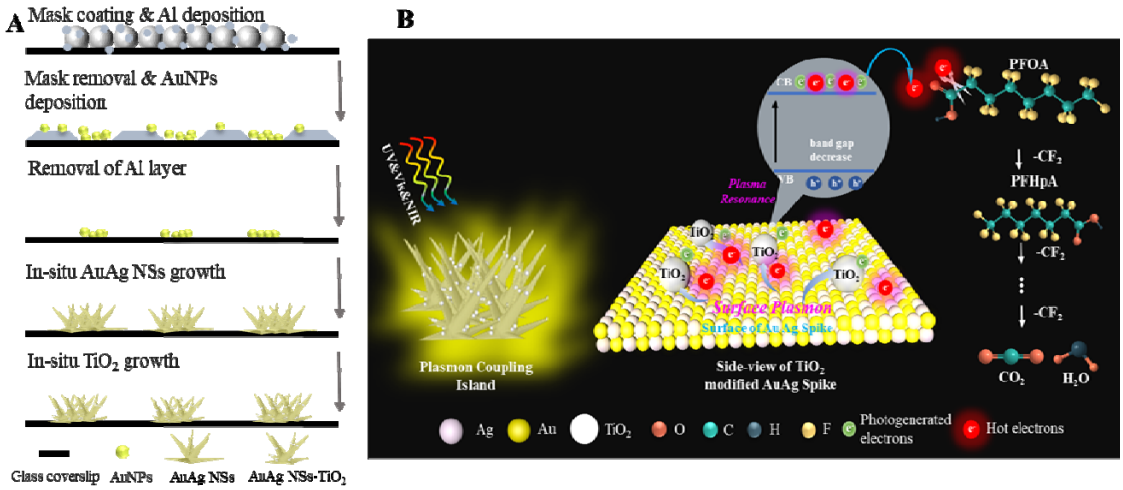


Figure 1. Raman imaging of patterned gold nanoparticles on glass surface under 532 nm laser irradiation. The micrometre scale self-assembled gold nanoparticle islands display evident electrical coupling under irradiation.

Furthermore, through fabrication of AuAg NSs-TiO_2 particles as isolated micro-scale islands, we developed an effectual strategy for obtaining chemically active hot electrons in UV-Vis-NIR full spectrum region. Our island synergistically coupled plasmon resonance of Au with electron-hole pairs of TiO2 can be used for efficient photocatalytic reactions in the UV-Vis-NIR full spectrum region. More remarkably, the island utilizes resonant hot-electrons directly trigger Kolbe decarboxylation reaction and remove C-F bonds of polyfluoroalkyl substances (PFAS) without conventional oxyradicals under sunlight irradiation, displaying a 95.51% photocatalytic degradation and 62.98% defluorination rates on perfluorooctanoic acid (PFOA) in 5 hours at 20 ppm which is 10-folds higher than commercial TiO_2 agents (Scheme 1).



Scheme 1. Schematic illustrations of the AuAg NSs-TiO_2 coupling islands. (A) Fabrication process of AuAg NSs-TiO_2 islands array with micro-sphere lithography on a glass coverslip (side view), (B) Illustration of the operation mechanism adopted in AuAg NSs-TiO_2 coupling island. Due to the LSPR effect, the absorption of Au Ag - TiO_2 to sunlight was broadened, which exhibited excellent full-spectrum catalytic performance and realized the efficient photocatalyst (left picture).

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Strong dipole-promoted N–O bond hydrogenolysis enables ampere-level electrosynthesis of methylamine

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The electrochemical hydrogenolysis of nitromethane in water could provide a sustainable route for accessing methylamine, one of the simplest alkyl amines and most commonly used bulk chemicals. However, present efforts only achieve methylamine selectivities below 10% due to the ineffective N–O bond activation of the N-methylhydroxylamine intermediate. We design a copper electrocatalyst with abundant low-coordinated sites to enable the conversion of nitromethane to methylamine with 99% selectivity and 97% Faradaic efficiency at a low potential[1]. The low-coordinated copper sites induce a large dipole moment upon N-methylhydroxylamine adsorption to promote N–O hydrogenolysis. In situ Raman spectra show that CH_3NHOH can adsorb on low-coordinated Cu from the open-circuit potential, whereas its adsorption on coordination-saturated Cu occurs at a more negative potential. Altering the pH changes the rate-determining step, resulting in a pH-dependent volcano trend for methylamine production. The ampere-level production of 1.5 mol of methylamine alongside easy product purification, gram-scale synthesis of deuterated methylamine and drugs, and hydrogenolysis of other N–O bonds demonstrate the universality of our approach and offer a promising, general approach to alkyl N–O bond hydrogenolysis that could compete with traditional thermochemical routines.

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Uncovering Excited-State Coupling in Conjugated Polymers through Resonance Raman Spectroscopy

Alkylthienyl substitution in conjugated polymers has led to major performance gains in organic photovoltaics, but the underlying photophysical reasons remain unclear. Here, we use resonance Raman and transient absorption spectroscopy to explore how molecular design influences charge generation. Comparing PBDB and PBDB-T in blends with ITIC-Th, we find that PBDB-T enables more efficient hole transfer and higher charge photogeneration yields.

Resonance Raman results reveal that the alkylthienyl groups strengthen the coupling of the excited S_1 state to the benzodithiophene (BDT) core, localizing electron density on this unit only in PBDB-T, particularly in interaction with ITIC-Th. This enhanced donor–acceptor coupling explains the improved charge separation observed.

Our findings highlight how vibrational signatures captured by Raman spectroscopy directly link molecular structure to charge-transfer dynamics, providing new insight into the design of next-generation organic photovoltaic materials.

Computational–Spectroscopic Insights into Chemical Effects in Plasmon-Enhanced Nanospectroscopy

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Plasmon-enhanced nanospectroscopy, including surface- and tip-enhanced Raman spectroscopy (SERS, TERS), provides molecular-level insight into light–matter interactions with single-molecule sensitivity. While the electromagnetic enhancement is well described by near-field confinement, the chemical effect, the quantum-mechanical contribution to spectral enhancement, remains less quantitatively understood. It originates from charge transfer and orbital hybridization between the molecule and the plasmonic interface, which alter the electronic structure and polarizability tensor of the adsorbed species.

In this contribution, we employ first-principles and TD-DFT simulations to mimic the realistic chemical environment, explicitly considering molecular geometries, metal–molecule interactions, and background charges that represent the metallic substrate or tip. Building on our recent combined spectroscopic–computational works on R6G in NPoM cavities [1] and $CoPcF_{16}$ in TERS junctions [2], we reproduce mode-specific Raman intensity variations, frequency shifts, and adsorption-dependent signatures. These results demonstrate that chemical enhancement arises from ground- and excited-state charge redistribution and metal-induced polarization, governing the vibrational selectivity in plasmonic nanocavities.

This unified computational–spectroscopic methodology provides a microscopic understanding of chemical effects in plasmon-enhanced nanospectroscopy and a predictive route for designing plasmonic architectures with tailored vibrational and photochemical responses.

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Bichiral Plasmonic Nanoparticles with Geometry-Dependent Circular Dichroism

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Plasmonic nanoparticles (NPs) with an intrinsic chiral structure have emerged as a promising chiral platform for applications in biosensing, catalysis, and photonics. Quantitative understanding of the correlation between particle structure and optical chirality becomes increasingly important but still represents a significantly challenging task. In this talk, we present an interesting class of bichiral structures with geometry-dependent circular dichroism (CD). Bichiral plasmonic NPs exhibited intriguing geometry-dependent CD reversal; however, the crucial factor that dominates the plasmonic CD is still unclear. Combined with CD spectroscopy and theoretical multipole analysis, we demonstrate that plasmonic CD originates from the excitation of electric quadrupolar plasmons. Moreover, we further develop synthetic strategies to achieve the control of bichiral geometry with increasing architectural complexity. Our work sheds light on the physical origin of plasmonic CD and provides guidelines for the design of chiral structures toward chirality-dependent applications.

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Design and Synthesis of Chiroplasmonic Nanostructures: From Induced Chirality to Intrinsic Chirality

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Chiroplasmonic structures, with their distinctive optical activity and surface-enhanced effects, have shown great potential in biosensing, enantiomer discrimination, and asymmetric catalysis. This presentation summarizes our recent progress in the design and synthesis of chiroplasmonic nanostructures, spanning from induced to intrinsic chirality [1–6]. In the case of induced chirality, we employed a plasmon-enhanced circular dichroism strategy, where chiral molecular ligands are employed to induce controllable chiroptical responses in silver nanostructures. By tuning the molecular adsorption configurations and nanostructure morphologies, we significantly improved the g-factor and system stability. For intrinsic chirality, we established a general synthesis strategy based on chiral nanoconfinement, overcoming the limitations of conventional amino acid–directed methods and enabling the precise fabrication of diverse intrinsically chiroplasmonic nanostructures. Furthermore, by regulating the dielectric coupling between chiral Au cores and Cu2O shells, we achieved strong chiroptical activity in the near-infrared region. These intrinsically chiroplasmonic structures exhibit excellent chiroptical properties and have been applied in sensing, plasmon-enhanced electrochemical enantiomer recognition, and enantiomer-selective surface-enhanced Raman scattering (SERS).

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Bottom-up Fabrication of plasmonic nanostrcture for Highly Sensitive SERS Detection

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Surface-enhanced Raman spectroscopy (SERS) have gained wide application in recent years in the fields of food safety, environmental testing, catalytic monitoring, materials characterization and medical diagnosis due to their unique fingerprint specificity, single molecule sensitivity and non-labelled detection properties. The high homogeneity and reproducibility of the SERS substrates are undoubtedly critical parameters for highly sensitive quantitative assay applications.

SERS substrates can be constructed by both top-down and bottom-up preparation strategies. The top-down method is highly accurate and has good structural order. However, most of them require large equipment, are relatively costly, take a long time to prepare and cannot be produced in large quantities. The bottom-up technique, also known as nanoparticle assembly, has the advantage that the size and shape of the building blocks can be tuned by chemical synthesis techniques with advantages of simplicity and cost-effectiveness. The signal homogeneity and batch reproducibility of such SERS substrates are closely related to the size homogeneity, shape regularity, assembly density and alignment order of the assembled units. For the preparation and application of highly sensitive and homogeneous bottom-up SERS substrates, we have carried out a series of work on (1) the precise synthesis of noble metal nanocrystals; (2) the highly reproducible preparation of nanoparticle monolayers; (3) the construction of functional substrates and the rapid in situ detection of contaminants.[1-5] We believe that these works can provide an experimental basis for the preparation of low-cost high-performance SERS substrates and the widespread dissemination of SERS technology.

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Unlocking Plasmonic Hot Electron Utilization on Palladium Nanoparticles via Modulation of Bimetallic Interface for Enhanced Photocatalysis

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ABSTRACT:

Plasmonically generated hot electrons hold significant promise as non-thermal energy sources for driving chemical transformations, yet their catalytic efficacy is fundamentally constrained by the intrinsic Fermi level (E_F) limitations of noble metals. Using palladium (Pd) as a model system—a material renowned for its exceptional catalytic activity but restricted by its low E_F (≈ -5.1 eV)—we demonstrate a rational interfacial engineering strategy to amplify hot electron energy and reaction performance. By integrating copper (Cu) into Pd nanostructures, we achieve a 0.45—0.75 eV elevation in hot electron energy through tailored Cu-Pd interfacial electronic modulation. This advancement unlocks previously inaccessible reaction pathways, most notably enabling a direct four-electron reduction process on CuPd Janus nanoparticles synthesized via in situ Cu growth on Pd(111) surfaces, a mechanism absent in pure Pd systems. Furthermore, the introduction of Pd (100) facets synergistically enhances catalytic efficiency, elevating Suzuki coupling conversion rates from 65% to 94% while achieving a 1.6-fold acceleration in reaction kinetics. Combining in situ electrochemical surface-enhanced Raman spectroscopy (SERS) and theoretical calculations, we quantify that the hot electron energy level of Pd increases from −5.11 eV to −4.66 eV, with an increase of 0.45 eV, thereby optimizing hot electron transfer dynamics and redox potentials. This work provides a paradigm-shifting approach to plasmonic photocatalyst design, emphasizing dual control over hot electron energetics and interfacial charge transfer pathways as critical levers for overcoming inherent material limitations in energy-conversion applications.

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Digital colloid-enhanced Raman spectroscopy by single-molecule counting

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Quantitative detection of various molecules at very low concentrations in complex mixtures has been the main objective in many fields of science and engineering, from the detection of cancer-causing mutagens and early disease markers to environmental pollutants and bioterror agents. Moreover, technologies that can detect these analytes without external labels or modifications are extremely valuable and often preferred [1]. In this regard, surface-enhanced Raman spectroscopy can detect molecular species in complex mixtures on the basis only of their intrinsic and unique vibrational signatures [2]. However, the development of surface-enhanced Raman spectroscopy for this purpose has been challenging so far because of uncontrollable signal heterogeneity and poor reproducibility at low analyte concentrations [3].

Here, as a proof of concept, we show that, using digital colloid-enhanced Raman spectroscopy (dCERS), reproducible quantification of a broad range of target molecules at very low concentrations can be routinely achieved with single-molecule counting, limited only by the Poisson noise of the measurement process [4]. As metallic colloidal nanoparticles that enhance these vibrational signatures, including hydroxylamine-reduced-silver colloids, can be fabricated at large scale under routine conditions, we anticipate that dCERS will become the technology of choice for the reliable and ultrasensitive detection of various analytes, including those of great importance for human health [5].

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Development of stable plasmonic materials for environmental analytical applications

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Noble metal nanoparticles exhibit unique optical properties, including localized surface plasmon resonance (LSPR) and surface-enhanced Raman scattering (SERS). By modulating physicochemical parameters such as morphology, size, and surface modifications, the absorption spectra and Raman enhancement effects of these nanoparticles can be tuned, enabling the development of advanced optical nanosensing platforms. Despite their high sensitivity and excellent selectivity, the application of such sensors in complex environmental samples remains challenging due to issues such as spontaneous nanoparticle aging and matrix interference [1].

To address these challenges in plasmonic nanosensing for environmental analysis, we have designed a series of optical nanosensors incorporating various strategies, including the synthesis of stable materials, functionalization of sensor interfaces, and the design of probe molecules. These approaches aim to facilitate on-site and online analysis of trace pollutants in various environmental matrices, particularly in seawater. This report highlights the development of on-site detection methods and online Raman spectroscopy techniques for typical environmental pollutants [2-3]. These advancements provide crucial technological support for studying environmental processes.

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Ultrasensitive Surface-Enhanced Raman Scattering Measurement of Macromolecules

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Usually, the gap configurations of nanoparticle pairs or nanoparticle-on-mirror geometries of noble metals have been predominantly adopted to the surface-enhanced Raman scattering (SERS) [1, 2]. Under this framework, it is difficult to continuously improve the enhancement factor (EF) of SERS and to initiate its substantial progress toward practical applications. There is an inherent contradiction that large SERS EF is premised on or at the cost of small gaps, such as 1 nm and below, which limits the detection of biological macromolecules such as RNA, DNA and protein samples. Technically, the fabrication of repeatable extreme narrow gaps is a great challenge to this day. Inspired by nonradiative methodology involving anapole states and bound states in the continuum, we optimally tailor geometries of metasurface with capabilities for manipulating electromagnetic field in space and in time. In this case, when the gap gets wider, the SERS EF of pure electromagnetic enhancement can reach the order of 10^{12} by virtue of the reduction of the effective mode volume accompanying with higher-order electric multipoles, including electric quadrupole, octupole, 32-pole, 64-pole, 128-pole, etc [3]. In such open architectures, previous severe restrictions that so many biomolecules have been screened out for SERS detection have naturally disappeared [3].

This breakthrough in overcoming the framework of traditional electric dipole enhancement mechanism resolves the long-standing limitation (since 1997) where single-molecule SERS measurements were constrained by ultra-narrow gap "hotspots" [1, 2]. It paves the road for detecting biomacromolecules, breathing life into the SERS area, and clearing the obstacles on the way to practical application of SERS substrates.

