Study on SERS Solvent Perturbation Effects of Several Typical Raman Probe Molecules

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Abstract: This study introduces solvent perturbation into surface-enhanced Raman spectroscopy (SERS) to systematically analyze dynamic spectral features by converting the random signal scintillation typically observed at single-molecule concentrations into a measurable range of medium to high concentrations. Using silver aerogel as the substrate, combined with in situ Raman spectroscopy and theoretical calculations, we demonstrate that solvent perturbation and laser testing activate dynamic information from rhodamine 6G, p-mercaptopyridine,

and methylene blue molecules that is typically obscured in conventional detection. At single-molecule concentrations, multipeak scintillation is observed, while, at medium to high concentrations, the intensities of characteristic peaks converge, forming a “flattening effect”. Additionally, anomalous satellite peaks appear near main peaks, leading to a peak splitting phenomenon. These dynamic spectral changes originate from the averaging of molecular orientations and the rotation of side-chain single bonds. This approach establishes an analytical method that links molecular structure, interfacial dynamics, and spectral response, providing a foundation for constructing a dynamic SERS fingerprint database.

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