

Supplementary Information

Study of graphene plasmons in graphene-MoS₂ heterostructures for optoelectronic integrated devices

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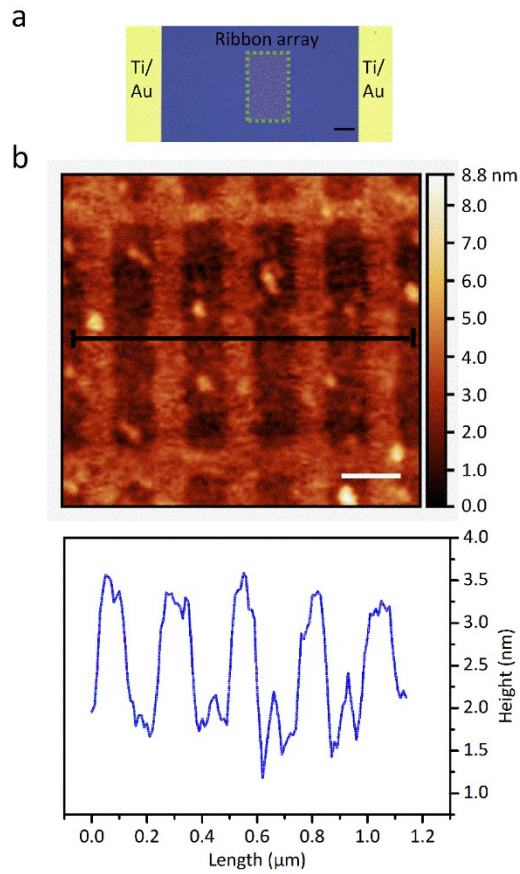


Fig. S1 (a) An optical image of the MoS₂/graphene device, both graphene and MoS₂ layers were patterned into nanoribbon arrays. Scale bar is 50 μm. (b) Top: AFM image of a MoS₂ nanoribbon array with ribbon width of ~100 nm. The scale bar is 200 nm. Bottom: Linescan profile of the top image corresponding to the black line. The MoS₂ nanoribbons had uniform thickness about 1.9 nm.

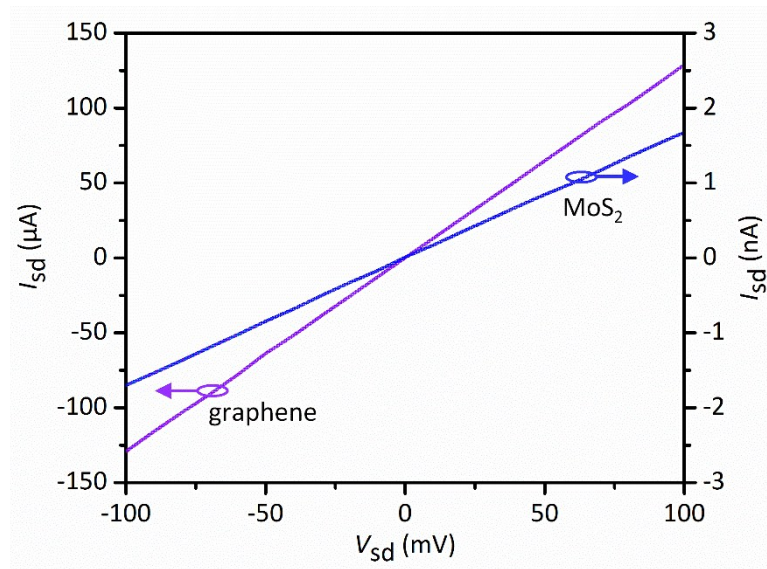


Fig. S2 Output curves of monolayer graphene and monolayer MoS₂ devices on SiO₂/Si, respectively. The linearity indicates that Ohmic contact was formed between Ti and both the graphene and MoS₂ layers.

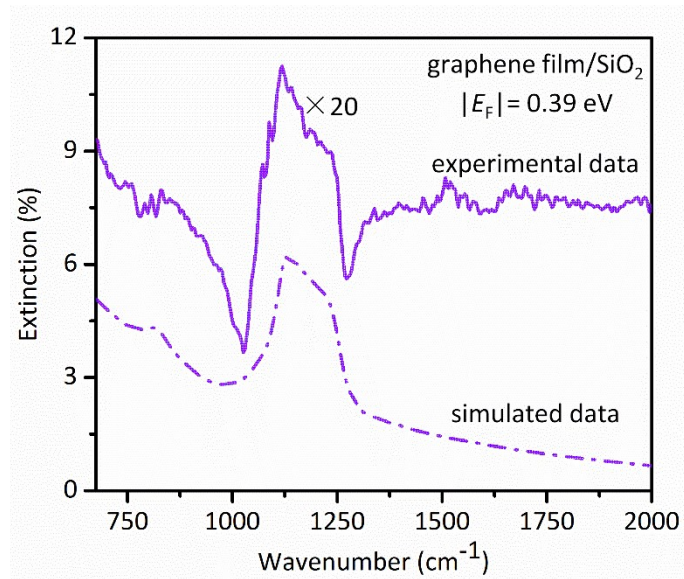


Fig. S3 Experimental and simulated extinction spectra for graphene film on SiO₂ substrate (defined as graphene film/SiO₂ device). The extinction spectra were obtained at $|E_F| = 0.39$ eV, using single-beam transmittance spectra at $|E_F| = 0$ as a background. The experimental data was multiplied by 20.

