Trapped mode control in an anisotropic MoS$_2$ metasurface

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Progress in developing advanced photonic devices relies on introducing new materials, discovered physical principles, and optimal designs when constructing their components. Optical systems operating on the principles of excitation of extremely high-quality factor trapped modes (also known as the bound states in the continuum, BICs) are of great interest since they allow the implementation of laser and sensor devices with outstanding characteristics. In this paper, we discuss how one can utilize the natural anisotropy of novel materials, particularly, the bulk molybdenum disulfide (MoS$_2$) composite, to realize the excitation of trapped modes in dielectric metasurfaces. The bulk MoS$_2$ composite is a finely-stratified structure characterized by averaged constitutive parameters possessing a form birefringence property. Our metasurface is composed of an array of disk-shaped nanoparticles (resonators) made of the MoS$_2$ composite under the assumption that the anisotropy axis of the MoS$_2$ composite can be tilted to the rotation axis of the disks. We perform a detailed analysis of eigenwaves and scattering properties of such anisotropic resonators as well as the spectral features of the metasurface revealing dependence of the excitation conditions of the trapped mode on the anisotropy axis orientation of the MoS$_2$ composite used.

I. INTRODUCTION

Thanks to astonishing advances in technology, electrically thin layers of materials can be fabricated with sub-wavelength periodic patterns to create planar metamaterials (also known as metasurfaces). Such two-dimensional structures make it possible to control the phase, amplitude, frequency, angular momentum, and polarization state of electromagnetic waves in a predetermined way [1, 2]. Due to abrupt phase changes on device surfaces rather than phases of light propagating inside the systems, this type of metamaterials can be ultra-thin and flat, which is highly desirable in integrated optics and photonics. The main task in this field is to design metasurfaces that provide the most efficient interaction of light with nanostructured matter. With the use of novel materials, like transition metal dichalcogenides (TMDs) [3], one can also expect to make such metasurfaces manageable.

Atomically thin TMDs of the form MX$_2$ (M = Mo, W; X = S, Se, Te) are a new class of semiconductor materials proposed for use in both fundamental physics exploration in two-dimensional systems and device applications. Among the TMDs, MoS$_2$ is an indirect bandgap semiconductor with large bandgap energy which can be transformed into a direct semiconductor in the monolayer limit [4, 5]. A bulk MoS$_2$ is considered as a layer-by-layer stack of MoS$_2$ monolayers, where strong interactions only exist within the basal plane of covalent bonds. Therefore, the bulk MoS$_2$ is an anisotropic crystal, which can be macroscopically characterized with tensor permittivity possessing in-plane $\varepsilon_{||}$ and out-of-plane $\varepsilon_{\perp}$ terms [6]. In particular, these extraordinary properties of MoS$_2$ have been utilized in constructing anisotropic resonators for lasing systems [7] and dielectric metasurfaces [8–11].

The optical features of dielectric metasurfaces depend on the excitation conditions of corresponding Mie-type modes [12, 13] arising in resonators. In particular, in the spectra of dielectric metasurfaces, there are two basic resonant states which correspond to the excitation of the magnetic dipole and electric dipole modes whose position on the frequency scale depends on the aspect ratio of the particles [14]. Moreover, when metasurfaces containing anisotropic particles are considered, an additional mode splitting may occur [15], which makes the physics of such nanostructures much richer. Performing tuning mode conditions by changing the aspect ratio of dielectric nanoparticles allows one to perform flexible manipulation by resonant states [14, 16] of the nanostructure, and realize, for example, Huygens metasurfaces [17] where destructive interference between the electric and magnetic dipole modes of comparable strength suppresses backward scattering making such metasurfaces to be fully transparent.

Among different designs of dielectric metasurfaces we further distinguish a particular class of structures that allow obtaining the strongest resonant response due to the excitation of so-called trapped modes [18, 19] (recently such modes are referred to as bound states in the continuum, BICs [20, 21]). In metasurfaces, such modes are related to non-radiating (dark) eigenwaves which cannot couple with the field of incident radiation (continuum). The origin of a particular trapped mode and its characteristics depend on the symmetry of a system and its
Spatial, geometric, and material parameters. In particular, a trapped mode can be excited in metasurfaces if their constitutive particles (resonators) are in some way perturbed [22]. In this case, a perturbation transforms inherently dark mode to a weakly radiative one when the spatial symmetry of the translation unit cell of the metasurface is broken.

From the point of view of electromagnetic theory, breaking the spatial symmetry of resonators forming a metasurface leads to the appearance of artificial anisotropy of their averaged constitutive parameters resulting in their anisotropic or bianisotropic electromagnetic response [24]. The effect of anisotropy enables the trapped mode coupling with the continuum transforming the dark mode into a quasi-trapped one. Despite the leakage of energy from the quasi-trapped mode due to anisotropy, the concentration of electromagnetic energy in the resonators can be maintained at a very high level if the introduced perturbation is small [23]. Nevertheless, technologically, the production of nanoscale resonators with the required small perturbation is a rather complicated task. Evidently, this issue can be solved with the use of naturally artificial materials, in particular, MoS$_2$ composites.

