物理学报 *Acta Phys. Sin.* **Vol. 73, No. 13 (2024) 138101**

# 《可调谐的声学型石墨烯等离激元增强纳米红外光谱*》的补充材料

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注释 1：计算色散关系的方法

我们通过菲涅耳反射系数$r_{\mathrm{p}}$（$q$，$\omega$）方法计算 AGP 的色散关系. 计算的结构为石墨烯/空气间隙/金的多层结构，如图 S3 所示.

该系统的$r_{\mathrm{p}}$由以下方程决定：

$$r_{\mathrm{p}} = r_{\mathrm{g}} + r_{\mathrm{m}} \mathrm{e}^{\mathrm{i}2k_{\mathrm{a}}^{z}d} \ / \ 1 + r_{\mathrm{g}} r_{\mathrm{m}} \mathrm{e}^{\mathrm{i}2k_{\mathrm{a}}^{z}d} \qquad \text{(S1a)}$$

$$r_{\mathrm{g}} = \left(\varepsilon_{\mathrm{a}\perp} k_{\mathrm{g}}^{z} - \varepsilon_{\mathrm{g}\perp} k_{\mathrm{a}}^{z}\right) / \left(\varepsilon_{\mathrm{a}\perp} k_{\mathrm{g}}^{z} + \varepsilon_{\mathrm{g}\perp} k_{\mathrm{a}}^{z}\right) \qquad \text{(S1b)}$$

$$r_{\mathrm{m}} = \left(-\varepsilon_{\mathrm{a}\perp} k_{\mathrm{m}}^{z} - \varepsilon_{\mathrm{g}\perp} k_{\mathrm{a}}^{z}\right) / \left(\varepsilon_{\mathrm{a}\perp} k_{\mathrm{m}}^{z} + \varepsilon_{\mathrm{g}\perp} k_{\mathrm{a}}^{z}\right) \qquad \text{(S1c)}$$

下标“g”，“a” 和 “m” 分别表示石墨烯、空气和金. $d$代表单层石墨烯的厚度. $r_{\mathrm{g}}$和$r_{\mathrm{m}}$分别代表石墨烯/空气和空气/金界面的反射率. $\varepsilon_{\mathrm{g}\perp}$和$\varepsilon_{\mathrm{a}\perp}$分别代表石墨烯和空气的外平面介电函数. $k_i^z$是沿 $z$ 轴传播波的动量分量：

$$k_i^z = \sqrt{\varepsilon_{i\perp}(\omega/c)^2 - \left[\left(\varepsilon_{i\perp}/\varepsilon_{i//}\right)\cdot q^2\right]} \qquad \text{(S1d)}$$

其中$i$ = g, a 和 m, $\omega$是入射光的频率，$c$ 是真空中的光速. $\varepsilon_{i\perp}$和$\varepsilon_{i//}$分别表示相应$i$材料的面外和面内介电函数.

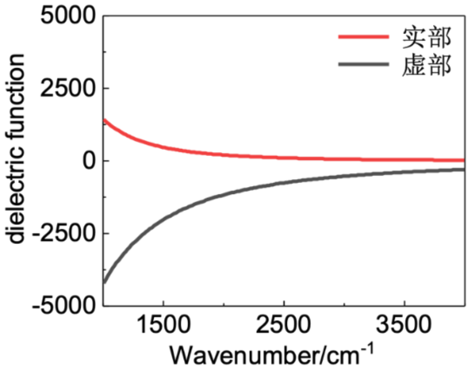

图 S1 金的介电函数

Fig.S1. Dielectric function of gold.

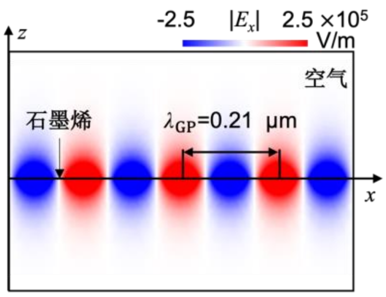

图 S2 石墨烯等离激元（graphene plasmon, GP）沿 $x$ 轴的的电场强度分布图（$E_x$）. GP 的共振频率为 1600 cm$^{-1}$

Fig.S2. Electric-field distribution of graphene plasmon (GP) in Graphene at a resonance frequency of 1600 cm$^{-1}$.

图 S3 单层石墨烯/空气间隙/金多层结构的侧视图

Fig.S3. Side view of the layered structure of single-layer graphene/ airgap/ Au.