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POSTER



Surface-Enhanced Raman Spectroscopy Combined with Advanced AI Algorithms for Liquid Biopsy in Cancer Diagnosis

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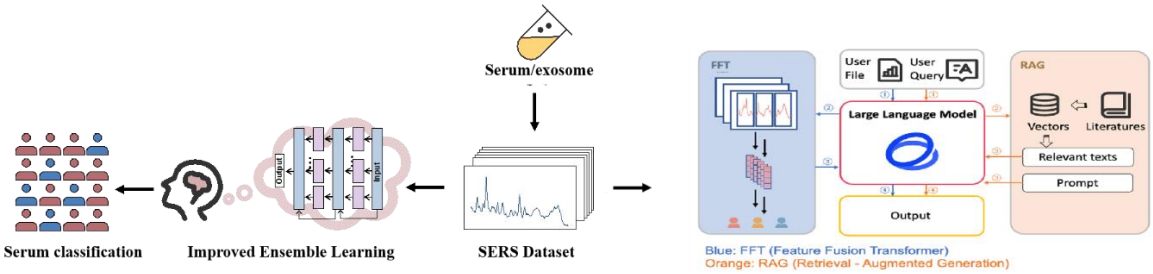
Liquid biopsy has emerged as a promising approach for non-invasive cancer early detection. Among various techniques, label-free surface-enhanced Raman scattering (SERS) provides a comprehensive molecular fingerprint of biofluids such as serum and exosomes. However, the clinical translation of SERS faces challenges including substrate inhomogeneity and the complexity of spectral data analysis.

To address these issues, two types of homogeneous SERS substrates were developed, which were combined with different machine learning algorithms respectively to achieve the diagnosis of lung cancer and hepatocellular carcinoma. For lung cancer detection, a platform was developed which combined with a uniform silver nanowire substrate and an improved ensemble learning model (SCSIEL)[1]. The system achieved 97.0% AUC and 93.4% accuracy on clinical serum samples (n=268), outperforming conventional biomarkers. For hepatocellular carcinoma, a feature fusion transformer model was designed to analyze SERS spectra of exosomes achieving 94.1% accuracy on clinical plasma samples (n=165)[2]. The model was further integrated into an AI agent (ChatExosome), which utilizes a large language model for interactive diagnosis and knowledge retrieval.

These studies demonstrate that the synergy between uniform SERS substrates and artificial intelligence algorithms could form a reliable and promising platform for cancer diagnostics, holding potential for broader application in diagnosing various diseases.



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Multi-stage screening and staging of obesity-induced T2DM via non-targeted SERS-AI platform with biochemical interpretability

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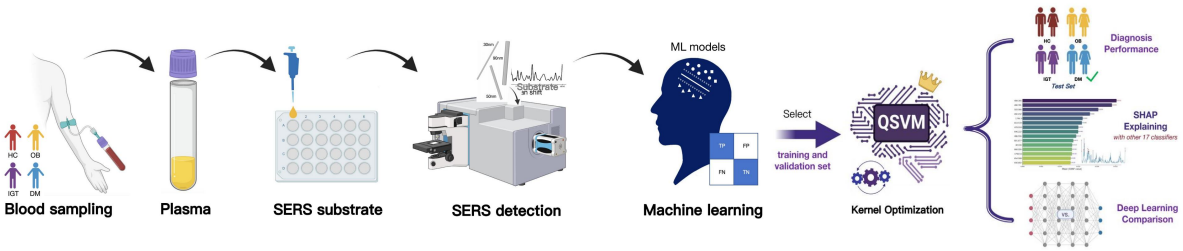
Type 2 diabetes mellitus (T2DM) is a prevalent chronic metabolic disorder characterized by progressive systemic changes, where reliable early-screening and rapid staging of obesity-induced T2DM stages (obesity [OBs], impaired glucose tolerance [IGTs], diabetes mellitus [DMs]) remains challenging due to the lack of stage-specific bio-markers.

Herein, we developed a robust non-targeted SERS-AI platform that integrated surface enhanced Raman scattering (SERS) and interpretable machine learning algorithms for multi-stage screening and staging of obesity-induced T2DM[1]. We analyzed 72,600 Raman fingerprint signals (300 spectra/sample) derived from plasma samples of 242 participants including 60 OBs, 60 IGTs, 62 DMs and 60 healthy controls using multiple candidate algorithms. Among all the models, Quadratic SVM achieved the highest quadruple-classification prediction accuracy of 94.5% after kernel optimization. Moreover, for the post-hoc interpretability of machine learning classification, SHapley Additive exPlanations (SHAP) analysis was applied on QSVM along with 17 other classifiers to identify the top 15 high-weight Raman shifts associated with stage-specific biochemical constituents, manifesting many possible bio-markers. Comparative evaluation also showed traditional models such as QSVM outperform neural networks in stability and interpretability under non-big-data conditions.

The ideal prediction accuracy of our effective and interpretable SERS-AI platform reveals the practical potential of such approach in multi-stage screening and staging where generalizable algorithms balance computational efficiency with in-depth insights, providing a foundation for clinical application as well as deepening our understanding of obesity-induced T2DM from a non-targeted biochemical perspective.



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Three-Dimensional SERS-Active Hydrogel Microbeads Enable Highly Sensitive Homogeneous Phase Detection of Alkaline Phosphatase in Biosystems

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Alkaline phosphatase (ALP) is a biomarker for many diseases, and monitoring its activity level is important for disease diagnosis and treatment. In this study, we used the microdroplet technology combined with an in situ laser-induced polymerization method to prepare the Ag nanoparticle (AgNP) doped hydrogel microbeads (HMBs) with adjustable pore sizes that allow small molecules to enter while blocking large molecules. The AgNPs embedded in the hydrogel microspheres can provide SERS activity, improving the SERS signal of small molecules that diffuse to the AgNPs. A specific hydrolysis reaction of ALP on 5-bromo-4-chloro-3-indolylphosphate (BCIP) was introduced and its product 5,5′-dibromo-4,4′-dichloro-1H,1H-[2,2’]bisindolyl-3,3′-dione (BCI) was employed to assess ALP activity due to its highly resonance Raman activity. The sensing platform was applied to model ALP activity in serum and evaluated ALP inhibitors. The SERS assay showed higher sensitivity than UV−vis absorption spectroscopy, with the lowest detectable ALP concentration of 1.0×10^{-20} M. In addition, the ALP activity in HepG2 cells was evaluated using this sensing platform, showing lower ALP-expressing activity than that of controls in response to hypoxia and ferroptosis. This SERS activated HMB shows great potential in detecting ALP and is expected to help analyze complex clinical samples [1].

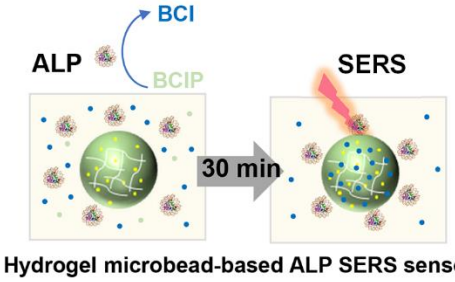

Figure 1. Schematic diagram of SERS active hydrogel for ALP detection

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Bioinspired Hierarchical Multi-synergistic Interface for the Capture and Phenotype Analysis of CTCs on a Multistage SERS-Microfluidic Platform

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Abstract: Accurate capture and phenotype identification of circulating tumor cells (CTCs) significantly contribute to cancer diagnosis and prognostic assessment. However, many CTCs isolation devices have been developed with sufficient capture efficiency, which suffers from cumbersome pre-processing, poor anti-interference ability and requires cumbersome release operations before CTCs analysis. Here, we drew inspiration from the filopodia-extending behavior and aggregate expression of biomarker on CTCs, a novel collaborative microfluidic device (CMD) integrated with a nanowire forests trap substrate (NFTS) was designed for the efficient capture of CTCs based on interface dual recognition and in-situ single-cell phenotype analysis in peripheral whole blood (Fig. 1). The nanowire forests on the surface of NFTS could “trap” the extended filopodia of CTCs. Moreover, aptamers modified on the NFTS surface acted as “baits” to promote the multi-interactions between the NFTS and CTCs, resulting in an efficient CTCs capture performance of 93.6% ± 3.5%. Finally, CMD can accurately capture CTCs from the blood of clinical cancer patient at different stages and perform in-situ analysis with SERS detection. The results of in situ single cell phenotype analysis for CTCs achieves high diagnostic sensitivity. Therefore, our CMD holds great potential as an effective device for the accurate capture and heterogeneity analysis of CTCs in clinical setting.

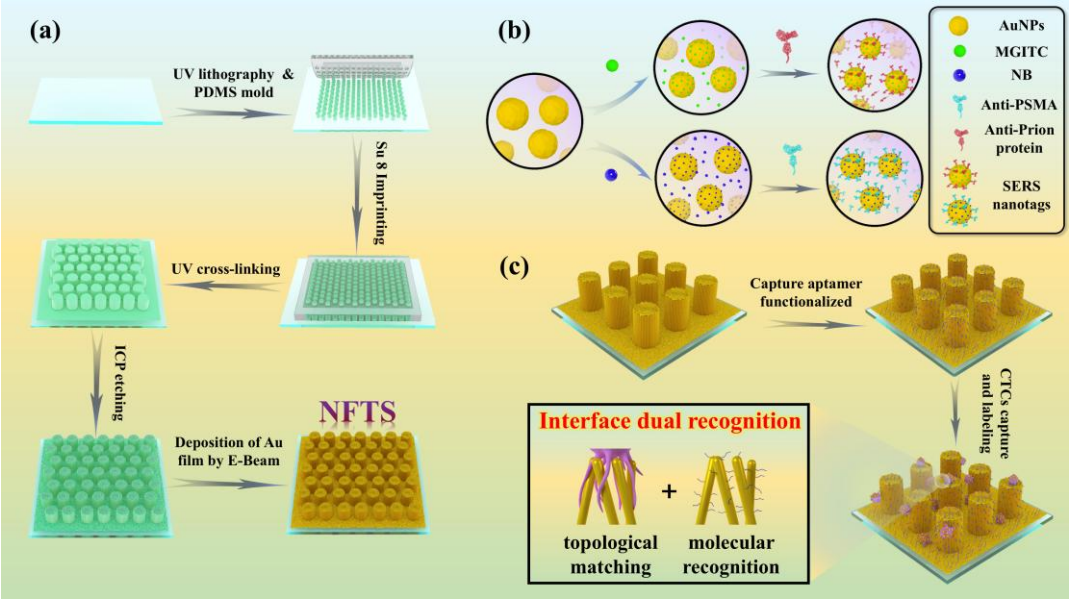

Fig. 1. The workflow of multistage capture and in-situ single-cell phenotype analysis with SERS measurement for CTCs on CMD.

Keywords: SERS; Microfluidic chip; Micro-nano hierarchical structure; Interface dual recognition; CTCs

A high sensitivity prostate-specific antigen SERS detection platform based on laser resonance nanoparticles

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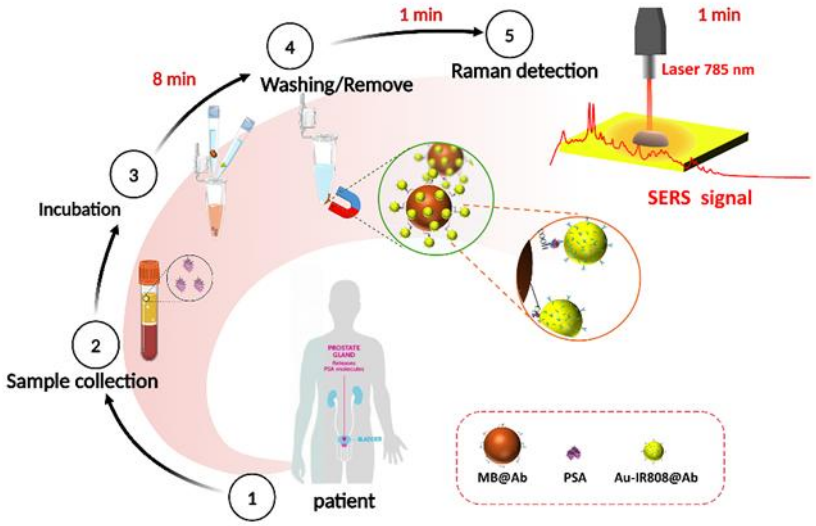
Accurate Quantitative Analysis of Cancer-Related Specific Biomarkers in Clinical Serum Is of Great Significance for Early Cancer Diagnosis and Treatment. Hospitals commonly use serum prostate-specific antigen (PSA) as a biomarker for prostate cancer diagnosis and prognosis. Prostate cancer cells produce more PSA than benign cells, leading to elevated PSA levels in the blood. In this study, an immunoassay for PSA detection was established, which is based on surface-enhanced Raman scattering (SERS) and combines magnetic beads with SERS nanotags. Currently, the PSA detection method used in hospitals has limitations: it takes 2 hours to obtain results, with high equipment and detection costs, resulting in low penetration in township hospitals in China. In contrast, the SERS-based method can deliver results in 10 minutes, with simple operation, low cost and portable equipment, making it suitable for township health centers. Seventy-five male clinical serum samples (most in the PSA "gray zone" of 4.0–10.0 ng/mL) were tested. The results showed good consistency with those measured by the electrochemical luminescence (ECL) system in hospital clinical laboratories, and the detection limit for actual patient samples reached 0.029 ng/mL. Therefore, this SERS-based clinical serum PSA marker detection method has great potential in township and rural markets.



Scheme 1 Schematic diagram of the PSA biosensor detection process based on SERS

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Microfluidic chip for myocardial infarction detection based on surface-enhanced resonance Raman spectroscopy

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Myocardial infarction (MI) is a severe cardiovascular disease, where early diagnosis is critical for patient rescue [1]. Surface-Enhanced Resonance Raman Scattering (SERRS) technology shows great potential for MI detection due to its high sensitivity and molecular specificity [2]. This study developed a SERRS-based microfluidic chip and a matched handheld Point-of-Care Testing (POCT) device for rapid, sensitive, and quantitative detection of MI-related biomarkers.First, a magnetic bead immunoassay was used: superparamagnetic beads modified with cTnT antibody A captured blood-borne cTnT, which then bound to SERRS-tagged Au@IR808 nanoparticles modified with antibody B, forming a sandwich immuno-complex. External magnetic field-enabled magnetic separation enriched these complexes for detection.Second, a microfluidic chip was designed to automate sample-magnetic bead complex mixing/reaction. Its fishbone-shaped protrusions, combined with flow splitting/merging, ensured efficient mixing for uniform reactions; magnetic adsorption of SERRS probes yielded stable signals.Finally, a one-click fully automated handheld POCT device was built for the chip. Results showed the chip-device system achieved high sensitivity and rapid detection, reliably identifying MI biomarkers within 5 minutes for qualitative analysis.In conclusion, this SERRS-based chip-device system offers high sensitivity and fast response, providing a feasible solution for early MI diagnosis. It provides new insights for microfluidic applications in cardiovascular diagnostics and references for bioanalysis/medical diagnosis research.

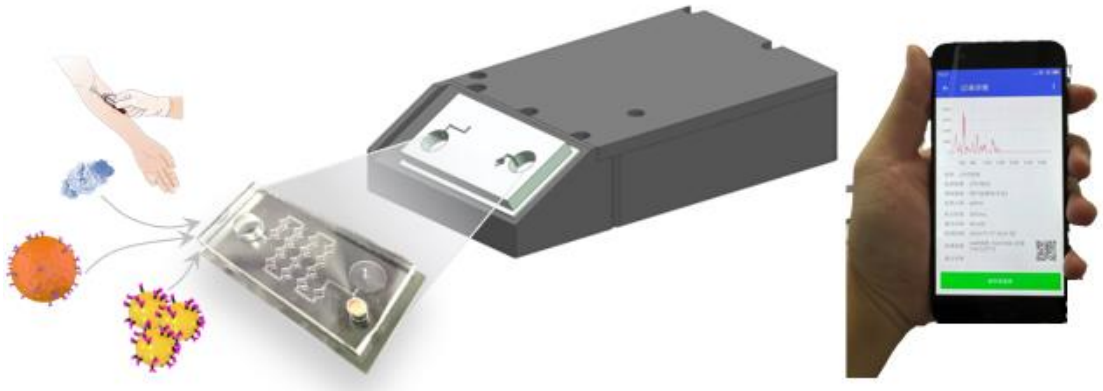

Figure 1: Detection process of myocardial infarction using microfluidic chip based on surface-enhanced resonance Raman spectroscopy in combination with Raman spectrometer

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Kill two birds with one stone: Cu_2O@Ag nanoparticles for SERS detection and inhibition of *Escherichia coli* O157: H7

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Escherichia coli (*E. coli*) O157:H7 is a common foodborne pathogen that can cause infections even at low dose. The rapid, sensitive detection and effective inhibition of *E. coli* O157:H7 in food is of great significance for ensuring public health and safety. However, there are many challenges in the actual detection process, such as poor selectivity, long time consumption, low sensitivity and many other interference factors. In this work, we synthesized silver-coated Cu_2O nanoparticles (Cu_2O@Ag NPs) by in situ growth of Ag NPs on the surface of Cu_2O NPs. After being functionalized with specific antibody together with magnetic beads (MBs), a sandwich structure sensor based on surface enhanced Raman spectroscopy (SERS) was further constructed for the detection and inhibition of *E. coli* O157:H7. Specifically, the constructed probes demonstrate (1) ultrasensitive SERS detection in contaminated milk samples, and (2) synergistically enhanced antibacterial activity of the composite material. A series of key conditions in the experiment were optimized and verified. Ultimately, the developed SERS sensing platform can achieve the isolation and detection of *E. coli* in milk within 22 min, with a limit of detection (LOD) for 1 CFU/mL, ranging from 1 to 10^4 CFU/mL. In addition, Cu_2O@Ag NPs exhibited excellent antibacterial activity, with minimum inhibitory concentrations (MIC) of 62.5 μg/mL and 125 μg/mL against *E. coli* and *Staphylococcus aureus* (*S. aureus*), respectively. Our work provides a strategy that combines bacterial sensitive detection with inhibition, which has great potential in the future monitoring of foodborne pathogenic bacteria.