In this paper, we combine the anisotropic properties of a bulk MoS$_2$ composite considered for particle fabrication and geometric parameters of these particles to construct a metasurface that demonstrates resonant conditions originating from the trapped mode. In particular, in our metasurface, we utilize disk-shaped resonators due to their amenability with modern lithography techniques used for producing metasurfaces operating in the THz range. All our numerical simulations are targeted on the third telecommunication window [26]. Our approach is based on the analysis of eigenwaves of such resonators and their electric and magnetic dipole responses revealing the dependence of the excitation conditions of the trapped mode on the anisotropy axis orientation in the bulk MoS$_2$.

II. EIGENWAVES ANALYSIS

In what follows, we consider a metasurface composed of MoS$_2$ anisotropic disk-shaped nanoparticles arranged in a two-dimensional array. The translation unit cell of this array is a square with the side size $p$. The radius and height of the disks are $a$ and $h$, respectively. The MoS$_2$ composite is a finely-stratified structure (superlattice), which is characterized by averaged (homogenized) constitutive parameters. In particular, the MoS$_2$ composite possesses a form birefringence property [26] being a nonmagnetic ($\mu = \mu_0$) uniaxial anisotropic crystal whose anisotropy axis ($c$-axis) is directed perpendicular to the plane of layers forming the superlattice, and permittivity is described by a tensor quantity $\varepsilon$. For the sake of definiteness, we assume that the $c$-axis of the crystal is tilted in the $y$-$z$ plane and can change its orientation on the angle $\varphi$ with respect to the $z$-axis of the chosen Cartesian coordinate frame, where the $z$-axis is also the rotation (axial symmetry) axis of the disks, as shown in Fig. 1. In the operating frequency range under study, material losses in the bulk MoS$_2$ composite are negligibly small (see Appendix A) and, therefore, we exclude them from our consideration. Without loss of generality, we assume that the particles are located in homogeneous surrounding space (air). The trapped mode manifestation is related to the in-plane symmetry breaking of the metasurface unit cell. The substrate presence does not break the in-plane symmetry and has no significant influence on the effects discussed. Therefore, in order not to overload our study, we consider that the substrate is made of an air-like material $\varepsilon_\infty \approx 1$. Accounting for the substrate can be performed later in the engineering implementation of the metasurface by adjusting the geometric parameters of the resonators used.

Initially, we perform an eigenwave analysis of the given metasurface. For our simulations, we use the RF module of the commercial COMSOL Multiphysics finite-element electromagnetic solver. In the solver, we construct one square unit cell of the metasurface imposing the Floquet-periodic boundary conditions on its sides to simulate the infinitely expanded two-dimensional array of nanoparticles. From the solutions found, we select those that correspond to the excitation of the lowest-order eigenwaves only. We classify these eigenwaves by considering the electromagnetic field configuration inside the resonator when the $c$-axis tilt angle $\varphi$ is zero and permittivity of the disk acquires the diagonal form $\varepsilon|_{\varphi=0}=\{\varepsilon_\parallel,\varepsilon_\parallel,\varepsilon_\perp\}$. For the chosen geometric parameters of the resonators, the eigenwaves arise as the transverse electric TE$_{11\delta}$, and hybrid EH$_{11\delta}$ and HE$_{11\delta}$ modes, sequentially arranged.
with increasing frequency (this classification is based on the mode nomenclature of cylindrical dielectric waveguides, see Ref. [27]). In the subscripts of the mode abbreviations, the first index denotes the azimuthal variation of the fields, the second index denotes the order of variation of the field along the radial direction, and the third index denotes the order of variation of fields along the $z$-direction. Since we do not fix the exact number of field variations along the $z$-axis, we substitute the third index with the letter $\delta$. In general, the characteristics of eigenwaves under study inherit the properties of the corresponding modes of an anisotropic nanowire derived in Appendix [B].

Moreover, as known from the theory of dielectric resonators [28], the $\text{TE}_{01,\delta}$ mode of an isolated cylindrical resonator radiates like a magnetic dipole $\mathbf{m}$ oriented along its rotation axis (out-of-plane), whereas the $\text{EH}_{11,\delta}$ and $\text{HE}_{11,\delta}$ modes radiate like an electric dipole $\mathbf{p}$ and magnetic dipole $\mathbf{m}$, respectively, oriented along the transverse direction (in-plane). Thus, each hybrid mode is complemented by its own degenerated state, depending on the direction in which the corresponding dipole moment is oriented, along either the $x$-axis or the $y$-axis in the chosen Cartesian coordinate frame. We distinguish these degenerated hybrid modes by adding the corresponding superscript $x$ or $y$ to the mode abbreviations. The appearance of all eigenwaves of our interest at the initial stage $\varphi = 0$ are collected in Fig. 2(a).