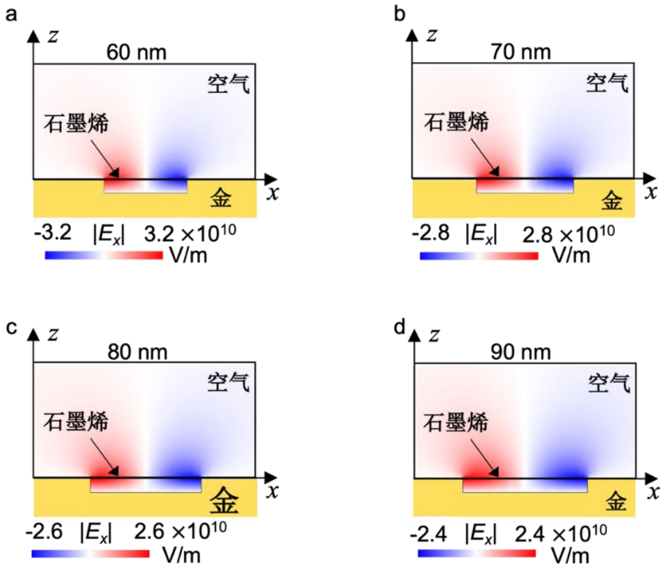

图 S4 基于不同金纳米腔室宽度的声学型石墨烯等离激元（nanocavity-Acoustic graphene plasmon, n-AGP）沿 $x$ 轴的电场分布图（$E_x$）. 当金纳米腔室宽度为 60 nm (a), 70 nm (b), 80 nm (c), 90 nm (d) 时，n-AGP 沿 $x$ 轴的 $E_x$

Fig.S4. Electric-field distribution ($E_x$) along the $x$-axis of nanocavity-Acoustic graphene plasmon (n-AGP) based on different gold nanocavity widths. When the width of the gold nanocavity is 60 nm (a), 70 nm (b), 80 nm (c), and 90 nm (d), $E_x$ of nanocavity-Acoustic graphene plasmon (n-AGP).

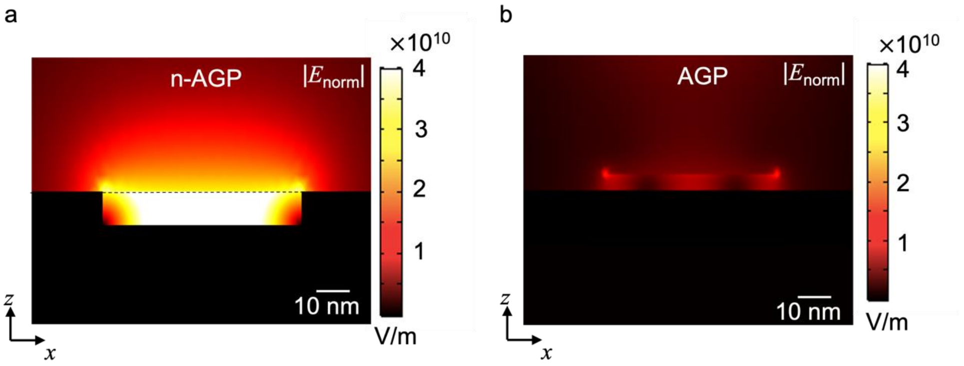

图 S5 n-AGP 和声学型石墨烯等离激元（acoustic graphene plasmon, AGP）的电场强度分布图. (a) n-AGP 的电场强度分布图（$|E_{\mathrm{norm}}|$）; (b) AGP 的电场强度分布图（$|E_{\mathrm{norm}}|$）. 石墨烯宽度为 60 nm，石墨烯与金之间存在 10 nm 空气间隔. $E_{\mathrm{norm}} = \sqrt{E_x^2 + E_z^2}$

Fig.S5. Electric-field distribution of n-AGP and acoustic graphene plasmon (AGP). (a) Electric-field distribution diagram of n-AGP ($|E_{\mathrm{norm}}|$); (b) Electric-field distribution diagram of AGP ($|E_{\mathrm{norm}}|$). Graphene has a width of 60 nm, and there is a 10 nm air gap between graphene and gold. $E_{\mathrm{norm}} = \sqrt{E_x^2 + E_z^2}$.