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Background-free Rolling Circle Amplification for SERS Bioassay Using Chimeric Hairpin Integrated CRISPR/Cas12a System

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Rolling circle amplification (RCA) has revolutionized nucleic acid detection owing to its isothermal simplicity. However, over two decades of clinical application have been hampered by off-target amplification and incompatibility with double-stranded DNA (dsDNA). Herein, a strategy, specifically cleavage of rationally designed DNA/RNA chimeric hairpin pre-primer by dsDNA-targeted CRISPR/Cas12a to release ssRNA for initiating RCA (SCOPE-RCA), is proposed for nucleic acid identification of African swine fever virus (ASFV). Leveraging the trans-cleavage capability of CRISPR/Cas12a, the SCOPE-RCA system achieves 99% ssDNA cleavage within 20 minutes, thus largely suppressing non-specific amplification. Eventually, cascaded with catalytic hairpin assembly (CHA) coupled surface-enhanced Raman scattering (SERS) signal amplification, the SCOPE-RCA system can detect ASFV in mock-infected samples as low as 59 copies/mL. With its ease of use and ultrasensitive detection capability, the SCOPE-RCA system demonstrates significant potential for nucleic acid research and clinical applications.

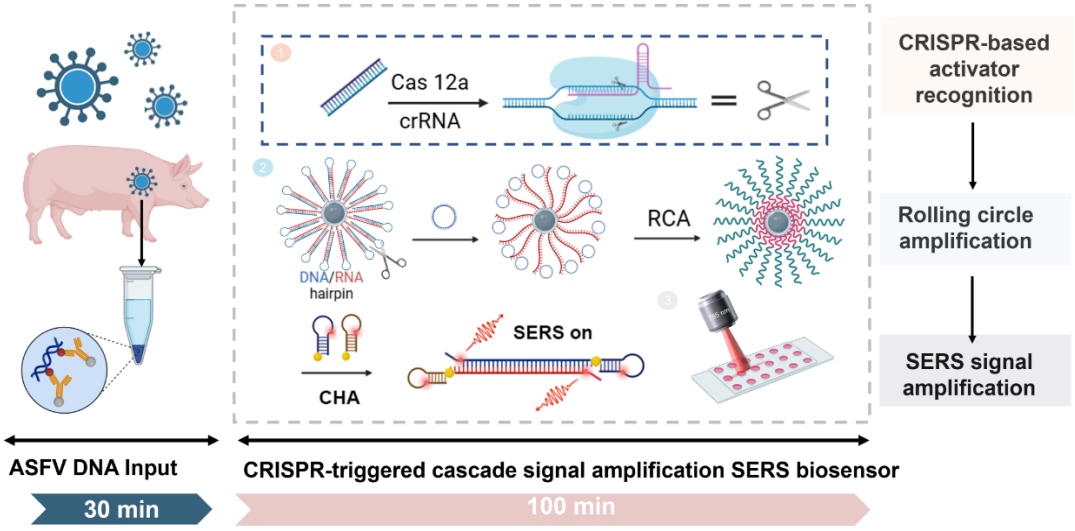

Figure 1： Schematic diagram of the principle of the SCOPE-RCA strategy。

Key words： ASFV, CRISPR, rolling circle amplification, SERS, chimeric hairpin.

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Application of SERS in Oxygen Reduction Reaction

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The combination of surface-enhanced Raman scattering (SERS) and electrochemistry (EC–SERS) provides a breakthrough research method for revealing the molecular mechanism of oxygen reduction reaction (ORR). As the core process of metal-air batteries, ORR involves complex multi-electron transfer paths and key intermediates (such as *O, *OOH, *OH), and traditional electrochemical methods are difficult to directly capture transient species. With its ultra-high surface sensitivity and unique "fingerprint" recognition ability, SERS realizes the in-situ dynamic tracking of ORR intermediates on the electrode surface through the local electromagnetic field enhancement effect generated by noble metal nanostructures[1]. Studies have confirmed that SERS can analyse the oxygen molecule adsorption mode (end/side), O–O bond vibration characteristics and intermediate product evolution path at different potentials in real time, and quantitatively correlate the active sites of the catalyst (such as single atom M–N_4 site) and reaction selectivity [2].

In this study, we effectively embedded the tetra-atomic zinc complex precursor on graphene nanosheets to obtain a tetra-atomic cluster catalyst (Zn_4-NSG) with a half-wave potential of 0.90 V, showing high ORR activity. The Zn_4-NSG zinc-air battery showed significant stability after 350 hours of continuous operation. In addition, X–ray photoelectron spectroscopy (XPS), SERS, and synchrotron radiation X–ray absorption fine structure (XAFS) measurements were used to observe the changes in the valence state of the active site, the coordination environment, and the reaction intermediates. Combined with theoretical calculations, it is verified that the electronic effect of the polyatomic configuration changes the length of the O–O bond of *OOH and adjusts the configuration of *OOH on the surface of the Zn-based catalyst. The O–O bond is more likely to break during the reaction, and then the basic steps in the ORR process are more likely to occur, thereby improving the ORR performance[3].

Keywords: SERS; ORR; Intermediate

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First Highly Sensitive Detection of 6PPD Using a SERS-Colorimetric Dual-Mode Method

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The global automotive industry's rapid expansion fuels annual growth in demand for N-(1,3-dimethylbutyl)-N'-phenyl-p-phenylenediamine (6PPD), a critical rubber stabilizer. Yet this surge in demand amplifies environmental risks posed by 6PPD and its toxic derivative N-(1,3-dimethylbutyl)-N′-phenyl-p-phenylenediamine-quinone (6PPD-Q), underscoring an urgent need for efficient, straightforward detection methods.

To address this gap, silver nanoparticles (Ag NPs) with excellent SERS enhancement effects were successfully synthesized for target SERS detection. It further integrated a colorimetric method—leveraging the visible red color from 6PPD's reaction with $CuSO_4$—to develop a dual-mode (SERS-colorimetry) platform, enabling quantitative analysis of 6PPD and its key oxidation product N-(1,3-dimethylbutyl)-N'-phenyl-p-phenylenediamine quinone imine (6PPD-QI). Both SERS and color-based detection of 6PPD-QI exhibited linear responses over 10^{-3} to 10^{-9} g/mL, with a SERS limit of detection (LOD) as low as 2.24×10^{-9} g/mL. Mutual validation of the two modes enhanced result accuracy and reliability, while application to lake water samples confirmed the platform's suitability for environmental detection.

This work provides a practical technical tool for monitoring 6PPD-related pollutants, supporting efforts to mitigate their ecological impact.

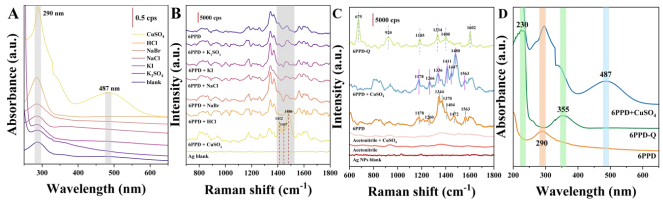

Fig. 1. (A) UV-vis images and (B) SERS images after different coagulants were mixed with 6PPD, (C) SERS signals of 6PPD-Q, 6PPD + $CuSO_4$ and 6PPD (silver nanosubstrate), (D) comparison of ultraviolet absorption peak results.

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Enhanced Non-Destructive SERS Detection in Muscle Tissue: Functionalizing Acupuncture Needles with Planar Silver Dendrites

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In vivo, non-destructive, and highly sensitive detection within biological tissues, particularly muscle, is of paramount importance for disease diagnosis and food safety. Surface-enhanced Raman scattering (SERS) is an ideal technique due to its ultra-high sensitivity and fingerprinting capability. However, developing implantable SERS sensors that withstand insertion, maintain stable signals, and are reusable remains challenging.

This study developed a high-performance, insertable SERS sensor based on planar silver dendrites-functionalized acupuncture needles (needle@P-AgD) fabricated via atomic layer deposition (ALD). The sensor was prepared by electrochemically depositing silver dendrites (AgD) onto needles, followed by a process combining ALD of an alumina protective layer, mechanical rolling, and chemical etching to transform the 3D dendritic structures into a dense, planar configuration strongly bonded to the substrate.

The results demonstrate that the needle@P-AgD sensor exhibits exceptional performance: 1) High Adhesion and Stability: The synergistic effect of ALD and rolling, coupled with subsequent thermal annealing, creates robust adhesion between the planar Ag dendrites and the needle. It withstands up to 50 insertion-withdrawal cycles in simulated muscle tissue (agarose gel) without significant degradation in microstructure or SERS activity, whereas conventional dendrite-modified needles (needle@AgD) suffer severe detachment and signal loss. 2) Excellent Detection Capability: The sensor achieves a detection limit of 10^{-8} M for Rhodamine 6G (R6G). Crucially, it enables non-destructive, in situ detection by successfully penetrating a gel with an R6G concentration gradient, acquiring depth-resolved chemical information from different depths (2-16 mm). 3) Versatility and Reusability: The sensor was successfully applied to detect the drug 6-Mercaptopurine (6-MP) and the banned dye Malachite Green (MG) in simulated muscle tissue, demonstrating broad application potential. Furthermore, an ALD-assisted thermal annealing cleaning cycle effectively regenerates the sensor, allowing stable SERS performance over at least 5 reuse cycles.

In summary, the needle@P-AgD sensor integrates high sensitivity, exceptional mechanical stability, non-destructive detection capability, and reusability. It presents a highly promising novel tool for in vivo and real-time SERS detection within muscle tissue.

Schiff base reaction-assisted highly sensitive SERS internal standard strategy for detection of vanillin derivatives in tea matrices

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Vanillin (4-hydroxy-3-methoxybenzaldehyde), an aromatic compound derived from vanilla pods, possesses a unique aroma and flavor. Currently, it is widely used as an additive in the food industry, including in tea, milk powder and ice cream. However, excessive consumption of vanillin can cause nausea, dizziness, allergies and vomiting. Various methods have been established to detect vanillin content. These methods exhibit good sensitivity in vanillin detection but are limited by complex pretreatment steps, time consumption, and expensive equipment, which significantly restrict their application in rapid on-site monitoring. Thus, there is an urgent need to develop a highly sensitive, rapid, simple, and low-cost method for monitoring vanillin concentration in food. In this work, a Schiff base reaction-based SERS detection method is proposed for the highly sensitive detection of vanillin in tea. Ag nanocubes (Ag NCs) are functionalized with 4-aminothiophenol (4-ATP), whose amino group undergoes a Schiff base reaction with the aldehyde group of vanillin to form a stable C=N imine group. Highly sensitive detection of vanillin is achieved by identifying the C=N stretching vibration peak at 1650 cm^{-1} after the Schiff base reaction. Using the C-S stretching vibration peak at 1077 cm^{-1} as an internal standard, a linear relationship is established between the value of I_{1650}/I_{1077} and vanillin concentration. The results show a satisfactory linearity between vanillin concentration and the value of I_{1650}/I_{1077}, with a correlation coefficient (R^2) of 0.995 and a low limit of detection (LOD) of 10 μg/L. Furthermore, this method requires no tedious pretreatment and achieves a detection limit of 10 μg/L for vanillin in real tea samples, exhibits good universality in the detection of aldehyde flavorants in different teas. Our work presents a universal strategy for the highly sensitive detection of aldehyde flavorants via the Schiff base reaction, which has great potential of SERS technology in flavorant molecule detection.

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Tunable Gold Nanocrystal Films for Ultrasensitive and Reproducible SERS Detection

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Surface-enhanced Raman scattering (SERS) is a powerful analytical technique [1], but conventional substrates often rely on sophisticated nanofabrication methods [2], limiting their cost-effectiveness and scalability [3].

We report a facile strategy for preparing gold nanocrystal (Au NC) films with tunable plasmonic and electronic properties, enabling highly sensitive and reproducible SERS detection. Au NCs (3–5 nm) with a typical plasmon resonance at ~510 nm were employed as building blocks. By employing a simple film assembly and subsequent chemical treatment, the interparticle spacing and coupling strength were effectively regulated, resulting in a controllable insulator–metal transition without altering the metal core. This ligand-exchange process simultaneously induced a porous network structure, which further enhanced molecular accessibility and hot-spot density. Such structural tunability provided an optimized dielectric environment for plasmon enhancement. SERS experiments using rhodamine 6G and crystal violet as probe molecules revealed both strong enhancement and excellent reproducibility (relative standard deviation <10%). Importantly, the substrates enabled quantitative detection with a linear response over a wide concentration range (10^{-4}-10^{-11} M), reaching a detection limit as low as 10^{-11} M. Moreover, the SERS activity remained stable over storage for at least two weeks.

This work demonstrates that, through a simple and reproducible preparation route, highly uniform Au NC films can achieve ultrasensitive molecular detection, offering strong potential for practical applications in environmental monitoring and biomedical sensing.

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Raman Scattering Measurement of Single Nanoparticle Collision

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Plasmonic nanoparticles have found widespread applications in fields such as biosensing and catalytic analysis due to their small size, ease of functionalization, good biocompatibility, and low toxicity [1]. Although existing synthesis methods can effectively control the overall morphology, surface ligands, size, and material composition of nanoparticles, unavoidable heterogeneity still exists among nanomaterials at the single-particle level. Therefore, conducting measurements at the single-particle level is crucial for gaining a deeper understanding of material properties and optimizing synthesis strategies.

The single-particle collision electrochemistry method utilizes ultramicro/nanoelectrodes under electrochemical confinement to monitor, in real-time and in situ, the electrochemical reactions occurring within the electron tunneling region of individual nanoparticles. This reveals statistical behaviors in heterogeneous systems, such as the size distribution [2], catalytic activity [3], and electronic band structure [4] of single particles. However, this method still struggles to directly monitor the distribution of ligands on the nanoparticle surface and the changes in electrochemical interfacial reactive species during the collision process.

To address this challenge, this study developed a single nanoparticle collision measurement system that combines optical and electrochemical techniques. When a noble metal nanoparticle collides with a plasmon-resonant substrate, a nanogap structure can form, creating "hot spots" with significant electromagnetic field enhancement effects. This greatly enhances the Raman signal of interfacial molecules during the collision process. By analyzing the intensity and peak position changes of the Raman signals within these "hot spot" regions, the distribution state of ligands on the nanoparticle surface and the dynamic information of interfacial chemical reactions occurring during the electrochemical collision process can be elucidated.

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In Situ SERS Probing the Structure Change and Interfacial Water on Monolayer 1T'-TMD during Acid HER

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Unconventional 1T' phase transition metal dichalcogenides (TMDs) stand out as one of the most promising non precious metal electrocatalysts for the hydrogen evolution reaction (HER) [1]. Herein, we employed in-situ electrochemical Raman spectroscopy to monitor dynamic changes in interfacial water and phonon modes during the HER process. We systematically compared the HER performance of four 1T'-TMDs, namely MoS_2, WS_2, $MoSe_2$, and WSe_2. Focusing on the A_g vibrational modes at the Γ-point (Gamma point) and the 2LA bands induced by double-resonance Raman scattering, we found that different TMDs counterparts exhibit distinctly varied structural strains and charge doping behaviors under HER conditions. By integrating density functional theory (DFT) calculations to analyze the evolution of interfacial water during the reaction, we further uncovered the intrinsic differences among 1T'-TMDs with varying elemental compositions [2]. This work deepens the fundamental understanding of the structure-activity relationship in 1T'-TMD-based electrocatalysts and provides valuable guidance for the rational design of high-performance HER catalysts.

