Supplementary Material

A Graphene Metasurface Inspired Optical Sensor for the Heavy Metals Detection for Efficient & Rapid Water Treatment

A. Graphene Conductivity Analysis

The graphene conductivity (σ_s) can be defined with the help of the following Equations (S1)-(S4) [1]:

$$\varepsilon\,(\omega) = 1 + \frac{\sigma_s}{\varepsilon_0 \omega \nabla} \tag{S1}$$

$$\sigma_{intra} = \frac{-je^2 k_B T}{\pi\hbar^2\,(\omega - j2\Gamma)}\left(\frac{\mu_c}{k_B T} + 2\,\ln\left(e^{\frac{\mu_c}{k_B T}} + 1\right)\right) \tag{S2}$$

$$\sigma_{inetr} = \frac{-je^2}{4\pi\hbar}\ln\left(\frac{2|\mu_c| - (\omega - j2\Gamma)\hbar}{2|\mu_c| + (\omega - j2\Gamma)\hbar}\right) \tag{S3}$$

$$\sigma_s = \sigma_{intra} + \sigma_{inter} \tag{S4}$$

Where permittivity and vacuum's permittivity are indicated by ε and ε_0, respectively. Angular frequency and thickness of single-layer graphene sheet are indicated by ω, and ∇, respectively. Graphene conductivity as derived in eq. (4) can be separated into intraband conductivity (σ_{intra}) and interband (σ_{inetr}) conductivity. Room temperature, Boltzmann constant, and reduced plank's constant are indicated by T, k_B, and $\hbar$ respectively. The graphene chemical potential (GCP) is specified by μ_c, and can be given as $\mu_c = \hbar\nu_F\sqrt{\pi C V_{DC} / e}$, where capacitance, gate voltage, and Fermi velocity are indicated by C, V_{DC}, and ν_F, respectively.

B. Performance Defining parameters for the Developed Sensor

There are several parameters such as Sensitivity (S), Figure of Merit (FOM), Q factor (Q), Sound to Noise Ratio (SNR), Dynamic Range (DR), Detection Accuracy (DA), Detection Limit (DL), Sensor Resolution (SR), Uncertainty (UC) are utilized to examine the sensor's performance and they can be derived as indicated in Equations (S5)-(S13) [2]–[4]:

$$S = \frac{\Delta f}{\Delta n} \tag{S5}$$

$$FOM = \frac{S}{FWHM} \tag{S6}$$

$$Q = \frac{f_r}{FWHM} \quad \text{(S7)}$$

$$SNR = \frac{\Delta f}{FWHM} \quad \text{(S8)}$$

$$DR = \frac{f_r}{\sqrt{FWHM}} \quad \text{(S9)}$$

$$DA = \frac{1}{FWHM} \quad \text{(S10)}$$

$$DL = \left(\frac{\Delta n}{1.5}\right)\left(\frac{FWHM}{\Delta f}\right)^{1.25} \quad \text{(S11)}$$

$$SR = S \times DL \quad \text{(S12)}$$

$$UC = \frac{2(\Delta f)^{0.75}(FWHM)^{0.25}}{9} \quad \text{(S13)}$$

Sensitivity is calculated by measuring the difference between the peak of two biomolecules and used as a performance measure for sensors. Sensitivity, quality factor, Q, and figure of merit are the key attributes that characterize a sensor's performance. As the difference between peak increases the quality of the sensor is enhanced due to the improved sensitivity.

A figure of merit (FOM) is the proportion of the sensitivity and the resonance frequency line width which is highly used to specify sensing proficiency.

Δf is the frequency difference between two transmittance peaks and Δn is the difference of refractive index between these two points.

s stands for the sensitivity and the FWHM indicates the full width at half maximum.f_r indicates the resonance frequency for which the lowest value of transmittance was observed.

References

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