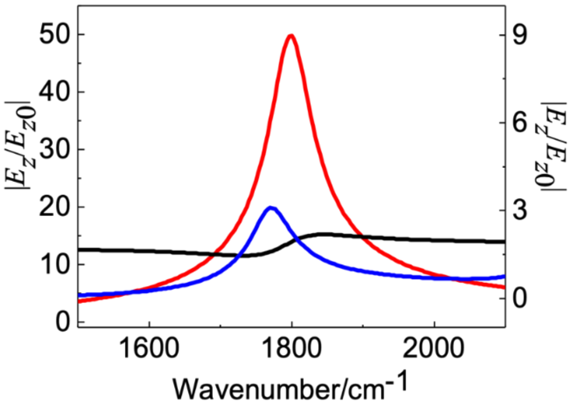

图 S6 不同石墨烯等离激元模式的归一化电场强度谱. 从石墨烯下方 5 nm 处提取归一化电场强度谱. 共振频率为 1800 cm$^{-1}$ 时，n-AGP 的最高电场增强倍数（$|E_z/E_{z0}|$）约为 50 (红色曲线). 共振频率为 1770 cm$^{-1}$ 时，GP 的最高电场增强倍数$|E_z/E_{z0}|$约为 3. (蓝色曲线）共振频率为 1843 cm$^{-1}$ 时，AGP 的最高电场增强倍数$|E_z/E_{z0}|$约为 2 (黑色曲线). $E_{z0}$ 为仅电偶极子存在时的电场强度

Fig.S6. Normalized electric-field spectra of different graphene plasmon modes. Normalized electric-field spectra from 5 nm below the graphene. The maximum electric field enhancement factor ($|E_z/E_{z0}|$) of the n-AGP is approximately 50 at a resonance frequency of 1800 cm$^{-1}$ (red curve). For the GP, the maximum electric field enhancement factor $|E_z/E_{z0}|$ is about 3 at a resonance frequency of 1770 cm$^{-1}$ (blue curve). The maximum electric field enhancement factor $|E_z/E_{z0}|$ of the AGP is approximately 2 at a resonance frequency of 1843 cm$^{-1}$ (black curve). $E_{z0}$ is the electric field intensity when the electric dipole is directly excited.

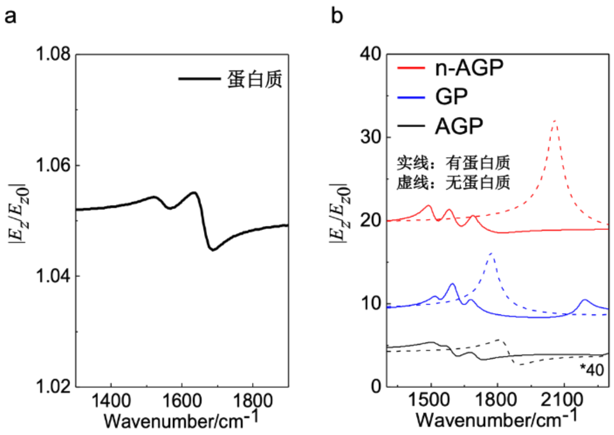

图 S7 蛋白质分子对不同石墨烯等离激元模式归一化电场强度谱的影响 (a) 宽度为 60 nm，高度为 10 nm 的蛋白质的归一化电场强度谱, $E_{z0}$ 为仅电偶极子存在时的电场强度; (b) 有（实线）无（虚线）蛋白质时，不同石墨烯等离激元模式的归一化电场强度谱的比较

Fig.S7. Effect of protein molecules on the normalized electric-field spectra of different graphene plasmon modes: (a) Normalized electric-field spectra of protein with a width of 30 nm and a height of 10 nm, $E_{z0}$ is the electric field intensity when the electric dipole is directly excited; (b) comparison of normalized electric-field spectra of different graphene plasmon modes with (solid line) and without (dashed line) proteins.

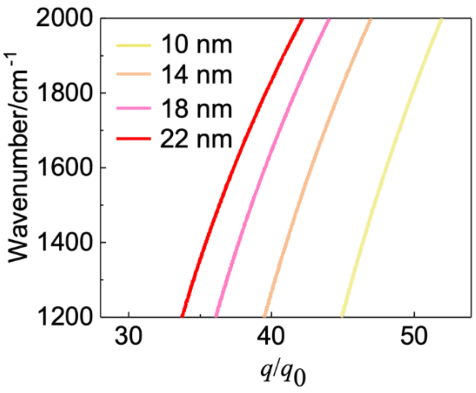

图 S8 石墨烯与金相距不同距离时(10 nm, 14 nm, 18 nm, 22 nm)，计算 AGP 的色散关系

Fig.S8. Dispersion of AGP at at different distances (10 nm, 14 nm, 18 nm, 22 nm) between graphene and gold.