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《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

段谕[1)2)] 戴小康[2)3)] 吴晨晨[2)3)†] 杨晓霞[2)3)‡]

1)（郑州大学，河南先进技术研究院，郑州 450001）

2)（国家纳米科学中心，中国科学院纳米科学卓越创新中心，中国科学院纳米光子材料与器件重点实验室，中国科学院纳米标准与检测重点实验室，北京 100190）

3)（中国科学院大学，材料与光电研究中心，北京 100049）

注释 1：计算色散关系的方法

我们通过菲涅耳反射系数r_p（q，ω）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_p由以下方程决定：

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

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

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

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_g和r_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：

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

其中i = g, a 和 m, ω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.

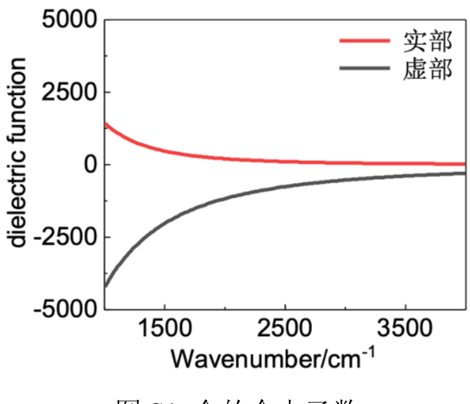

图 S1 金的介电函数

Fig.S1. Dielectric function of gold.

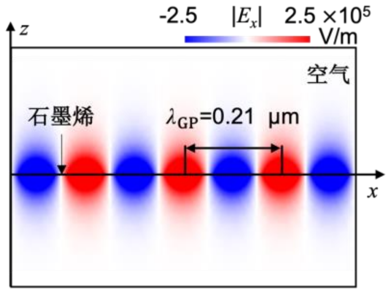

图 S2 石墨烯等离激元（graphene plasmon, GP）沿 x 轴的的电场强度分布图（E_x）. GP 的共振频率为 1600 cm^{-1}

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.

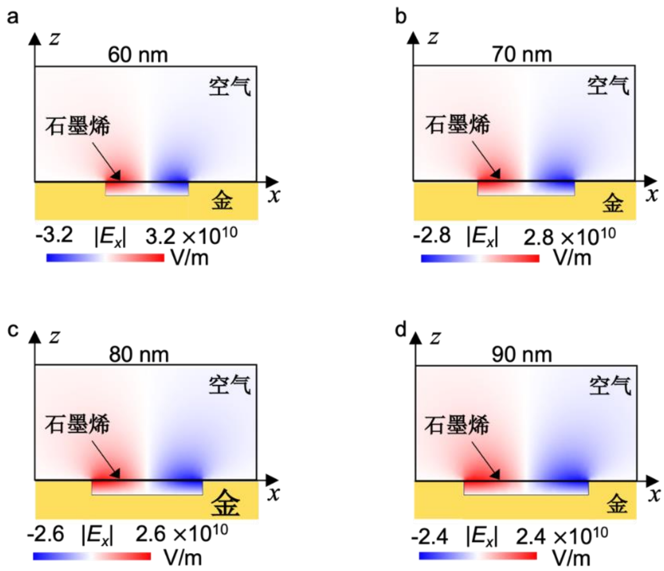

图 S4 基于不同金纳米腔室宽度的声学型石墨烯等离激元（nanocavity-Acoustic graphene plasmon, n-AGP）沿 x 轴的电场分布图（E_x）. 当金纳米腔室宽度为 60 nm (a), 70 nm (b), 80 nm (c), 90 nm (d) 时，n-AGP 沿 x 轴的 E_x

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).