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Interfacial water regulation enables efficient Zn^{2+} transport and electrode stability

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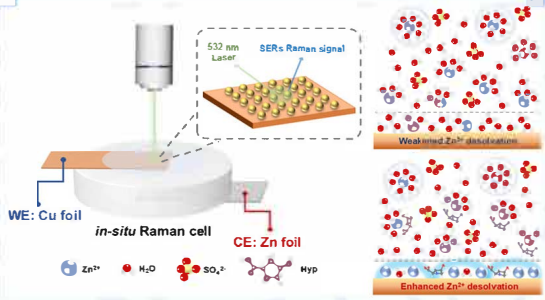
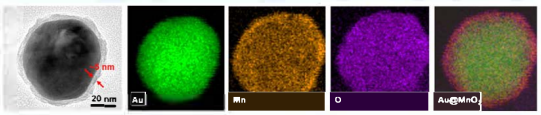
WHAT WE CONCERNED

- Aqueous zinc-ion batteries (AZIBs) have emerged as a promising next-generation energy storage technology due to their inherent safety and environmental sustainability.
- The dynamic evolution of the solvation structure at the electrode/electrolyte interface plays a critical role in AZIBs, influencing complex issues such as the hydrogen evolution reaction (HER) and parasitic side reactions.
- These challenges are intrinsically linked to perturbations of interfacial water molecules and associated hydrogen-bond network rearrangements during Zn^{2+} solvation/desolvation.

METHODS





- In situ monitoring of Zn^{2+} deposition dynamics via SERS and MD.
- Unveiling the underlying mechanism of MnO_2 lattice evolution in AZIB cathodes using Au@MnO_2 probes.
- Dynamic interfacial water control strategy to achieve stable and long cycle life of AZIBs.

RESULTS

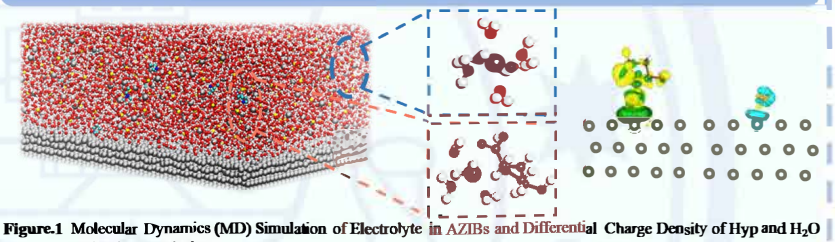


Figure.1 Molecular Dynamics (MD) Simulation of Electrolyte in AZIBs and Differential Charge Density of Hyp and H_2O on (002) Crystal Plane

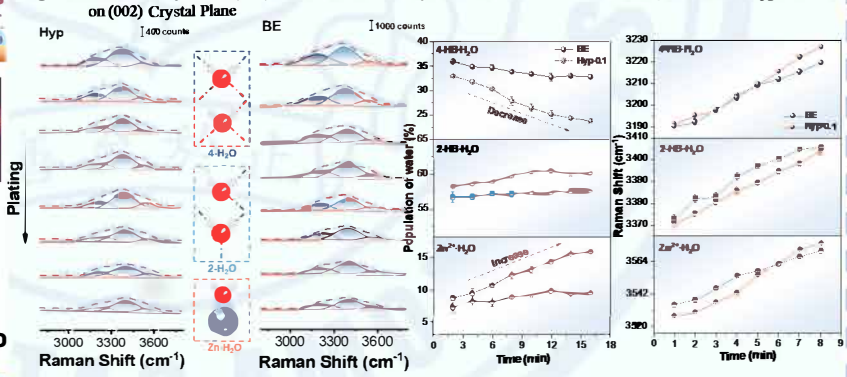


Figure.2 In situ SERS spectroscopy of interfacial water on Zn electrode, Gaussian fitting and ratio comparison of stretching modes (ν(O-H)) for 4-H_2O, 2-H_2O and Zn-H_2O.

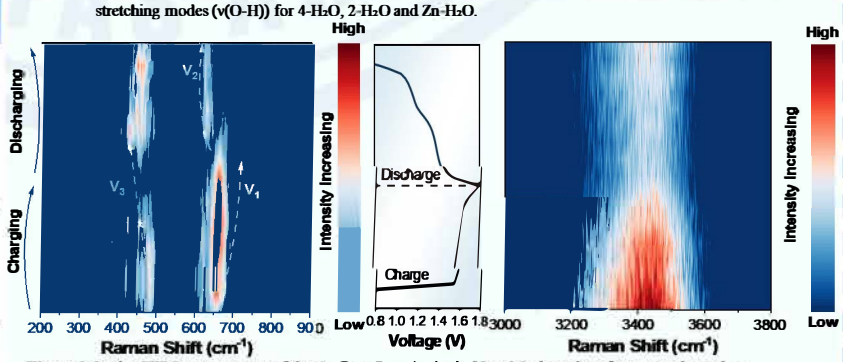


Figure.3 In situ SERS spectroscopy of the Au@MnO_2 cathodes in Hyp-0.1 electrolyte for one cycle testing.

CONCLUSION

- The Zn^{2+} solvation structure was effectively reconfigured by Hyp, leading to a stabilized interfacial physicochemical field.
- *In situ SERS* monitoring elucidated the evolution of interfacial water during Zn deposition, revealing a characteristic decline of 4-H_2O and the increase of Zn^{2+}-H_2O.
- Efficient interfacial water regulation mechanism enabled the AZIBs to achieve exceptional cycling stability for over 8,000 h.

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Template-based fabrication of plasmonic nanopore for integrated optical-electrochemical sensing

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Integrated nanopore electrochemistry-Raman spectroscopy techniques have attracted considerable attention due to their capability of providing molecular information on analytes. The key to detecting Raman signals in nanopores lies in the construction of plasmonic nanopores. However, achieving stable and rapid fabrication of plasmonic nanopores with high localized surface plasmon resonance (LSPR) remains a major obstacle hindering the further advancement of nanopore–Raman spectroscopy technique integration. Herein, we introduce a template-assisted strategy for the fabrication of plasmonic nanopores, in which porous noble-metal materials are employed as enhancement templates to be integrated with quartz nanopipettes. Using Au Nanocage (Au NC) as template, we utilized a centrifugation-based method to precisely anchor Au NCs at the nanopipette. The porous structure of Au NCs serves both as plasmonic hot spot and channels for molecules, thereby enabling electrochemical-Raman spectroscopy detection of λ-DNA. We anticipate that this approach will promote the further advancement of nanopore electrochemistry-Raman spectroscopy techniques.

Fast Ion Dynamic Exchange at Electrochemical Interfaces

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Since their first commercialization in the 1990s, lithium-ion batteries (LIBs) have overwhelmingly dominated the energy storage landscape for more than three decades [1, 2]. Typical LIB electrolytes comprise a lithium salt, solvents, and/or functional additives, which collectively determine both the bulk electrolyte properties and the electrode/electrolyte interfacial chemistry. At the negative electrode, the solid electrolyte interphase (SEI) forms via reductive decomposition of the electrolyte. The electrical double layer (EDL) is the region where electrochemical reactions occur, however, the impact of lithium salt concentration variations within the EDL on solvation structures and Li^+ transport remains insufficiently understood. In this work, we employ electrochemical atomic force microscopy (EC-AFM), gap-enhanced Raman spectroscopy, and machine learning molecular dynamics simulations to investigate how lithium bis(fluorosulfonyl)imide (LiFSI) concentration in tetraglyme (G4)-based solvated ionic liquids influences interfacial solvation structures and ion transport in LIBs. We reveal that anion participation in the primary solvation sheath suppresses solvent decomposition at the interface, modulates Li^+ transport mechanisms, and enables reversible Li^+ intercalation/deintercalation. These findings highlight the critical role of solvation tuning in interfacial electrochemistry, as validated by advanced characterization techniques, and provide insights toward the development of durable, high-performance lithium-ion batteries.

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In-Situ SERS Insights into Tailoring Key Intermediates and Interfacial Water in $Ag_{92}Ru_8$ Aerogel for Sustainable Nitrate Reduction to Ammonia

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The pursuit of efficient ammonia production through electrochemical nitrate reduction reaction (NO_3RR) at ambient conditions is a significant demand in green and energy-saving industries. Rational tailoring of the competing yet complementary processes of water splitting and nitrate activation at reducing potentials is pivotal for manipulating the efficiency and selectivity of ammonia synthesis. Herein, $Ag_{92}Ru_8$ aerogel has been synthesized via a one-step reduction strategy, demonstrating remarkable in tuning the reaction intermediates and interfacial water dynamics. Based on $Ag_{92}Ru_8$ aerogels, a high NH_3 Faradaic efficiency (FE) of 97.16%, and a superior yield rate of 2.49 mmol h^{-1} $mg_{cat.}^{-1}$ were achieved at −0.5 V. And the corresponding Zn-NO_3^- battery exhibited potential as a power source for practical application. More importantly, in-situ SERS tests captured the signal of interfacial water and Ru–H intermediates generated from water splitting promoted by Ru species, which demonstrated the crucial rule of *H intermediates in the hydrogenation process of NO_3RR with direct spectral evidence. Density functional theory (DFT) results further demonstrate that *H intermediate generated from interfacial water are promoted by Ru species in the hydrogenation process of NO_3RR, offering valuable insights for the targeted design of efficient catalysts[1].

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[1] Junjie Chen[a,b], Xiaomei Xing[a], Sisi Wen [c], Mengyuan Li[a], Di Liu[a], Wenji Jiang [a], Xinyi Shao[a], Ruikai Qi[d], Yumei Yang[a], Ming Mu[a], Zheng-jie Chen[e,]*, Bing Zhao[a] and Wei Song[a]*, “Tailoring key intermediates and interfacial water at $Ag_{92}Ru_8$ aerogel toward sustainable ammonia synthesis from nitrate” Chemical Engineering Journal xxx (xxxx) 167002.

TiO_2-Coated Glass Fiber Membranes with Ag/rGO for Instantaneous and Sensitive Detection of Sulfasalazine

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Abstract: Sulfasalazine (SSZ) is a sulfonamide that belongs to the important class of medications called anti-inflammatories. It is commonly used in the treatment of inflammatory bowel disease such as ulcerative colitis and Crohn's disease[1]. Current detection methods often encounter challenges such as limited sensitivity and prolonged detection times[1-3]. Therefore, the development of a highly sensitive, rapid-response sensor capable of in-situ detection of Sulfasalazine holds considerable promise for practical applications.

In this study, we propose a novel sensor based on TiO_2-coated glass fiber membranes, polyelectrolyte, and Ag/rGO composites for the highly sensitive and real-time detection of Sulfasalazine. The sensor significantly enhances the adsorption capacity and charge transfer efficiency of the antibiotic molecules through the synergistic effect of the Ag/rGO composites and the aggregation-induced polyelectrolyte interaction with Ag, enabling ultra-low concentration detection of Sulfasalazine, with a detection limit of 10^{-11} M. Additionally, the flexible composite membrane exhibits excellent uniformity (RSD = 1.27%) and outstanding temporal stability (>30 days). Notably, the TiO_2 membrane exhibits photocatalytic degradation properties, effectively breaking down antibiotic residues during the detection process, which allows for the repeated use of the material. After five cycles, the TiO_2 membrane retains 96.56% of its initial spectral intensity.The sensor demonstrated exceptional performance in practical applications, successfully detecting Sulfasalazine on the surfaces of fruits and in river water samples, with recovery rates ranging from 95.81% to 111.74%. Most importantly, this method enables real-time, on-site detection of Sulfasalazine in various samples, overcoming the timeliness issues associated with traditional detection techniques. This approach provides a convenient, efficient tool for environmental monitoring and food safety testing.

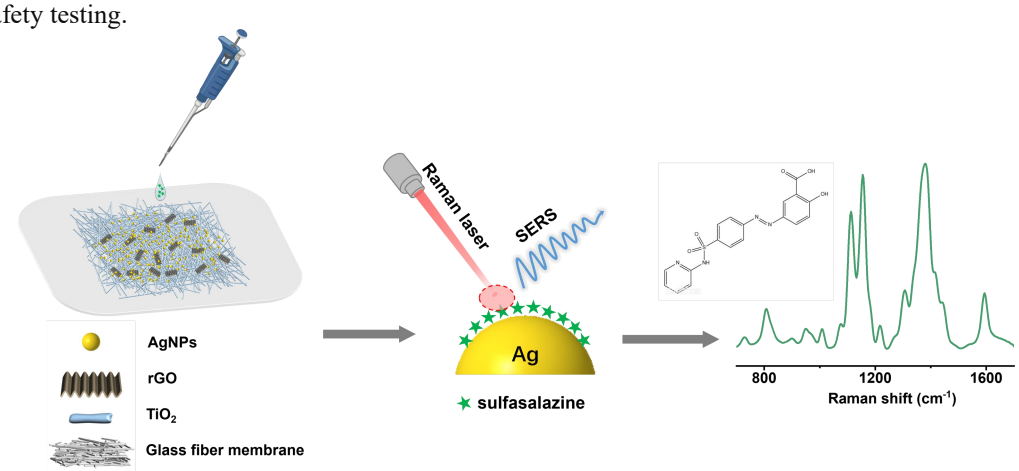

Figure 1. Schematic illustration of TiO_2-Ag/rGO composite membrane for rapid detection of sulfasalazine.

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Designing Your Own Smart SERS Sensor (DYOSSS): An AI-Assisted Smart Agent for Discovering New Quantitative Biosensing Mechanisms

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Surface enhanced Raman spectroscopy (SERS) offers rich molecular fingerprint information and holds great potential for quantitative chemical analysis in biosensing, diagnostics, and environmental monitoring. The development of quantitative SERS sensors remains largely empirical, relying on chemists' intuition to select key spectral indicators.[1] This reliance hampers efficiency, particularly for analytes with low Raman scattering cross sections. Thus, we propose DYOSSS (Design Your Own Smart SERS Sensor), an autonomous agent for rapid SERS sensor design. This agent integrates high-throughput acquisition of Raman spectra at varying analyte concentrations, machine learning-based spectral classification, and interpretability algorithms to identify the most influential spectral features for analyte quantification. The identified features can be applied as new quantitative sensing indicators for the analyte after validation using chemical expertise. Using urea as a model analyte, DYOSSS uncovered new spectral indicators for quantitative sensing and achieved a detection limit of 10^{-8} M, surpassing most previously reported urea biosensor based on SERS. DYOSSS has the potential to accelerate the discovery and development of novel, high performance SERS sensors.

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Raman-based 3D Reconstruction of Tissue Lesions Using Tetrahedral Unstructured Mesh Refinement

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Three-dimensional reconstruction of tissue lesions based on Raman optics provides a promising approach for noninvasive deep-tissue imaging. However, the complex geometry and optical heterogeneity of biological tissues impose strict requirements on numerical precision and computational stability[1, 2]. To address the limitations of traditional structured grids in geometric adaptability and computational cost[3], this study proposes an **unstructured mesh partitioning method based on tetrahedral elements with local adaptive refinement**, applied to Raman source localization and 3D reconstruction. The proposed method dynamically adjusts mesh density in potential light-source regions to achieve high local accuracy while maintaining global computational efficiency. Two refinement modes—4-subdivision and 8-subdivision—were designed, providing approximately fourfold and eightfold improvements in spatial resolution, respectively. A unique node-mapping and volume-conservation mechanism ensures topological consistency and continuity of physical parameters across refined regions.
Results demonstrate that the proposed mesh refinement method effectively reduces the size of the finite element system matrix and enhances reconstruction stability, achieving an optimal balance between accuracy and efficiency. In numerical simulations, the reconstruction error using unstructured meshes was significantly lower than that of uniform grids. Combined with a feasible-region pre-partitioning strategy, the localization error of Raman sources was reduced to the millimeter level. This work establishes an efficient and scalable numerical framework for high-precision Raman-based 3D lesion reconstruction, offering potential applications in rapid and accurate deep-tissue optical imaging.

