

Towards improved precision in the Quantification of Surface-Enhanced Raman Scattering Enhancement Factor: A Renewed Approach

(supporting information)

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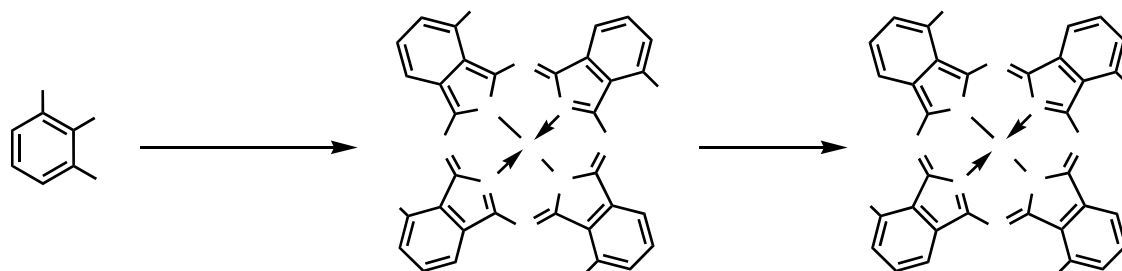
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Scheme S1 synthesis of 1,8,15,22-Tetraaminophthalocyanatocobalt(II)

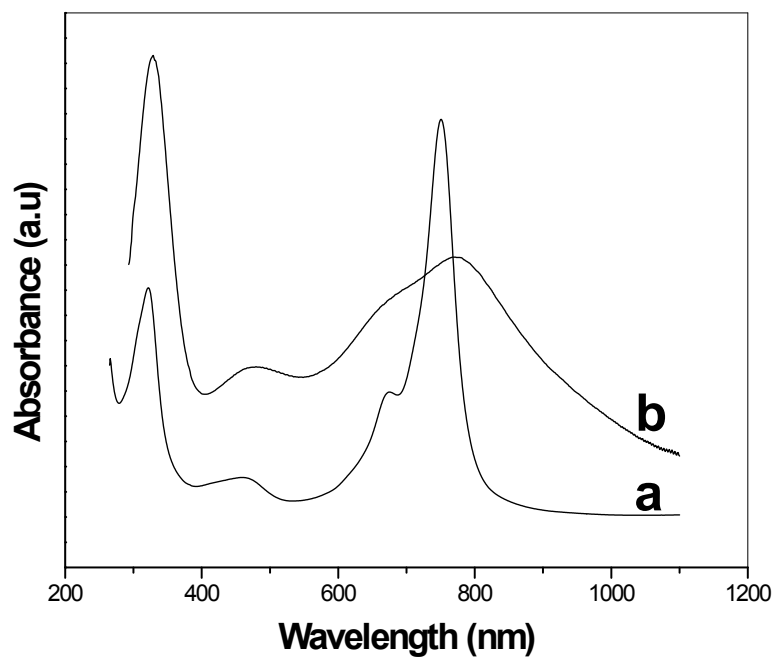


Fig. S1 UV–visible spectra obtained for (a) 4α-Co^{II}TAPc in DMF and (b) SAM of 4α-Co^{II}TAPc on ITO surface.

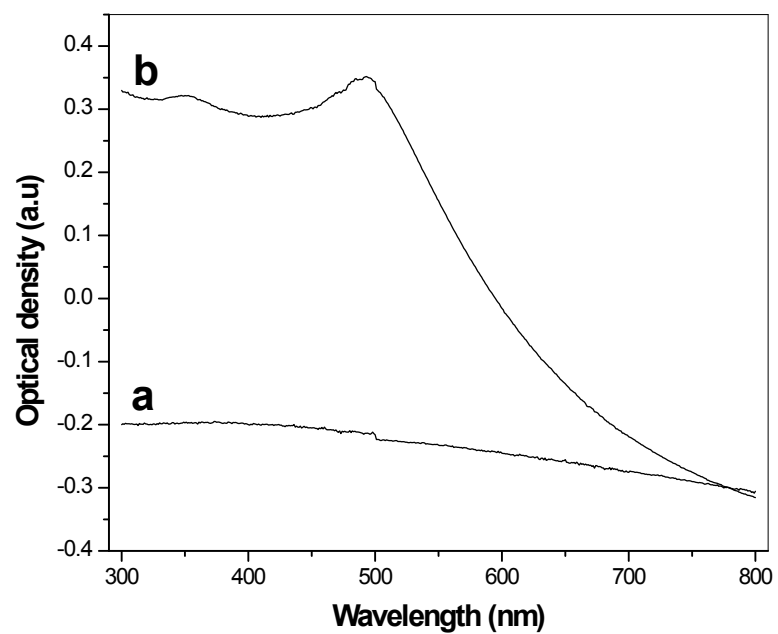


Fig. S2 Reflectance UV-visible spectra of (a) bare GC and (b) nanostructured Au electrodeposited substrates.