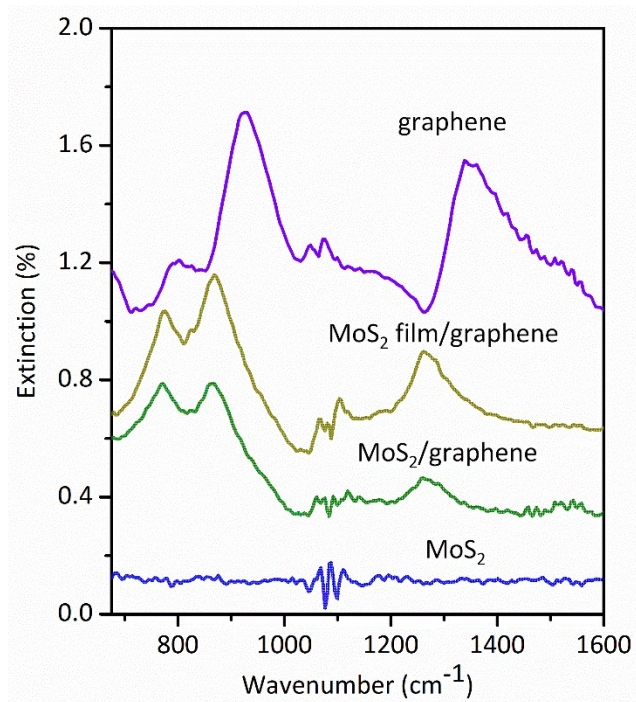


Fig. S4 Extinction spectra of graphene, MoS₂ film/graphene, MoS₂/graphene, and MoS₂ nanoribbon array devices. The first three ones were measured at equivalent Δ_{CNP} (= 100 V). No distinct plasmon resonance was observed in the spectrum of MoS₂ nanoribbon array device which was measured at $V_g=100$ V (corresponding to maximum current), using single-beam transmittance spectra at $V_g=-37$ V (corresponding to its minimum current) as a background. The ribbon width was 100 nm.

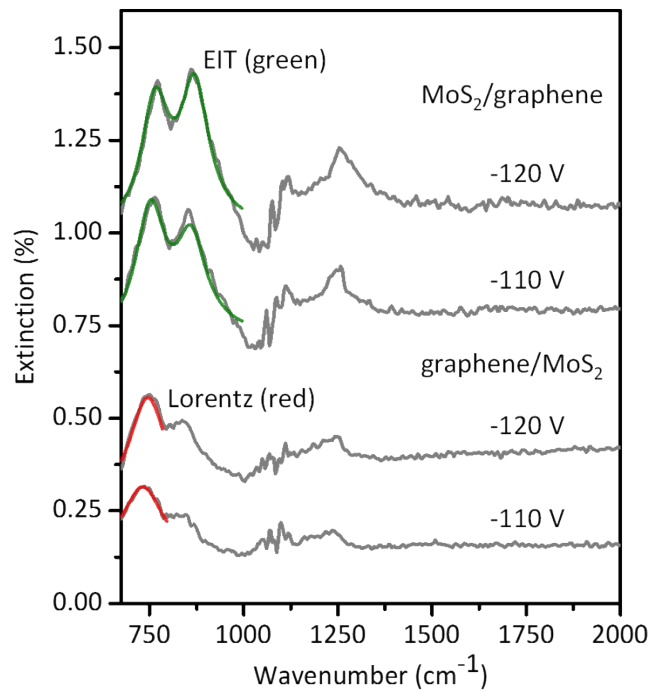


Fig. S5 Illustration of the curve analysis methods to extract the full width at half-maximum (FWHM) (Γ) of resonance peaks. Electromagnetic induced transparent (EIT) model is adapted when MoS₂/graphene plasmon frequency is close to the phonon frequency of substrate SiO₂ (green curves). And the plasmonic peak is fitted by a Lorentz shape (red curves) for graphene/MoS₂ heterostructure. The detailed fitting method is following ref. 35 in the main text.¹ The calculated lifetime values for MoS₂/graphene at -120 V and -110 V are 86 fs at 824 cm⁻¹ and 99 fs at 802 cm⁻¹, respectively, and for graphene/MoS₂ are 83 fs at 748 cm⁻¹ and 78 fs at 734 cm⁻¹, respectively.