Key word: Raman Optics, Three-Dimensional Reconstruction, Local Adaptive Refinement

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A dual-signal SERS biosensor based on magnetic nanoparticles for sensitive exosome detection

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The precise detection of exosomes in biofluids offers great potential for non-invasive cancer diagnostics[1, 2], yet achieving high sensitivity and reproducibility in complex matrices remains challenging[3]. Herein, we developed a self-calibrating magnetic SERS aptasensor for accurate quantification of oral cancer-derived exosomes. The sensor was synthesized via a layer-by-layer assembly approach to form an internal standard encoded core-satellite structure ($NiFe_2O_4$@PB@Ag), which was subsequently conjugated with SH-modified complementary DNA (cDNA) to form $NiFe_2O_4$@PB@Ag-cDNA. This was then hybridized with a ROX-functionalized aptamer to construct the final $NiFe_2O_4$@PB@Ag-dsDNA SERS aptasensor. Magnetic-induced assembly of the sensor, combined with surface plasmon effects, significantly enhanced the SERS performance. Furthermore, the SERS sensor demonstrated a broad detection range (5.0×10^3~5.0×10^{11} particles/mL) for exosomes, with a limit of detection (LOD) as low as 1.15×10^3 particles/mL. This method can be employed for the detection of exosomes in plasma, providing a robust and reliable platform for exosome-based liquid biopsy in clinical applications.

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Raman Spectroscopy Combined with Machine Learning for the Classification of Authentic versus Adulterated Xinjiang Honey

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As a widely used technique for material identification, Raman spectroscopy poses certain challenges in intuitively and empirically distinguishing substance-related components. The differentiation between authentic and adulterated honey is a typical case of particular importance in the food industry. In this study, a method combining Raman spectroscopy with deep learning algorithms was proposed to analyze the characteristic data of authentic and adulterated Xinjiang honey. A deep learning model based on convolutional neural network (CNN) integrated with an attention mechanism was developed, and random Gaussian noise was added to expand the dataset. This model achieved an accuracy of 98.2% in classifying authentic and adulterated Xinjiang honey. By combining Raman spectral data with deep learning technology, this study provides a new and effective approach for solving similar substance identification problems, which holds significant application prospects[1].

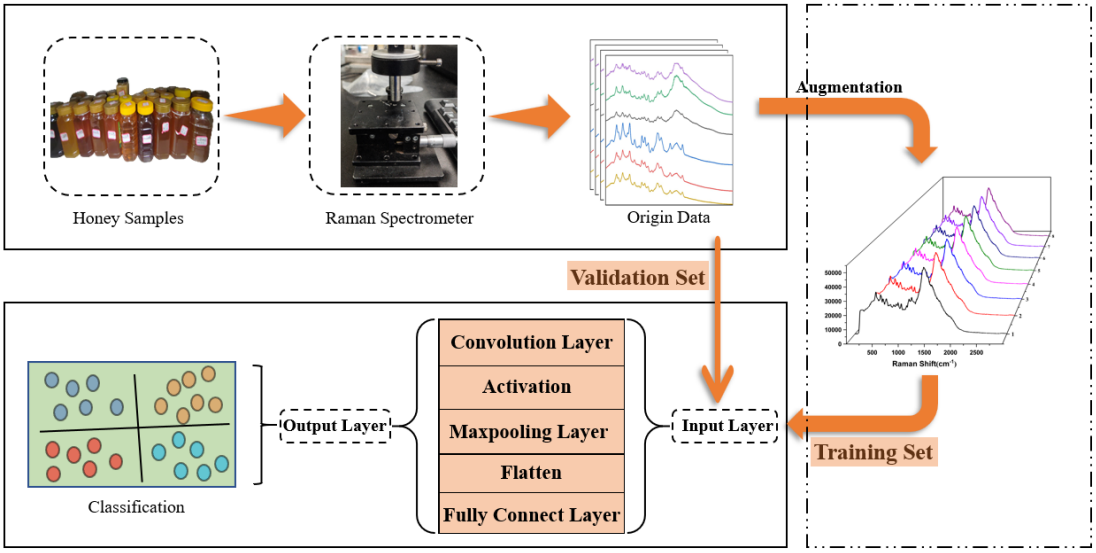

Figure.1 Flowchart of authentic and adulterated Xinjiang honey classification using machine learning

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SpecRecFormer: Similarity-driven methods for adaptive open-set recognition of complex spectra

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Abstract: In practical mixed-spectrum recognition tasks, it is common to encounter spectral categories that were not present during training, which gives rise to the open-set recognition problem. Most conventional deep learning classification models rely on the closed-set assumption, presuming that all test categories have been observed during training. As a result, they often misclassify unknown categories as one of the known classes, leading to distorted outcomes or even severe misidentifications. A common strategy to address this issue is to introduce an additional "unknown" class and apply an error threshold to detect unseen samples[1,2]. This method works reasonably well when the spectral features of unknown samples differ substantially from those in the training set. However, in cases where known and unknown components coexist within a mixed spectrum, it becomes challenging to determine an appropriate threshold, often resulting in the failure to reliably identify the unknown components.

This paper proposes SpecRecFormer, an open-set recognition model based on similarity measurement. The model architecture combines the local feature extraction capability of a dual-channel convolutional neural network with the global dependency modeling of a Transformer. To facilitate effective learning of complex mixed spectra, positive and negative augmented spectra are first generated from single-component polycyclic aromatic hydrocarbons reference spectra using data augmentation techniques. These augmented spectra pairs are then used in contrastive training, enabling the model to learn similarity representations between unknown mixed spectra and known single-component reference spectra in the database. Furthermore, the relationship between decision threshold setting and spectral complexity is investigated, leading to the introduction of a dynamic threshold adjustment strategy that enhances the generalization capability of the model in complex scenarios. Experimental results demonstrate that SpecRecFormer achieves rapid analysis of 16 mixed categories formed by arbitrary combinations of four single-component polycyclic aromatic hydrocarbons reference spectra, attaining 93.75% accuracy in closed-set testing. When evaluated on an extended polycyclic aromatic hydrocarbons test set containing categories unseen during training, the model achieves 89.21% accuracy, confirming its effectiveness in recognizing target classes while rejecting non-target classes in open-set scenarios. Moreover, on a real-world polycyclic aromatic hydrocarbons surface-enhanced Raman scattering test set incorporating various environmental disturbances and measurement noise, the model maintains a high accuracy of 93.63%, demonstrating robust recognition performance under practical conditions. These results collectively indicate that SpecRecFormer holds promising potential for reliable spectral analysis in complex environmental monitoring applications.

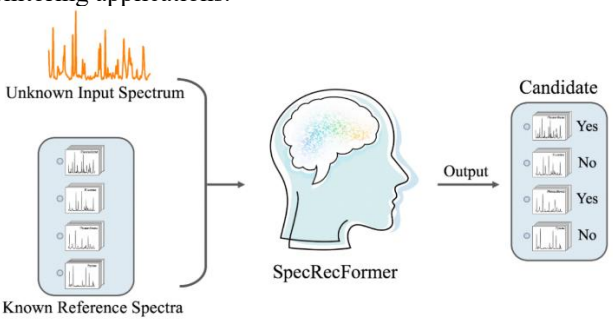

Figure 1. Schematic illustration of similarity-based open-set recognition approach.

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SERS-Based Rapid Quantification of Propofol for Real-Time Perioperative Precision Sedation Monitoring

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Propofol is the most commonly used intravenous (IV) anesthetic and sedative in the clinical practice due to its rapid onset and short distribution half-life[1]. However, its narrow therapeutic window and high inter-individual pharmacokinetic variability pose challenges in achieving appropriate sedation levels in diverse patients[2]. Moreover, residual circulating propofol during the early recovery phase has been associated with oversedation, prolonged mechanical ventilation, and an increased incidence of postoperative delirium (POD), particularly in elderly patients or those with organ dysfunction[3]. These concerns highlight the urgent need for rapid and accurate quantification of propofol to ensure clinical safety. In this work[4], we developed a sensitive and rapid surface-enhanced Raman scattering (SERS) platform based on vertically aligned Au nanorods array with enhancement factor $>10^7$ was fabricated for directly propofol detection in unprocessed postoperative blood samples. Propofol was rapidly and selectively derivatized with 2,6-dichloroquinone-4-chloroimide (DCQ) under alkaline conditions, yielding a strong characteristic SERS peak at 1278 cm^{-1}. This assay displayed a linear response from 1 ng mL^{-1} to 20 μg mL^{-1} with a limit of detection of 0.38 ng mL^{-1} in 2 min for each sample. Both the artificial simulated serum and clinical postoperative blood samples testing demonstrated excellent quantification performance of as-prepared SERS platform. Significantly, comparative validation with high-performance liquid chromatography (HPLC) showed a Deming slope of 0.95, confirming analytical interchangeability. Moreover, a subsequent cohort of 32 patients demonstrated a robust inverse correlation between SERS-derived propofol levels and Richmond Agitation-Sedation Scale scores (Spearman ρ=-0.80, $p<0.0001$), a single threshold of 1.17 μg mL^{-1} predicted moderate sedation to deep sedation with 100 % sensitivity and 100 % specificity. This work presents the first clinically validated, reagent less-cleanup SERS assay for intravenous anesthetic monitoring, providing a practical framework for real-time therapeutic drug management in critical care and anesthesia.

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In–situ Surface–enhanced Raman spectroscopy monitoring of Rhodamine 6G Degradation in Agricultural Products by TiO_2@COF@Au multifunctional photocatalyst

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Rhodamine 6G (Rh6G), a major industrial dye pollutant, causes environmental hazards via discharge, bioaccumulates in food/agricultural products to threaten human health, while existing detection/degradation technologies and regulatory supervision are inadequate.

To address this research gap, a TiO_2@COF@Au composite photocatalyst with excellent photocatalytic performance and high surface-enhanced Raman scattering (SERS) activity was synthesized for the photocatalytic degradation and in-situ SERS monitoring of Rh6G. By integrating UV-vis and SERS as a dual-detection strategy, cross-validation via significant color changes ensured the accuracy and reliability of the results. Under xenon lamp irradiation, the TiO_2@COF@Au composite achieved complete decolorization of 10 mg/L Rh6G solution within 60 min. For Rh6G SERS detection, the composite exhibited a wide linear range of 10^{-3} to 10^{-11} g/mL with a limit of detection (LOD) as low as 2.0×10^{-11} g/mL. Application of the catalyst in detection and degradation experiments on milk, fruit peel, and vegetable leaf samples confirmed its practical value for the detection and efficient degradation of Rh6G residues in food and agricultural products.

The developed multifunctional nanoplatform provides a practical approach for organic dye photodegradation and in-situ SERS monitoring, contributing to environmental pollutant remediation and real-time surveillance.

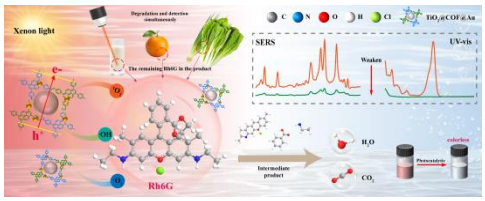

Fig. 1. The photocatalytic degradation of Rh6G by TiO_2@COF@Au and the real-time SERS monitoring were carried out.

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Preparation and Humidity Sensitive Properties of NH2-MIL-125/Silicon Nanoporous Pillar Array

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A Sulfhydryl-β-cyclodextrin (HS-β-CD) modified Ag/porous silicon (HS-β-CD/Ag/PS) substrate was successfully prepared and used for the detection of acetophenone. The amount of HS-β-CD modification could be controlled by its concentration, which had a significant impact on the SERS performance of the substrates. The substrate with the optimal amount of HS-β-CD modification exhibited a strong SERS response to acetophenone molecules. It also displayed good homogeneity with a relative standard deviation (RSD) of 9.56 %, a SERS enhancement factor of up to 2.3×10^{7}, and a detection limit of low to 1×10^{-8} M. The high SERS performance of the substrate can be attributed to the effective enrichment of acetophenone by HS-β-CD, which can form an inclusion complex with acetophenone, trapping it in the cavity. These results suggest that HS-β-CD/Ag/PS substrates hold great potential for SERS analysis of the breast cancer marker acetophenone.

Keywords: Surface-enhanced Raman scattering (SERS); Ag/porous silicon; Acetophenone; Sulfhydryl-β-cyclodextrin (HS-β-CD)

Enantioselective Surface-Enhanced Raman Scattering by Chiral Au Nanocrystals with Chiral Fields and Internal Standards

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The chiral discrimination of enantiomers is crucial for drug screening and agricultural production. Surface-enhanced Raman scattering (SERS) is proposed for discriminating enantiomers benefiting from chiral plasmonic materials. However, the mechanism of enantioselective SERS is unclear, and fluctuating SERS intensities may result in errors. Herein, this work demonstrates a reliable SERS substrate using chiral Au nanocrystals with finely modulated chiral fields and internal standards [1]. Chiral electromagnetic fields are enhanced after modulation, which is conducive to increasing the difference in the enantiomeric SERS intensity, as evidenced by the experimental and simulation results. Furthermore, the SERS stability is improved by the corrective effect of the internal standards, and the relative standard deviation is significantly reduced. Using finely modulated chiral fields and internal standards, L- and D-phenylalanine exhibit a stable six times difference in SERS ratio. Theoretical simulations reveal that linearly polarized light can also excite the chiral fields of chiral Au nanocrystals, indicating non-chiral far-field light is converted into chiral near-field sources by chiral Au nanocrystals. Thus, the mechanism of enantioselective SERS can be elucidated by the scattering difference of chiral molecules in chiral near fields. This study will pave the way for the development of enantioselective SERS and related chiroptical technologies.

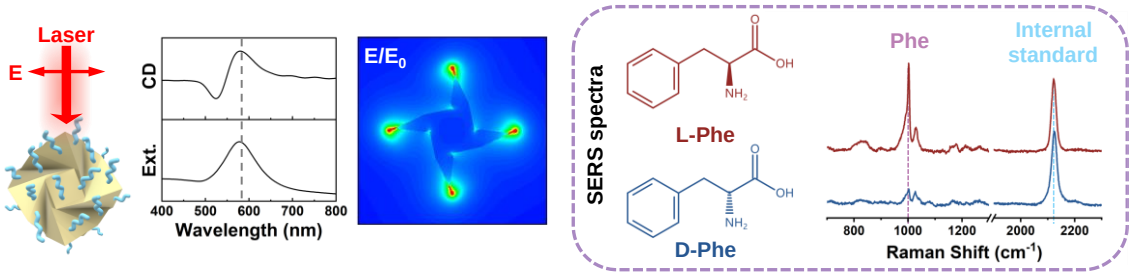

Figure 1. Enantioselective SERS based on chiral Au nanocrystals.

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Single-cell SERS profiling of IL-6-Associated Pyroptosis in Breast Cancer Subtypes

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Breast cancer remains one of the leading causes of cancer-related death among women worldwide. Its molecular subtypes—including hormone receptor-positive, HER2-positive, and triple-negative breast cancer (TNBC)—exhibit distinct signaling pathways, treatment responses, and prognoses. Pyroptosis, an inflammatory form of programmed cell death characterized by membrane rupture and cytokine release, has emerged as a promising target in cancer therapy. Among these cytokines, interleukin-6 (IL-6) plays a central role in modulating tumor progression, immune activation, and the inflammatory tumor microenvironment. Understanding IL-6 dynamics at the single-cell level is thus essential for revealing the functional heterogeneity of cancer cells in response to therapeutic stimulation.

In this study, we developed a microfluidic droplet-based platform integrated with surface-enhanced Raman spectroscopy (SERS) for high-throughput single-cell detection of IL-6 and reactive oxygen species (ROS). To construct a dual-response immunosensor for IL-6 and ROS, we designed a dual-probe system. The detection probe was synthesized by co-modifying silver nanoparticles with anti-IL-6 antibodies and reactive oxygen species sensitive molecule 4-mercaptophenylboronic acid (4-MPBA). The capture probe was prepared by anti-IL-6 antibodies and the Raman active molecule Nile Blue onto magnetic nanoparticles. In this configuration, the 4-MPBA acts as the ROS-responsive linker. The abundance of silver nanoparticles enriched around the magnetic beads is directly proportional to the amount of captured IL-6 and can be quantitatively evaluated by the stable signal strength of Nile Blue, thereby providing a reading of IL-6 release. Using this platform, we analyzed two breast cancer cell lines representing different subtypes: MDA-MB-231 (triple-negative) and SKBR3 (HER2-positive). Cells were subjected to electrical stimulation alone and in combination with cisplatin to assess subtype-specific pyroptotic responses. The platform enabled real-time monitoring of IL-6 and ROS at the single-cell level, revealing marked heterogeneity in cytokine secretion between subtypes and treatment conditions. Notably, combined electrical and cisplatin stimulation significantly enhanced IL-6 secretion in a subtype-dependent manner. These findings highlight the value of single-cell analysis in uncovering distinct pyroptotic regulatory mechanisms and suggest a potential role for IL-6 as a functional biomarker in subtype-specific cancer therapy. This platform offers a powerful tool for advancing personalized approaches in cancer treatment.