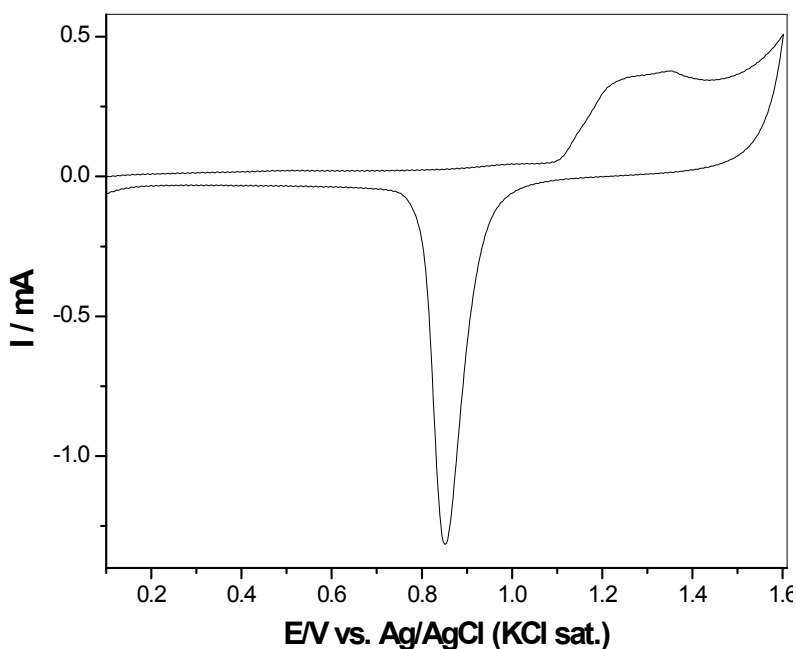


Fig. S3 Cyclic voltammogram obtained for GC/Au electrode in 0.1 M H₂SO₄ at a scan rate of 0.1 V s⁻¹.

Quantification of real surface area

The working geometrical area is 1 cm diameter electrode is 0.785 cm²

For 1 cm² Au₂O₃ reduction charge = 400 μC (*Analytical Chemistry* **2000**, 72, 2016-2021)

Therefore, for 0.785 cm², the Au₂O₃ reduction charge = 314 μC

Thus 314 μC should be the Au₂O₃ reduction charge for the flat 0.785 cm² gold surface

The experimental Au₂O₃ (Fig. S3) reduction charge obtained for nanostructured Au on GC
= 1250 μC

Roughness factor = Real charge/geometric charge = 1250 / 314 = 3.98

Therefore, the real surface area = 0.785 cm² × 3.98
= 3.02 cm²

Quantification of surface coverage of 4 α -Co^{II}TAPc

Surface coverage of 4 α -Co^{II}TAPc on electrode surface has been calculated using the below equation