Calculation of carrier density, Fermi level, and mobility

For bare MoS₂ and bare graphene device, their carrier density were obtained using a standard parallel plate capacitor model, where $ne = C_g V_g$,² and $V_g - V_{CNP} = \hbar |v_F| \sqrt{\pi n} / e + ne / C_g$,³ respectively. n is carrier density, C_g is the gate (SiO₂) capacitance of $1.2 \times 10^{-8} \text{ F cm}^{-2}$,⁴ V_g is the gate voltage, V_{CNP} is the charge neutrality point voltage, $v_F = 1.1 \times 10^6 \text{ m s}^{-1}$ is the fermi velocity. The carrier density of MoS₂ and graphene can be converted to their Fermi level using $E_F = \hbar^2 \pi n / 2m_e$ and $E_F = \hbar |v_F| \sqrt{\pi n}$, respectively. Where $m_e = 0.35m_0$,⁵ m_0 is the electron mass.

The field-effect mobility, μ , is calculated by the formula: $\mu = \frac{L_{ch}}{W_{ch} C_g V_{ds}} |g_m|$,⁶ where L_{ch} and W_{ch} is the effective width and length of MoS₂ and graphene channel between drain and source electrodes, respectively. C_g is the gate (SiO₂) capacitance of $1.2 \times 10^{-8} \text{ F cm}^{-2}$,⁴ V_{ds} is the drain-source voltage. g_m is transport transconductance, $g_m = \left(\frac{\partial I_{ds}}{\partial V_{bg}} \right) V_{ds}$, Where I_{ds} is the drain-source current, V_g is the bottom-gated voltage.

Simulation method for extinction spectra

Finite element method was used to calculate the plasmonic behavior of graphene in bare graphene, MoS₂/graphene, and graphene/MoS₂ devices. In the simulation setup, the plane waves were incident from normal directions with the electric field perpendicular to the nanoribbons. We used an effective electrical ribbon width of 68 nm, equal to the physical ribbon width 100 nm minus the width of 'inactive' edges 32 nm⁷ and the width-to-pitch ratio of 1:2. For the optical constants in the simulation, surface conductivity of graphene was defined by Kubo formula in a complex form consisting of interband and intraband contributions.⁸ The charge mobility of graphene was used as $1000 \text{ cm}^2 / (\text{V} \cdot \text{s})$. The dielectric constant of monolayer MoS₂ of 3.7 was adopted.⁹ The thickness of graphene and MoS₂ were used as 0.35 nm and 0.6 nm, respectively.^{10, 11} The spacing between graphene ribbons and the MoS₂ was chosen to be 0 nm, neglecting the influence of small gap between layers caused by the residual polymethyl methacrylate (PMMA) polymer during the device fabrication process. The mesh of 0.25 nm was chosen for simulation.

Calculation of charge distribution in heterostructures via Thomas-Fermi charge screening theory

The Thomas-Fermi (T-F) charge screening theory has been widely used to calculate the charge distribution in multilayer graphene and multilayer MoS₂ field-effect transistors via the following two formulas.^{10, 12}

$$\frac{Q_i}{Q_{i-1}} \approx \exp\left(-\frac{d_i - d_{i-1}}{\lambda}\right) = \exp\left(-\frac{d_{ML}}{\lambda}\right)$$

$$\sum_{i=1}^N Q_i = Q_{gate}$$

Where Q_i is the charge in the i th layer, d_i denotes the distance from bottom layer material to the i th layer, d_{ML} is the distance between layers, λ is T-F screening length, Q_{gate} is the total charge induced by gate.

In MoS₂/graphene device, the charge distribution can be calculated via

$$\frac{Q_{MoS_2}}{Q_{graphene}} = \exp\left(-\frac{d_{MoS_2}}{\lambda_{graphene}}\right) = 0.37, \text{ where } d_{MoS_2} \text{ is the thickness of monolayer MoS}_2 \text{ (0.6 nm),}$$

$\lambda_{graphene}$ is the charge screening length of graphene (0.6 nm). Likewise, in graphene/MoS₂ device, the charge

distribution can be calculated via $\frac{Q_{graphene}}{Q_{MoS_2}} = \exp\left(-\frac{d_{graphene}}{\lambda_{MoS_2}}\right) = 0.95$, where $d_{graphene}$ is the thickness

of monolayer graphene (0.35 nm), λ_{MoS_2} is the charge screening length of MoS₂ (7 nm). Thus, the charge density in graphene layer in MoS₂/graphene and graphene/MoS₂ devices were calculated as ca. 73% and ca. 49% of that in bare graphene device.

Notes and references

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