This work was supported by the National Natural Science Foundation of China (22373041 and 22173035), National Key Research and Development Program of China (2023YFC3706002), Science and Technology Development Program Projects of Jilin Province (20220101046JC), the Fundamental Research Funds for the Central Universities, and Innovative research project of State Key Laboratory of Supramolecular Structure and Materials.

Keywords: SERS, Droplet microfluidics, Single-cell analysis, Pyroptosis, Interleukin-6

Layered Biometal Nanoporous Platforms for SERS Sensing

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Abstract

Nanoporous metals are extensively investigated as platforms for applications in plasmonics. They present high surface areas and strong local electric fields that can be tuned at different energies, playing with the choice of the metals and the morphology of the porous layers. Until recently, research in the field of plasmonics has primarily focused on porous metals composed of a single element, with limited attention given to the impact of alloy composition. The investigation of bi-metallic systems has only just begun to emerge in the literature. Combining two or more different plasmonic metals, it could be possible to explore the interactions between two metals excited at specific energies. This involves plasmonic coupling, electron transfer, band hybridization at the interface, electromagnetic field interactions, and possibly thermal and electronic energy transfer depending on separation, size, and materials involved. The analysis of bi-metal systems can also be interesting in biomolecule detection, such as in the case of Surface Enhanced Raman Scattering (SERS). Here we report, for the first time, a detailed study (comprising morphological analyses, numerical modelling, and optical spectroscopies) on bi-metal nanoporous platforms prepared with a dry-synthesis method enabling the easy and controllable fabrication of bilayers combining different metals such as Au, Ag, and Cu.

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Ultrafast photoelectron imaging of spatiotemporal plasmonic vortices

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Introduction

Spatiotemporal vortices intertwine orbital angular momentum (OAM) with both space and time, offering new opportunities for fundamental physics and advanced applications [1,2]. Achieving spatiotemporal vortices in interface-bound waves beyond free space represents a significant frontier in nanophotonics, with great potential for revolutionizing on-chip devices. Here, we introduce a distinct class of two-dimensional structured wave in the optical regime, that is spatiotemporal plasmonic vortex (STPV), via a general chronotopic engineering approach. Using interferometric time-resolved photoemission electron microscopy (ITR-PEEM) [3], we directly image their evolution with nanometer–attosecond resolution, and demonstrate tunable vortex charge and position. Quantum-path analysis of coherent two-photon photoemission process further reveals their nonlinear harmonics and angular-momentum conservation.

Method

Theoretical formulation of STPVs

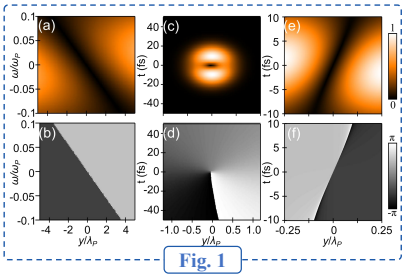

Fig. 1

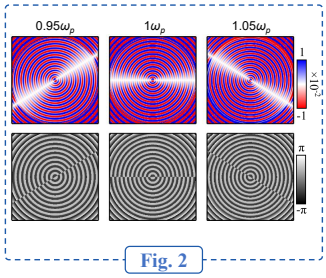

Fig. 2

The chronotopic field engineering for STPVs can be described in terms of space-frequency coupling and its Fourier-transformed counterpart in the space-time domain, which is achieved via interfering a pair of surface plasmon polariton (SPP) wave packets with distinct OAM and a controlled temporal delay. Their differential OAM ΔL_P and frequency-dependent inter-plasmon delay Δt_P give rise to space-frequency coupling, manifesting as a spatial chirp with a characteristic π-phase dislocation in the space–frequency domain [Figs. 1(a), (b)], and wraps into a vortex field with a donut-shaped profile and spiraling phase in the space-time domain via a U(1) mapping [Figs. 1(c), (d)]. By the focusing action, the field can be reshaped into Hermite–Gaussian like modes with vanishing OAM and a symmetry-enforced phase inversion at the focal point, accompanied by the re-emergence of a line defect [Figs. 1(f), (g)].

Such chronotopic coupling is conveniently described by the location of the frequency-dependent destructive interference: $y_{null}(\omega) \approx (\pi - \omega\Delta t_P)/\Delta L_p$, where the spatial and temporal coupled by the slope $\Delta t_P/\Delta L_p$, which directly determines the line-defect [Fig. 2]. In the space-time (y-t) domain, the surface normal electric field of STPVs can be formulated as:

$$E_P(y,t) \propto \left[\frac{t}{\sigma_t^2} + i\frac{\Delta L_P}{\Delta t_P}y\right] exp\left[-\frac{t^2}{2\sigma_t^2} - \frac{y^2}{2\sigma_y^2} - i\omega_0 t\right],$$

where σ_y and σ_t represent the spatial and temporal full width half maximum of the vortex pulse.

Results

ITR-PEEM Imaging of STPV dynamics

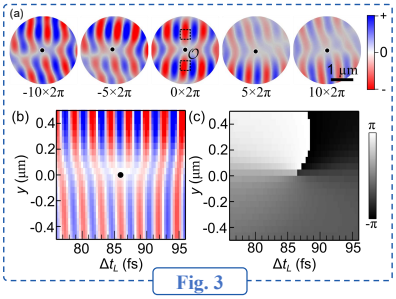

Fig. 3

Figure 3(a) shows a sequence of PEEM images capturing the propagation a STPV at the plasmon group velocity toward the focal point $\mathcal{O}$. A fork-shaped interference pattern with l=1 is observed prior to $\mathcal{O}$. At $\mathcal{O}$, the vortex collapses into a line defect, and subsequently revives with reversed chirality beyond it, a consequence of parity inversion. The evolution of the STPV in the y-t plane is reconstructed in Fig. 3(b), and its corresponding demodulated phase is presented in Fig. 3(c). The distinct fork-shaped pattern, together with spiraling phase structure, confirms a vortex carrying unit OAM.

Results

Control over STPV generation

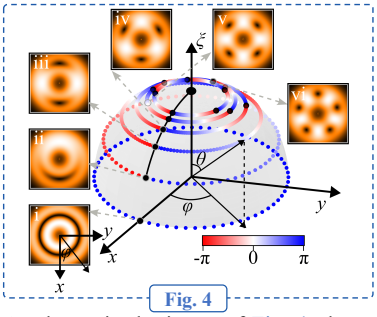

Fig. 4

The generation mechanism can be generalized to provide tunable control over both the number and positions of STPVs [Fig. 4]. The number of observed STPVs is governed by the ΔL_p between the interfering SPP wave packets, which is trigonometrically projected on the ξ-axis of the parameter hemisphere as:

$$\xi = cos\left[\frac{\pi}{2} - tan^{-1}(\Delta L_P/2)\right].$$

As shown in the insets of Fig. 4, the number increases with $|\Delta L_p|$: no vortex forms at $|\Delta L_p| = 0$; a single STPV with a charge of 1 appears at $|\Delta L_p| = 1$, manifesting as a crescent-shaped dark region; and higher-order singularities fractionalize into multiple fundamental vortices for $|\Delta L_p| > 1$. Their azimuthal positions are determined by the phase-slip and rotational symmetry of the wave field, and can be gradually tuned by adjusting the inter-plasmon delay Δt_p, as:

$$\varphi_N = \frac{(2N+1)\pi - \omega_P \Delta t_p}{\Delta L_p}.$$

Harmonics of STPV and OAM conservation

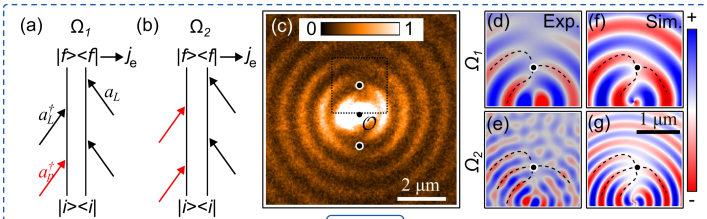

Fig. 5

We probe the nonlinear harmonics of STPVs and their OAM conservation via quantum-path-resolved photoemission. Figures 5(a)-(b) show the double-sided Feynman diagrams of two quantum pathways that can transport electrons to the final state for photoemission during the 2PP process. The Ω_1 component corresponds to the STPV field at the fundamental spatial-temporal frequencies arising from one-plasmon excitation, while the Ω_2 compoenent originates from pathways with two successive plasmon interactions, producing the upconverted STPV field at twice of the fundamental spatiotemporal frequency. By applying Fourier filtering to our ITR-PEEM movies [a snapshot shown in Fig. 5(c)], we isolate distinct quantum pathways in the 2PP process. The filtered Ω_1 image [Fig. 5(d)] displays the characteristic fork-shaped distribution with l=1, while the Ω_2 image [Fig. 5(e)] reveals the second harmonic, exhibiting a characteristic splitting that confirms OAM up-conversion to l=2. This direct observation of OAM doubling is accurately reproduced by our density-matrix simulations [Figs. 4(f), (g)], establishing that the spatiotemporal topology is imprinted directly into the nonlinear surface polarization, mapping onto progressively higher-order harmonics.

Conclusion

- We have introduced chronotopic engineering as a general framework for generating spatiotemporal vortices in reduced-dimensional systems, and demonstrated their experimental realization through nonlinear photoelectron imaging of tunable, on-chip STPVs and their OAM-conserving harmonics with nano–atto resolution.
- Beyond establishing a new synthetic route for structured surface waves, our results highlight the topological nature of the underlying spatiotemporal defects and the power of quantum-path–sensitive imaging to access their dynamics.

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Portable Raman-Combined Microfluidic Sensor with Femtosecond Laser-Fabricated VCSAS for SERS Detection of Trace Pb^{2+} and Cd^{2+} in Seawater

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Abstract: Rapid and sensitive detection of heavy metal ions such as Pb^{2+} and Cd^{2+} in seawater is critical for environmental monitoring and public health. In this study, we present a novel surface-enhanced Raman scattering (SERS) microfluidic sensor integrating a femtosecond laser-fabricated volcanic crater-shaped array substrate (VCSAS). As illustrated in Fig. 1, the VCSAS was constructed via UV lithography and femtosecond laser processing on PMMA@AuNPs composites, forming a hierarchical micro/nano structure that significantly enhances electromagnetic field coupling and Raman signal amplification. The substrate features periodic nano-craters with embedded AuNPs, enabling uniform hot spot distribution and superior signal reproducibility. Coupled with a portable Raman system and pump-free microfluidic chip, the sensor achieves label-free detection of Pb^{2+} and Cd^{2+} in seawater with detection limits as low as 10^{-12} M and 10^{-11} M, respectively. The entire detection process is completed within 150 seconds without external pumping, making it highly suitable for on-site environmental analysis.

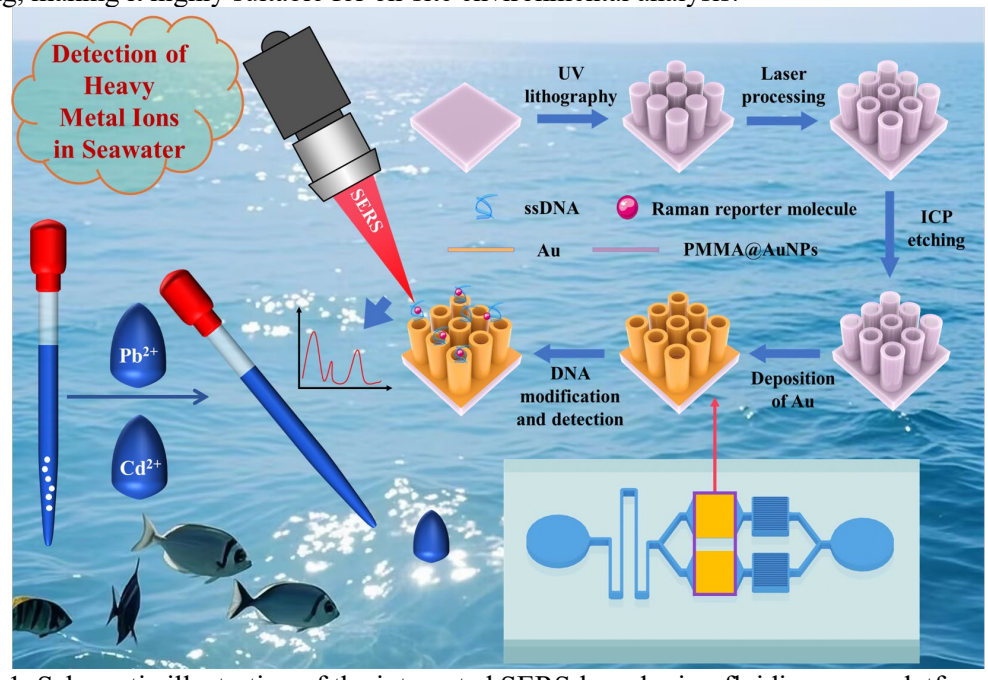

Fig. 1. Schematic illustration of the integrated SERS-based microfluidic sensor platform. The VCSAS substrate, fabricated by femtosecond laser processing of PMMA@AuNPs, is embedded within a pump-free microfluidic chip for rapid and sensitive detection of Pb^{2+} and Cd^{2+} in seawater samples.

Keywords: SERS; Microfluidics; Femtosecond laser; Heavy metal ions; Portable detection.

Nano-micro hierarchical anemone-like substrates integrated SERS-based microfluidic sensor for highly sensitive detection of Hg^{2+} in seawater

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Abstract: With the continued advancement of global industrial manufacturing and heavy metal–based economic activities, the excessive discharge of heavy metal ions has become an increasingly severe environmental issue. In response to the needs of ecological monitoring and human health protection, this study focuses on the trace detection of mercury ions in seawater using surface-enhanced Raman scattering (SERS). As illustrated in **Fig. 1**, a novel anemone-like array substrate (ALAS) with hierarchical micro-nano structures was designed and fabricated to achieve multidimensional enhancement through electric field coupling. The ALAS substrate forms an ordered nanoantenna array on polystyrene (PS) nanospheres, improving light-trapping efficiency and inducing surface plasmon resonance, thereby significantly enhancing the Raman scattering signals of reporter molecules. Meanwhile, the microfluidic chip designed with a capillary pump enables complete loading of the internal channel with the test sample within 100 seconds. The results demonstrate that the integrated chip exhibits excellent responsiveness across a mercury ion concentration range from 10^{-7} to 10^{-12} M, offering valuable insights for coastal environmental monitoring and ecological restoration.

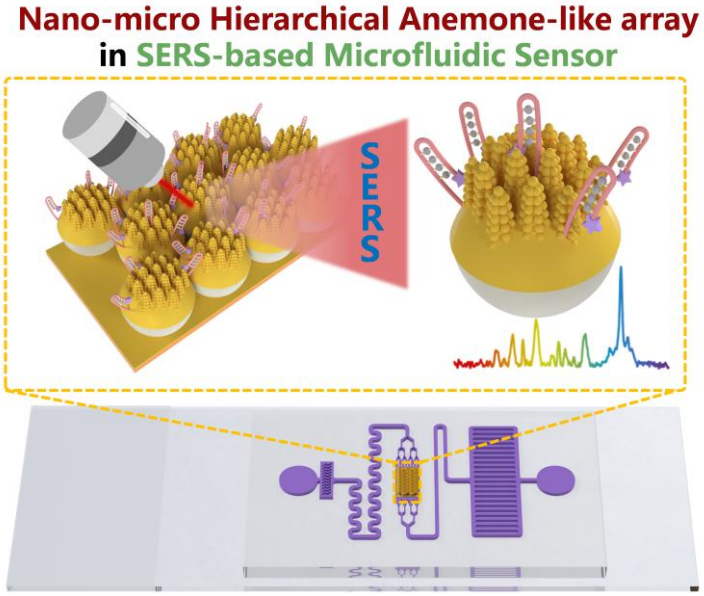

Fig. 1. Schematic diagram of a microfluidic chip with integrated with an anemone-like array SERS substrate for the sensitive detection of mercury ions in seawater.