$$\text{Surface coverage } (\Gamma) = Q/nFA$$

Here, Q = charge under the oxidation/reduction peak

n = number of electrons involved in the oxidation/reduction process

F = Faraday constant

A = real surface area of the electrode

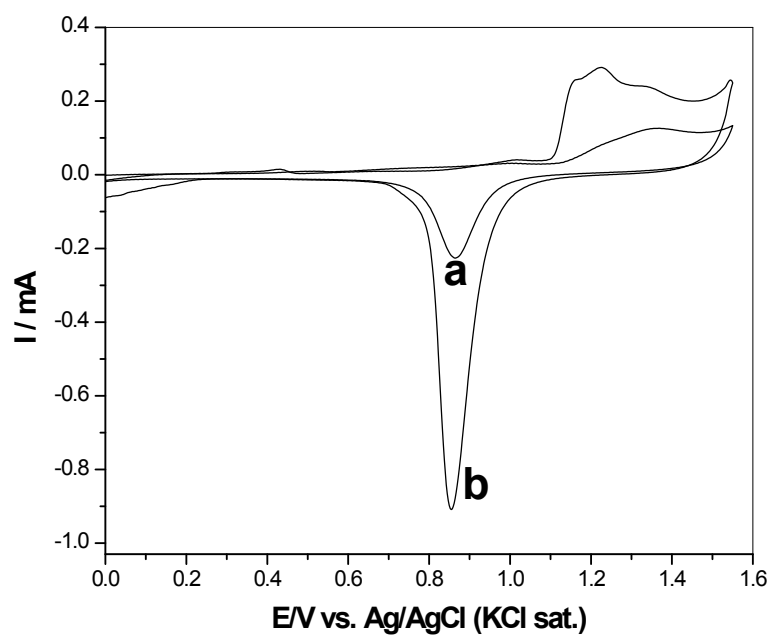


Fig. S4 Cyclic voltammograms obtained for (a) pAu and (b) pAu/Au electrodes in 0.1 M H₂SO₄ at a scan rate of 0.1 V s⁻¹.

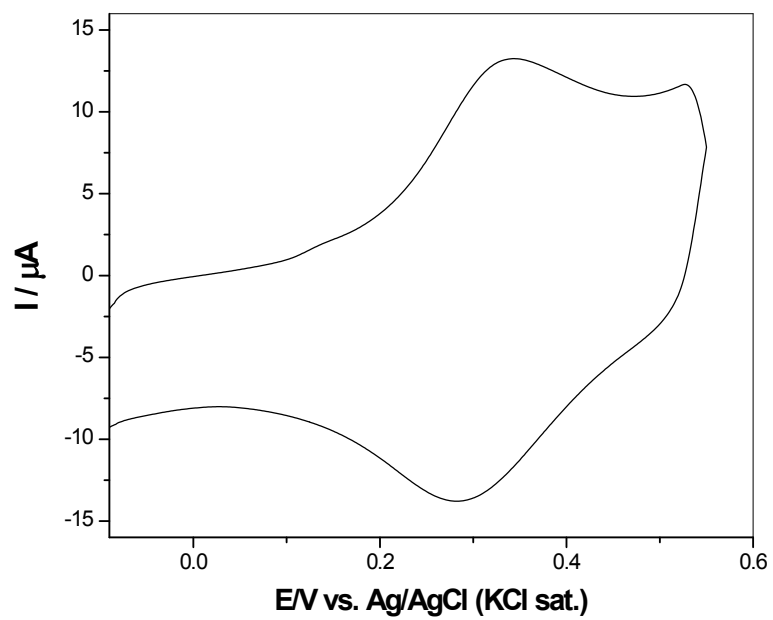


Fig. S5 Cyclic voltammogram obtained for self-assembled monomolecular films of 4 α -Co^{II}TAPc on pAu/Au electrode in 0.1 M H₂SO₄ at a scan rate of 0.1 V s⁻¹.

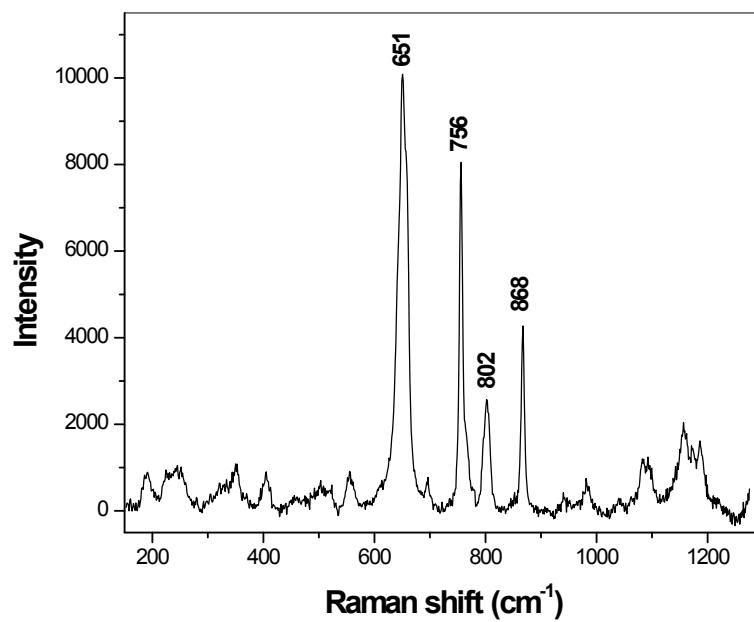


Fig. S6 Raman spectrum of 50 μM solution of 4 α -Co^{II}TAPc in DMF using 785 nm laser line as excitation source.