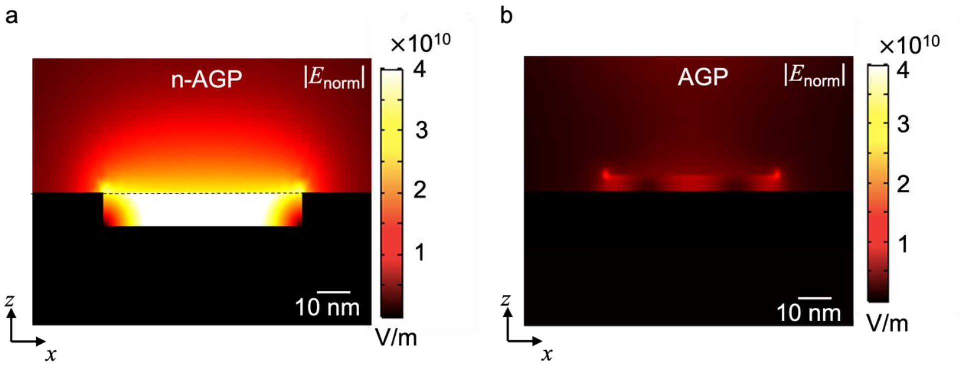

图 S5 n-AGP 和声学型石墨烯等离激元（acoustic graphene plasmon, AGP）的电场强度分布图. (a) n-AGP 的电场强度分布图（$|E_{norm}|$）; (b) AGP 的电场强度分布图（$|E_{norm}|$）. 石墨烯宽度为 60 nm，石墨烯与金之间存在 10 nm 空气间隔. $E_{norm} = \sqrt{E_x^2 + E_z^2}$

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

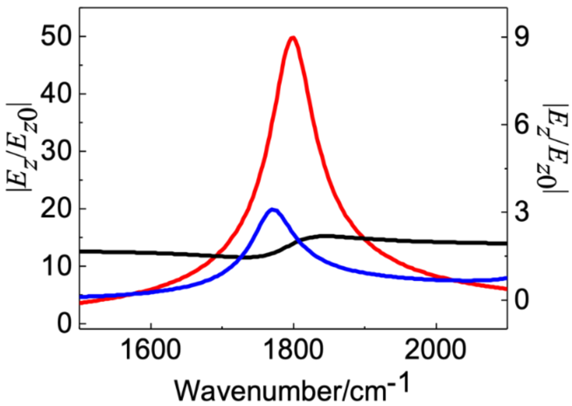

图 S6 不同石墨烯等离激元模式的归一化电场强度谱. 从石墨烯下方 5 nm 处提取归一化电场强度谱. 共振频率为 1800 cm^{-1} 时，n-AGP 的最高电场增强倍数（$|E_z/E_{z0}|$）约为 50 (红色曲线). 共振频率为 1770 cm^{-1} 时，GP 的最高电场增强倍数$|E_z/E_{z0}|$约为 3. (蓝色曲线）共振频率为 1843 cm^{-1} 时，AGP 的最高电场增强倍数$|E_z/E_{z0}|$约为 2 (黑色曲线). E_{z0} 为仅电偶极子存在时的电场强度

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.

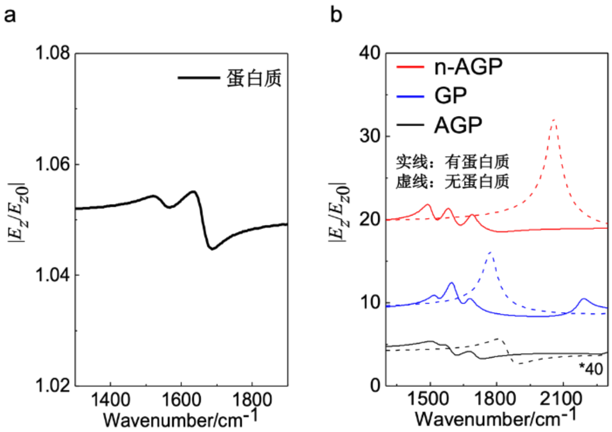

图 S7 蛋白质分子对不同石墨烯等离激元模式归一化电场强度谱的影响 (a) 宽度为 60 nm，高度为 10 nm 的蛋白质的归一化电场强度谱, E_{z0} 为仅电偶极子存在时的电场强度; (b) 有（实线）无（虚线）蛋白质时，不同石墨烯等离激元模式的归一化电场强度谱的比较

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.

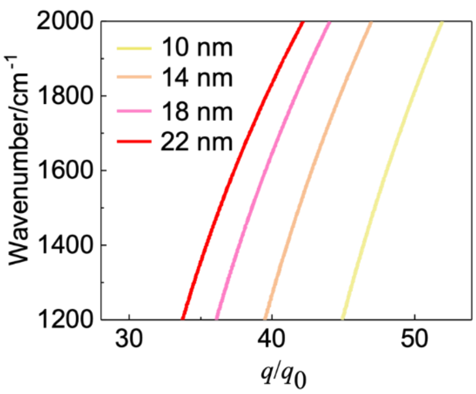

图 S8 石墨烯与金相距不同距离时(10 nm, 14 nm, 18 nm, 22 nm)，计算 AGP 的色散关系

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