Keywords: SERS; Anemone-like array; Nanoantenna; Multi-dimensional enhancement; Pump-free microfluidic chip.

Stretchable Plasmonic SERS Hydrogel Patch for Versatile Metabolite Sensing on Bio-interfaces

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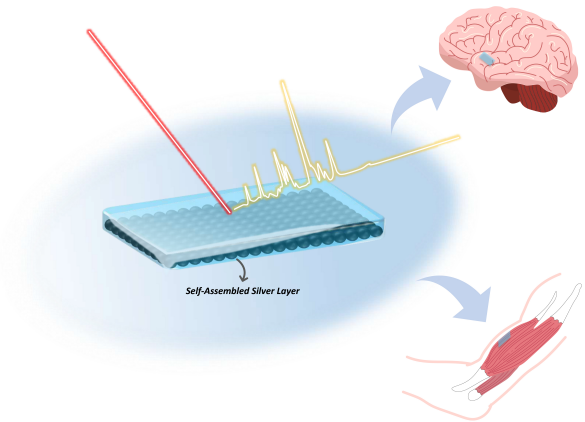
Real-time monitoring of biomedical metabolites has become increasingly demanded in recent years. Among existing techniques, surface-enhanced Raman spectroscopy (SERS) possesses unique advantages with high specificity, ultralow detection limits and low cost. Recently, rigid SERS substrates have made significant progress, high-performance SERS substrates can be mass-produced through simple self-assembly method [1], but lack of mechanical property, storage stability and conformal adhesion.

Herein, we design a flexible SERS patch for label-free detection of metabolites at bio-interfaces. The patch is composed of a self-assembled silver nanofilm and an ultrathin polyvinyl alcohol hydrogel layer coated on that. The hydrogel layer provides mechanical protection and prevents oxidation, which offers the patch strong skin conformity, mechanical durability, and excellent stability. . The SERS signal enhancement factor (SEF) reaches 10^7, enabling label-free quantitative detection of key metabolites including urea, lactate, and uric acid, with detection limits reaching 1mM, 10μM and 1μM levels, respectively. We further demonstrate the versatility of the patch by performing ex vivo experiments on porcine cerebral cortex and porcine muscle, simulating real-world application scenarios in brain-machine interfaces and organic metabolites sensors. This work demonstrates the feasibility of SERS-based flexible platform for real-time metabolites monitoring at different bio-interfaces.



Reference

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Construction of Micro−Nano Hierarchical Structures with Collective Properties for SERS Sensing

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In the process of translating surface-enhanced Raman scattering (SERS) technology into practical application scenarios, traditional two-dimensional (2D) nano-substrates are difficult to meet the requirements for high sensitivity and high specificity in complex sample detection due to issues such as sparse distribution of "hotspots", limited molecular capture efficiency, and poor signal reproducibility. To address this, the precise construction of three-dimensional (3D) nanostructures can significantly optimize SERS performance. Specifically, the localized surface plasmon resonance (LSPR) effects of adjacent nano-units in the 3D space generate synergistic coupling, which greatly enhances the "hotspot" density and the intensity of the localized electromagnetic field. This enables the SERS enhancement factor (EF) to break through the order-of-magnitude limitation of traditional 2D substrates.

On this basis, the introduction of machine learning technology can realize the intelligent upgrading and performance breakthrough of the SERS detection process. Aiming at problems such as noise interference and overlapping characteristic peaks in SERS spectral data, machine learning models such as convolutional neural networks (CNN) and support vector machines (SVM) are employed to achieve accurate identification of similar substances. Meanwhile, machine learning can be adopted to construct quantitative prediction models, which solves the problem of Raman intensity saturation at high concentrations in the traditional least squares method and enables wide-range concentration prediction of molecules.

Ultimately, through the technology integration pathway of "3D nanostructure construction-machine learning empowerment", the SERS technology based on micro-nano hierarchical structures can be promoted to achieve practical applications in two key fields including food contaminant monitoring and early cancer diagnosis.

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Highly Spherical, Single Crystalline Au Nanospheres for Uniform and Reproducible Hot Spots in Surface-Enhanced Raman Scattering at the Single-Particle Level

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Hot spots can generate intense local electromagnetic (EM) fields, thereby boosting diverse innovative applications. However, these applications may face challenges due to their subtle structural changes that can significantly impact their EM field strength. Herein, we report a large-scale synthesis of monodisperse, highly spherical, single crystalline (SC) Au nanospheres (Au NSs) with tunable sizes ranging from 38 to 92 nm for constructing uniform and reproducible hot spots with a nanosphere-on-mirror (NSoM) configuration. Surface-enhanced Raman scattering tests reveal that single NSoM hot spots generate homogeneous EM fields with intensity variation of <4.0% due to their identical "point-to-mirror" configuration. Moreover, the SC nature of the Au NSs can further increase the EM field by 9% because of their higher quality factor, resulting in less energy dissipation in the plasmon. Therefore, these Au NSs may serve as ideal building blocks for the construction of hot spots with homogeneous EM fields.

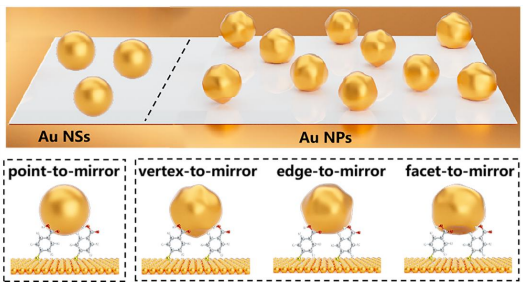

Fig. 1 Schematic diagram of highly spherical, single-crystalline Au NSs replace facet, polycrystalline Au NPs to construct individual highly uniform and reproducible hot spots.

Keywords: plasmonics; SERS; highly spherical Au NSs; single-crystalline; hot spots

Reference

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Angstrom-level resolution detection of hot electron transport distance in silver cube nanogaps

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In the field of nanotechnology, plasmonic nanocavities are the core objects for exploring light - matter interactions at the nanoscale. In plasmonic nanostructures, free charge carriers resonate with photons to generate collective oscillations. After dissipating energy through non - radiative transitions, hot electrons are formed. The transport distance of hot electrons in the nanogap is a key parameter, which directly affects the utilization efficiency of hot electrons and the performance of related devices. Traditional detection techniques are often limited by resolution when studying the transport distance of hot electrons and are difficult to provide high - precision information. Achieving Ångström - level resolution to detect the transport distance of hot electrons in plasmonic nanogaps plays a crucial role in deeply understanding the transport mechanism of hot electrons.

In this study, silver nanocubes were modified with a series of saturated alkylthiol molecules. The nanogap was regulated by the length of the carbon chain, and a gold film substrate was used to support hot - electron probe molecules, improving the detection resolution to 2 Å. Tests using a 633 - nm laser to match the plasmon coupling mode of silver cubes showed that as the carbon chain grew and the nanogap increased, the plasmon resonance blue - shifted, and the main dipole vibration mode was enhanced. Through the coupling conversion experiment of probe molecules, the longest transport distance of hot electrons was measured to reach 20 carbon positions.

Based on the above results, we established a theoretical model for hot - electron transport at the Ångström scale. At a high spatial resolution level, we revealed the direct transfer mechanism of plasmon - induced hot electrons, constructed nanophotonic cavities at different distances, and clarified the relationship between the hot - electron transfer efficiency and distance.

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Resonance SERS probe based on bifunctional molecule IR808 combined with SA test strips for highly sensitive detection of monkeypox virus

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As a high-risk zoonotic virus, highly sensitive detection of monkeypox virus is crucial for its prevention and control. Based on the principle of antigen-antibody specific recognition, this paper prepared an ultrasensitive surface-enhanced resonance Raman scattering (SERRS) biosensing probe (Au NPs@IR808@Ab) using the bifunctional molecule IR808 with resonance Raman effect and antibody-capturing ability. Combined with the strong affinity of the Biotin-streptavidin (Bio-SA) system, Bio-antibody and SA test strips were fabricated, and a Raman probe with a strip-shaped spot was designed—its 0.2 mm spot ensures full coverage of the test strip's T-line and stability of the obtained SERS spectrum. Experimental results showed that the detection sensitivity of this bifunctional probe sensor is at least 2 orders of magnitude higher than that of other highly sensitive molecular probes. In the pharyngeal swab system, 0.5% S9 surfactant effectively reduced false positives caused by complex matrix interference by virtue of its excellent hydrophobicity, ultimately achieving a detection limit of 1 pg. Relying on the bifunctional Raman probe and Bio-SA system, this approach ensures the intensity of SERS signals, more efficient antibody loading, and the test strip's probe-capturing capability; it also verified the effectiveness of S9 in suppressing false positives. The experiment confirmed that this scheme provides reference value for realizing on-site, highly sensitive point-of-care testing of monkeypox virus based on SERS technology [1].

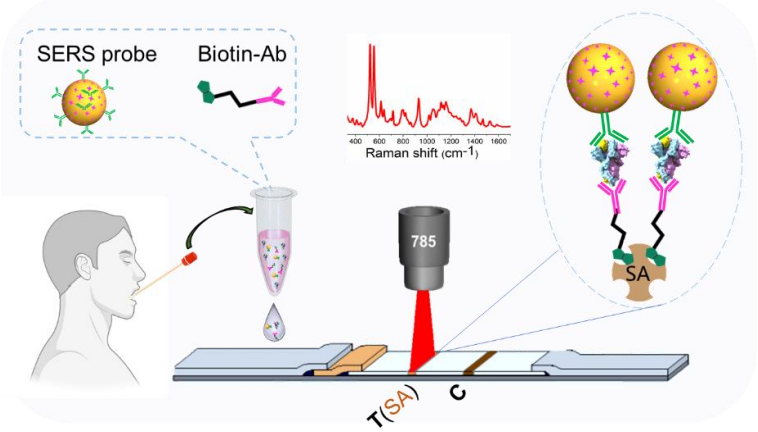

Figure.1 Flowchart of Au NPs@IR808@Ab SERS probe combined with SA test strip to detect monkeypox virus protein

Reference

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Construction of a magnetic dual-signal SERS aptasensor for the ratiometric detection of acetamiprid in tea samples

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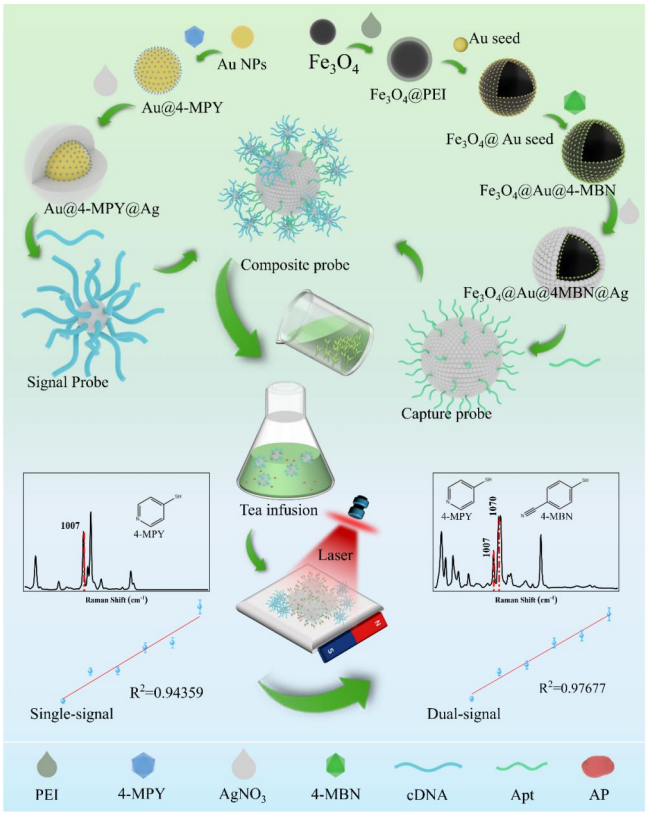
Research background

Acetamiprid (AP) is commonly used in combination to control pests and diseases and increase crop yield. However, as a systemic pesticide, its residue does not easily degrade and is toxic to the human body. Therefore, it is urgent to establish a sensitive, rapid and specific method for the detection of AP. Here, a novel magnetic SERS aptasensor with dual signal was designed through capture probes and signal probes for the ratiometric detection of AP.

Design& methods



Scheme. 1. The construction of SERS aptasensor for detecting AP in tea

Results and discussion

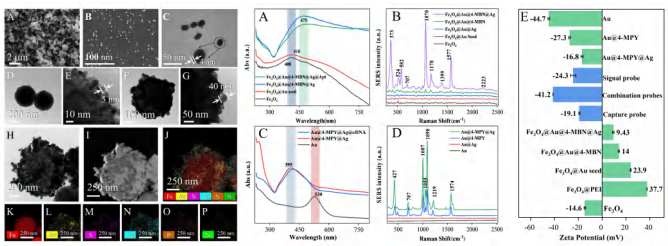


Fig. 1 Characterization of electron microscopic, Vis-UV, SERS and Zeta-potential

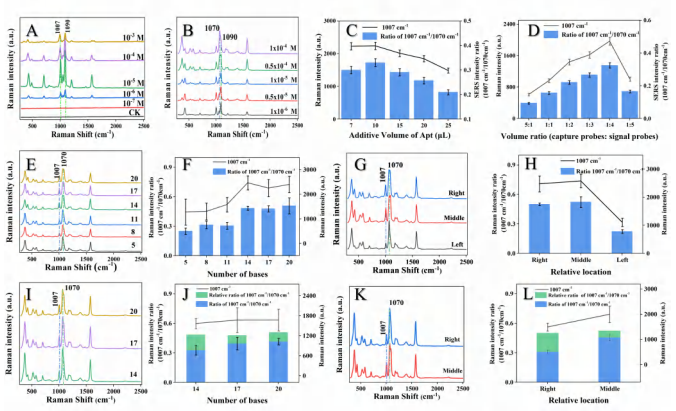


Fig. 2 SERS aptasensor conditions optimisation of 4-MPY, 4-MBN, aptamer, signal probe, cDNA length and position of complementary bases

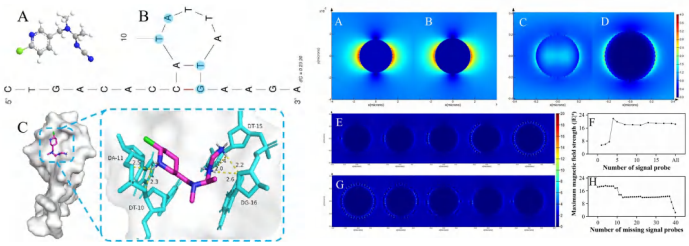


Fig. 3 Analysis of molecular docking of AP with aptamer and 3D-FDTD (Three-dimensional Finite-Difference Time-Domain Method) simulation

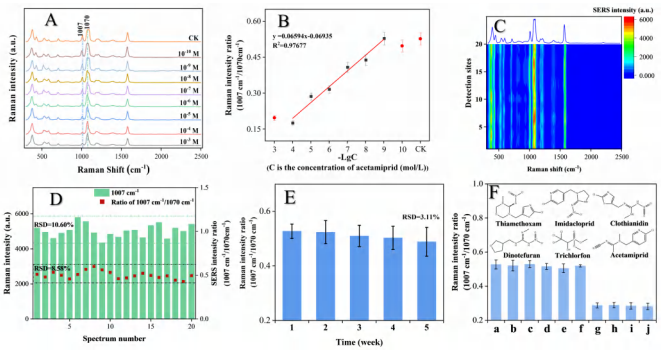


Fig. 4 SERS spectra of aptasensor for sensitivity, reproducibility, stability, specificity

Conclusion

- A novel ratiometric SERS method was developed for interference-free AP detection in complex matrices like tea infusions.
- Magnetic separation of the capture probe provides a convenient assay, resulting in excellent specificity, sensitivity, and reproducibility for this sensor.
- Applications to AP residue detection in green tea yielded recoveries from 82.41% to 94.17% with relative errors of 3.23% to 12.51%, comparable to HPLC results.

Acknowledgement

This work was supported by the National nature science foundation of China(NO.32202540), Wuhan Natural Science Foundation Exploration Program (Morning Light Program) in Hubei Province, China(NO.2024040801020298).

