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Decoding the topographical features of more realistic SERS active substrates in presence of the probe molecules from statistical considerations: An in-depth study bridging Microscopy with Spectroscopy

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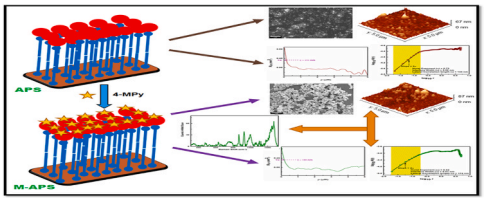
HIGHLIGHTS

- Surface topographies of the SERS active substrates have been explored in detail.
- Topographical features of the substrates were mapped in presence of 4-MPy molecule.
- Bare SERS substrates are compared with the same substrate in presence of 4-Mpy.
- The chaotic behavior of the substrates has been revealed from Lyapunov exponents.

GRAPHICAL ABSTRACT



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ABSTRACT

This paper reports for the first time the topographical parameters of SERS active substrates, fabricated through Langmuir-Blodgett and self-assembly techniques, in presence of the probe 4- Mercapto Pyridine (4-Mpy) molecules. Prior to this study the topographical parameters of bare SERS active substrates in absence of probe molecules had been investigated. However, correlating the topographical parameters of bare SERS active substrates with the corresponding SERS responses may be incomplete and imprecise, as in reality the SERS signals are collected from the probe molecules only upon adsorption on the substrates. The adsorption of probe molecules on the SERS active substrates can modify their overall morphologies in comparison to the pristine counterparts. The present paper thus reports the topographical features of the SERS active substrates in presence of 4-Mpy molecule from the statistical considerations in terms of lateral correlation length (ξ), Hurst or roughness exponents (α), root mean square surface roughnesses (ω) and fractal dimensions (D_f). Attempts have been made to correlate the topographical features of the substrates in presence of 4-Mpy molecule with their corresponding SERS responses. The chaotic behaviors of the substrates in pristine form and in the presence of 4-MPy molecules are also revealed from the Lyapunov exponents and the 2D phase space trajectories. We believe that the present report will help to correlate the topographical features of more realistic SERS active substrates in presence of probe molecules with their corresponding SERS activities and render significant advancement towards successful fabrications of efficient SERS active substrates in future endeavors.

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