Supporting Information:

Localized Surface Plasmons in Nanostructured Monolayer Black Phosphorus

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S1. Simulation Methods

The proposed structures are simulated with finite-difference time-domain methods with Lumerical FDTD solutions, a commercialized software package. All the structures including periodic nanoribbons and nanopatches are simulated in xy planes with periodic boundary conditions while the broadband plane waves are incident from z directions. Along the propagation directions (z directions), perfect matched layers (PML) are used to absorb all the light coming out to the boundaries. Electrical field distribution is gathered by 2D field profile monitors at the resonant wavelength just above the BP monolayer.

In the simulation, the audacious choice of 1 nm thickness will indicate the real response of the 2D monolayer film since it is still small enough compared with the wavelengths we are considering. To verify this, we consider the triple-layer structures with two layers of dielectric separated by BP film. In this setting, the dispersion relations reads¹:

$$e^{-2k_1 a} = \frac{\frac{k_1}{\epsilon_1} + \frac{k_2}{\epsilon_2} \frac{k_1}{\epsilon_1} + \frac{k_3}{\epsilon_3}}{\frac{k_1}{\epsilon_1} - \frac{k_2}{\epsilon_2} \frac{k_1}{\epsilon_1} - \frac{k_3}{\epsilon_3}}$$

where indices indicate the monolayer BP (1), dielectric (2) and dielectric (3) separately. The 2D dielectric function of the BP can be modeled with thickness a :

$$\epsilon_1 = \epsilon_{jj} = \epsilon_r + \frac{i\sigma_{jj}}{\epsilon_0 \omega a}$$

where ϵ_r is the dielectric constant of bulk BP. Since 1 nm is still quite small, we can expand the dispersion into dominant terms and plug in the dielectric function to get:

$$\frac{\epsilon_3}{k_3} + \frac{\epsilon_2}{k_2} = -\frac{i\sigma_{jj}}{\epsilon_0 \omega}$$

which is identical compared with the case treating BP in either directions as monolayer material without thickness².

S2. Electric field distribution for y case

In Figure S1, we show the side-view electric field distribution for the ribbons patterned along y direction. Compared with Figure 1 in the main text, the field resembles the x case however with lower amplitude.

Figure S1. (a,b) Side-view electric field distribution of one BP ribbon along y direction. Electromagnetic field is localized around two edges of the ribbon.

S3. Absorption of freestanding BP nanoribbons and dielectric thickness effect

Figure S2 shows the absorption of freestanding BP nanoribbons and graphene nanoribbons with the structure parameters described for Figure 1 in the main text. Compared with Figure 1b, the absorption in both armchair and zigzag cases has decreased, which is due to the weak light-matter interaction in the atomically thin BP film. The peak positions have also moved to new wavelengths, which is caused by the changing of environmental index below the BP film. In this

case, the overall shape of the spectrum keeps similar. Compared with freestanding graphene, BP interacts much weaker with light, which could be confirmed from the permittivity data. We've run the simulation for free standing graphene nanoribbons³ with Fermi level 0.64eV and mobility 10000cm/(V s). The resonance appears at smaller wavelength with much sharper shape.

To enhance the light-matter interaction as well as absorption, we design the Fabry-Perot setup below the BP film. In the simulation setup, the thickness of the dielectric between the BP ribbons and the bottom metal will influence the absorption in the BP. With various dielectric thickness, the electric field as well as the absorption in BP film can be tuned. Figure S3 shows the absorption spectra for both x and y cases with thickness changing from 1 μm to 30 μm . The period and widths kept at 250nm and 150nm separately. The absorption resonance for the ribbons along x direction is at about 31.5 μm and it keeps at the same position when we change the dielectric thickness since it is just determined by the size of the BP nanostructures. We observe the absorption reaches maximum at certain thickness. Figure S4 provides the explanation for the thickness dependency. The electric field intensity is plotted for the x cases with thickness 4.6 μm , 9.2 μm and 13.8 μm . The first and third one indicates the absorption at the maximum, while the second shows the absorption minimum. Since the dielectric constant is chosen at 1.7, the effective wavelength of the resonance is about 18.5 μm . These three numbers of the thickness are just the lengths of the quarter, half and three quarter effective wavelengths. At 4.6 μm and 13.8 μm , the electric field intensity reaches maximum which increases the absorption either. At 9.2 μm , the electric field intensity is almost 0 and the absorption is mainly reduced.

Figure S2. Absorption spectrum of the freestanding BP nanoribbons along x and y direction and freestanding graphene nanoribbons.

Figure S3. (a) Schematics of periodically patterned BP ribbons with t indicating the dielectric

thickness. (b,c) Absorption maps of two directions with fixed period $250nm$, fixed widths $150nm$ and various dielectric thicknesses

Figure S4. (a,b,c) Schematics and electric field intensity with three particular thicknesses. The BP is placed exactly at either the maximum or the minimum of the field intensity in these thicknesses.

S4. Plasmonic resonance dispersion of large period case and the anomalous phase shift upon reflection

We've run additional simulations for the case of large period. The resonance position is mainly determined by the ribbon width only. So we've run the sweep with different nanoribbon widths (changing from $100nm$ to $450nm$) and large period (period to width set as 3:1). Then we marked the plasmonic dispersion by picking up the resonance peak positions (similar method used to obtain the dispersion relations of graphene ribbons⁴).

There could be the anomalous reflection phase at the ribbon edges. And the exact formula could possibly be written as $q = (\text{constant}) \times \frac{\pi}{W}$, such as graphene ribbon case⁵. Since we don't have any experimental data, it is not fair to assume an arbitrary phase here to calculate the actual wave vector q . We just plot the dispersion by comparing the “plasmon resonance” vs “ $\frac{\pi}{W}$ ”, which mimics the plasmon behavior shown in BP (Figure S5).

Figure S5. Dispersion relations of BP nanoribbons in armchair and zigzag direction.

S5. Supporting Video

The supporting video shows how the light propagates through the ribbons structure. The electrical field is highly confined in the BP film.

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