P-40

In-situ Raman Spectroscopy Reveals the Mechanism of Enantioselective based on Chiral Plasmonic Gold Nanoparticles

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Abstract
Enantiomer discrimination is of crucial importance in various fields, including environmental science, analytical science, and pesticide science. Surface-enhanced Raman scattering (SERS), known for its high sensitivity, selectivity, and signal stability, has been used to identify enantiomers with the aid of chiral plasmonic materials[1,2]. However, the mechanism underlying enantioselective SERS remains unclear. In this work, we use electrochemistry, in-situ Raman spectroscopy, and computational simulations to investigate the SERS mechanism of chiral Au nanoparticles in identifying enantiomers (R/S-MA). Experimental and theoretical results demonstrate that under an applied electric field, the electron clouds of enantiomer molecules change, leading to selective differences in the adsorption behavior and charge distribution of R/S-MA enantiomers on chiral gold crystal surfaces.

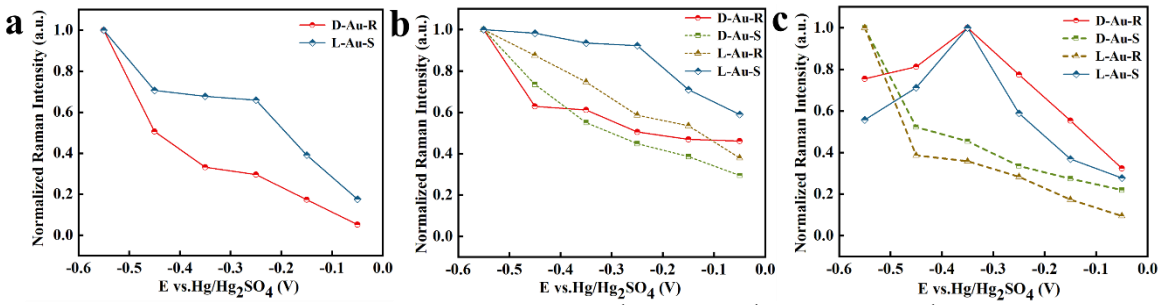

Figure 1. (a-c) SERS intensity of R/S-MA at 992 cm^{-1}, 1002 cm^{-1} and 1078 cm^{-1} positions on L-Au and D-Au substrates.

Reference

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Construction of a self-cleaning SERS aptasensor based on TiO_2 foam for efficient separation and rapid detection of multiple pyrethroid pesticides

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1. Abstracts

Pyrethroid pesticides are widely used in agricultural production due to their effective control of pests, but the abuse of them would cause pesticides residue, which may be harmful to human body and environment. Herein, it is necessary to develop a sensitive and stable method for detect pyrethroid pesticides residue. Here, a self-cleaning SERS aptasensor platform was constructed based on TiO_2 foam for efficient separation and rapid detection of multiple pyrethroid pesticides. Specifically, aptamer was modified on the surface of TiO_2 foam as capture probe, which can hybridize signal probes (Au@4-MPY@Ag-cDNA) with via complementary base pairing to form composite probes. Pyrethroid pesticide molecules can compete with cDNA for aptamers, leading to a regular decrease in Raman signal intensity of 4-MPY on TiO_2 foam platform by easily separation and achieving quantitative detection of pesticides. More importantly, the aptasensor platform based on TiO_2 foam is capable of self-cleaning under UV light catalysis, resulting in the reusability of material. Under optimal conditions, the aptasensor exhibits a excellent sensitivity, good reproducibility and superior specificity, showing a promising application potential in food safety.

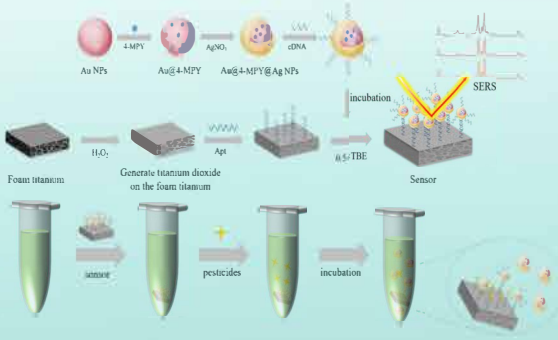

Fig. 1. Construction of SERS aptasensor

2. Results and discussion

2.1 Preparation and characterization

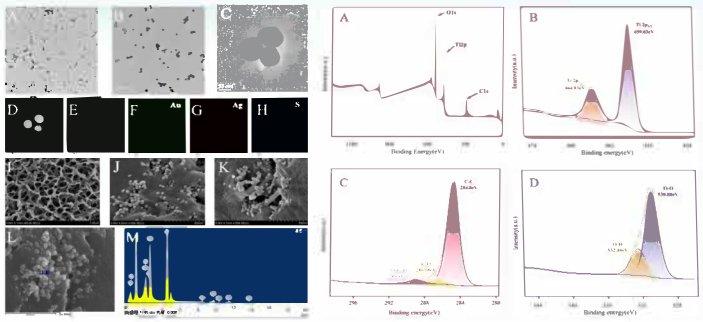

Fig. 2 The SEM image, EDS mapping image of Au@4-MPY@Ag NPs, and XPS image of TiO_2 on the foam titanium

2.2 Parameters optimization

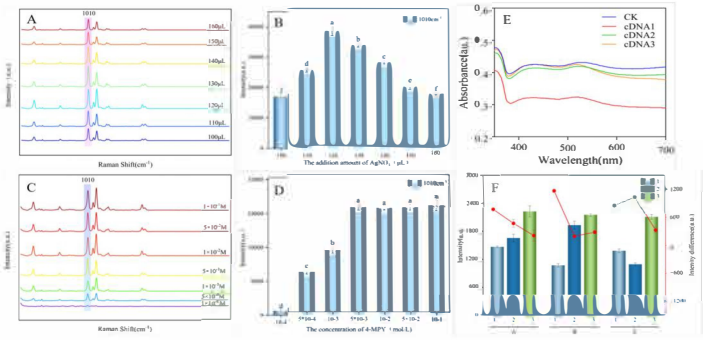

Fig. 3 Optimization of SERS sensors (silver shell thickness, concentration of 4-MPY, and the position of cDNA that interacts with the aptamer)

2.3 Molecular docking

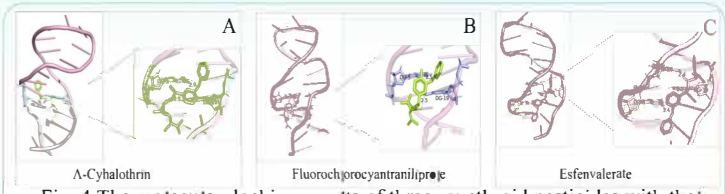

Fig. 4 The molecular docking results of three pyrethroid pesticides with their aptamers

2.4 Results of detection

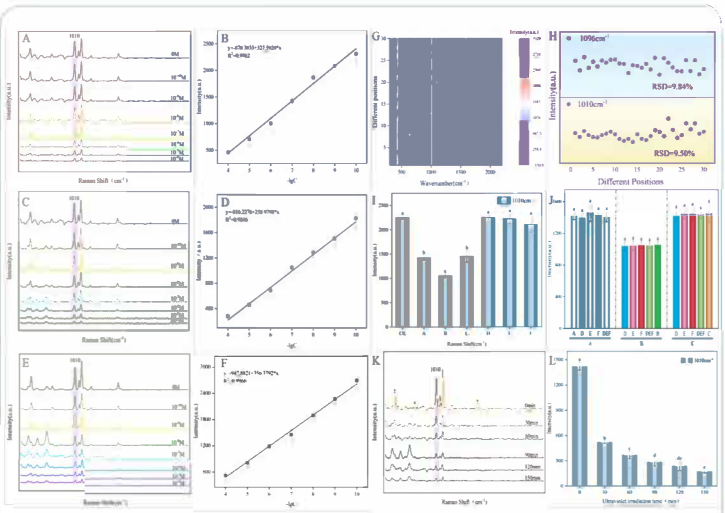

Fig. 5 SERS spectra of sensor for detection performance

3. Conclusions

1. This study designed a surface-enhanced Raman scattering (SERS) sensor with a novel foam metal (foam titanium) as the capture probe, which is expected to enable the sensor to be reusable.
2. Utilizing the new type of foam metal material as the capture probe, a simple detection and separation process can be achieved.
3. By using multi-pesticide aptamers, rapid detection of three common pyrethroid pesticides can be achieved. The detected pesticides have high sensitivity, repeatability and specificity.

In-situ Study of Lithium-ion Battery Operating Conditions Based on Fiber-Enhanced Raman Spectroscopy

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Lithium-ion batteries (LIBs) utilized in high–energy-density applications impose increasingly stringent requirements on the stability of the anode interface, where the formation and evolution of the solid electrolyte interphase (SEI) critically determine cycling longevity and safety[1]. Yet, the anode surface reaction processes are highly complex, and conventional characterization techniques suffer from limited spatial resolution and inadequate in situ monitoring capability. In this study, we propose a novel in situ characterization strategy that combines fiber-optic probe–based detection with core–shell structure enhancement. By constructing metal–dielectric core–shell nanostructures on the anode surface, we effectively strengthen the local electromagnetic field and significantly improve the sensitivity of spectral signals. Coupled with the high-precision spatial localization enabled by the fiber-optic probe[2], this approach allows real-time monitoring of lithium-ion insertion/extraction, SEI formation, and side-reaction kinetics. Experimental results demonstrate that this method achieves approximately an order-of-magnitude enhancement in signal intensity within key reaction zones, enabling the differentiation of characteristic spectral evolution corresponding to different lithiation states. Moreover, the core–shell structure is revealed to facilitate electron transfer and modulate interfacial reactions.[3] This work provides a new experimental tool for probing anode surface reaction mechanisms in greater depth and offers valuable insights for interface engineering and optimizing electrochemical performance.

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Development of high time resolution HPLC-SERS using concentrated SERS array for trace samples

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Analysing vitamins which are essential substances for maintaining a healthy life is important for the food industry. For example, niacin, also known as vitamin B3, is an essential nutrient. The aim of this study is to increase the amount of information obtained by combining surface-enhanced Raman spectroscopy (SERS) with high-performance liquid chromatography (HPLC) [1]. Combining HPLC with a mass spectrometer is a popular way to enhance the data quality, but a MS requires specialized training and is relatively cumbersome. SERS is, however, a relatively simple technique. We have fabricated SERS substrates using the metal film on nanosphere (MFON) method, in two configurations: (1) a multi-spot type substrate with 50 SERS regions formed on a slide glass, (2) a superhydrophobic SERS substrate, in which a superhydrophobic region surrounding a hydrophilic SERS spot allows sample concentration on the silver surface. For analytes, SERS analysis was attempted on BPE, a model molecule with high Raman activity, as well as adenine and niacin. Adenine is one of the main bases that make up nucleic acids, which are widely distributed in the body, and it exhibits strong Raman activity. Using the superhydrophobic SERS substrate, it was possible to collect and analyse the entire fraction corresponding to the UV peak of the chromatogram. From each fraction, a 2 µL sample droplet was placed on each of the SERS spots. The array was maintained at 60 degrees Celsius for complete drying. The 735 cm^{-1} adenine peak was successfully detected even in fractions that could not be measured using a normal substrate. Furthermore, we performed HPLC-SERS measurements of adenine and guanine in chicken liver and vegetable juice. It is hoped that this technique will find a wide range of applications in industry.

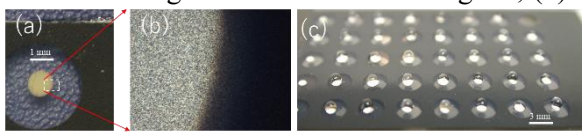

Fig. 1 Superhydrophobic SERS array

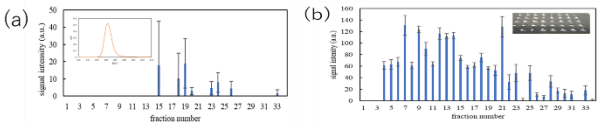

Fig. 2 The adenine peak detected with (a) normal and (b) superhydrophobic SERS arrays

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Morphology and depletion force-based assembly of nanocubes

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The self-assembly of nanoparticles is a highly efficient way to form functional nano-, micro- and macro-superstructures. Here, we present a uniform morphology-induced and depletion force-directed nanoparticle assembly on surface (MIDAS) method with gold nanocubes as building blocks. Morphology-sensitive depletion forces trigger the assembly of uniformly sized and shaped gold nanocubes into 2D monolayers and 3D superlattices. In order to understand their formation, in situ optical microscopy was used to track their nucleation and growth in real time. We observe that superstructure growth can be explained by principles derived from the growth of crystalline materials. In particular, the interaction of nanocubes with the substrate relative to interparticle interactions is revealed as the key to directing superstructure growth modes, with stronger interactions driving the formation of two-dimensional monolayers and weaker interactions leading to three-dimensional supercrystals. Based on this mechanistic understanding, modification of surface roughness is suggested as a new lever for directly controlling the superstructure growth mode. The MIDAS approach is a versatile method for the self-assembly of nanoparticles, as demonstrated by its application to various nanocrystal morphologies, compositions, and sizes. Furthermore, the assembly process generates uniform nanogaps over a large area, highly suitable for surface-enhanced Raman scattering applications.

Chiral Light Emissions from WSe_2 Monolayer Enhanced by (Chiral Nanoparticle)-on-Mirror Structures

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Chiral light emission holds significant importance in modern optics and material science. Transition metal dichalcogenide (TMDC) monolayers possess two degenerate inequivalent valleys K and K' at the Brillouin zone, allowing the selective excitation of carriers within a particular valley to produce circularly polarized light[1]. In TMDC monolayers, both A and localized excitons can exhibit chiral properties. In particular, localized excitons can enhance chiral emission by confining the carrier motion to a small spatial region[2]. Localized excitons in TMDC monolayers not only have the potential to display strong chiral characteristics but also possess quantum-emitter properties. Although recent studies have shown that chiral emission can be further enhanced, achieving significant chiral emission from localized excitons often requires stringent conditions, such as low temperatures and external magnetic fields, which limit practical applications[3][4]. Herein, we address these challenges by integrating a WSe_2 monolayer into a (chiral nanoparticle)-on-mirror structure to study the chiral emission of localized excitons. The degree of circular polarization ($DCP=I_{LCP}-I_{RCP}/I_{LCP}+I_{RCP}$) is used to represent the intensity of chiral emission. In our preliminary results, the DCP value can achieve a maximum of 0.7 at room temperature.

The (chiral nanoparticle)-on-mirror configuration can generate an enhanced electric field within the cavity. A excitons and localized excitons in the WSe_2 monolayer can be detected and modulated by this kind of structure at room temperature. Several factors can affect the chiral light emission. Preliminary results indicate that the DCP of localized excitons varies with the roughness of the Au film surface. Flatly placed chiral nanoparticles exhibit lower DCP values compared to tilted ones. When circularly polarized light is incident, there will be larger DCP values. This research provides crucial experimental evidence and technical methods for understanding and controlling the chiral emission of TMDC monolayers. The chiral emission of localized excitons can be significantly enhanced at room temperature, laying a theoretical and experimental foundation for developing novel chiral photon devices and optical sensing technologies.

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Highly precise nanocomposite coating fabrication using PVD-ALD technologies for SERS detection

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Surface-enhanced Raman scattering (SERS) requires nanostructured surfaces with controlled nanoparticle distribution and manufacturing reproducibility. We present a scalable bottom-up hybrid fabrication approach based on the formation of dewetted metal nanoparticles via physical vapor deposition (PVD), followed by conformal dielectric encapsulation and separation using atomic layer deposition (ALD). Integrated PVD–ALD processing without vacuum interruption enables the repeatable formation of stable mono- and multilayer metal–dielectric nanocomposites. By precisely controlling metal deposition and anchoring in the dielectric environment, we are able to tune plasmonic coupling and hot spot density on centimeter-scale substrates.

Preliminary SERS experiments using 10^{-5} M rhodamine 6G (λ = 633 nm) reveal clearly detectable Raman signatures under low excitation laser power, with enhancement strongly dependent on the nanocomposite configuration. Double-layered metal nanoparticles in an ALD matrix exhibit the highest integrated intensity, demonstrating potential for further optimization in the nanocomposite design.

This hybrid PVD-ALD platform offers a robust pathway to reproducible SERS nanocomposites substrates suitable for chemical and biosensing applications, with further optimization potential to improve detection limits.