Among these eigenwaves, the field for the $\text{TE}_{01,\delta}$ mode is axisymmetric and thus has no azimuthal variation, whereas the fields of the hybrid modes $\text{EH}_{11,\delta}^{x,y}$ and $\text{HE}_{11,\delta}^{x,y}$ are azimuthally dependent. This property of the $\text{TE}_{01,\delta}$ mode leads to the appearance of conditions corresponding to the existence of the trapped mode in our lossless metasurface signifying that the corresponding eigenfrequency ($\omega = \omega^\prime + i \omega^\prime\prime$) is a purely real quantity ($\omega^\prime\prime = 0$).

Further in our study, we vary the value of the tilt angle $\varphi$. When $\varphi \in (0^\circ, 90^\circ)$, there are off-diagonal components in the tensor $\hat{\epsilon}$, whereas when $\varphi = 90^\circ$, the $c$-axis is directed along the $y$-axis, and permittivity of the disk becomes diagonal $\hat{\epsilon}|_{\varphi=90^\circ} = \{\epsilon_\parallel, \epsilon_\perp, \epsilon_\parallel\}$ (see Appendix [B]). We track the change in the values of the real part of the eigenfrequency ($\omega^\prime$) and quality factor ($\omega^\prime / 2 \omega^\prime\prime$) of the selected eigenwaves. The corresponding results of
FIG. 3. Transmission coefficient as a function of frequency $f = \omega/2\pi$ and $c$-axis tilt angle $\varphi$ for the (a) $x$-polarized and (b) $y$-polarized incident waves. The markers at the bottom of the figure are the eigenfrequencies of the $\text{TE}_{01}\delta$, $\text{EH}_{11}\delta$, and $\text{HE}_{11}\delta$ eigenwaves, where the size of the markers represents their quality factor. (c) Patterns of the electric and magnetic fields plotted at the corresponding resonant frequencies for the $\text{TE}_{01}\delta$, $\text{EH}_{x,y}\delta$, and $\text{HE}_{x,y}\delta$ modes of the metasurface at three different values of $\varphi$. The red and dark blue arrows represent the flow of electric and magnetic fields while brown and gray arrows represent the electric $\mathbf{p}$ and magnetic $\mathbf{m}$ dipole moments, respectively. Parameters of the metasurface are the same as in Fig. 2.

III. SPECTRAL FEATURES

In this section, we reveal specific spectral features of the MoS$_2$ metasurface caused by the material anisotropy. For this study we consider that the metasurface is illuminated by a plane electromagnetic wave under the normal incidence conditions ($\mathbf{k} = \{0, 0, -k_z\}$) with the electric field polarized along either the $x$-axis ($\mathbf{E} = \{E_x, 0, 0\}$, $x$-polarization) or the $y$-axis ($\mathbf{E} = \{0, E_y, 0\}$, $y$-polarization). In the framework of the RF module of the COMSOL Multiphysics solver, we dispose of the radiating and receiving ports above and below the metasurface, respectively. The port boundary conditions are placed on the interior boundaries of the perfectly matched layers, adjacent to the air domains. Perfectly matched layers on the top and bottom of the unit cell absorb the excited wave from the radiating port and prevent unwanted re-reflection inside the computational domain. The port boundary conditions automatically determine the reflection and transmission characteristics of our calculations are presented in Figs. 2(b) and 2(c), respectively. One can see that the hybrid $\text{EH}_{x,y}\delta$ and $\text{HE}_{x,y}\delta$ modes lose their degeneracy and split apart with a change in the tilt angle $\varphi$ of the anisotropy axis, while the $\text{TE}_{01}\delta$ mode does not. Moreover, the quality factor of the $\text{TE}_{01}\delta$ mode changes from infinity to finite values undergoing a transformation from the trapped to a radiative state. Hereinafter, our task is to reveal the manifestation of these eigenwaves in the transmitted spectra of our metasurface.
the metasurface in terms of S-parameters. After simulation, we retrieve values of the transmission coefficient \(|T|^2 = |S_{21}|^2\) as a function of frequency and c-axis tilt angle \(\varphi\) for two orthogonal polarizations of the incident wave. The results of our calculations are summarized in Figs. 3(a) and 3(b) for the \(x\)-polarized and \(y\)-polarized waves, respectively.

When \(\varphi = 0^\circ\), the metasurface is polarization-independent. In the frequency band of interest, there are two resonant states related to the excitation of the degenerated hybrid EH\(_{11,\delta}\) and HE\(_{11,\delta}\) modes. The identified resonances appear due to an existing electromagnetic coupling between the linearly polarized incident wave and transversely located electric and magnetic dipoles inherent to the corresponding eigenwaves. Since the TE\(_{01,\delta}\) mode is axially symmetric with the corresponding magnetic resonances appearing due to an existing electromagnetic coupling with the field of the incident wave, the field of the incident wave does not interact with this mode and there is no corresponding resonance in the spectra of the transmitted wave.

Variation of the c-axis tilt angle \(\varphi\) breaks the in-plane symmetry of the structure, resulting that the metasurface becomes to be polarization-dependent. Although the degeneracy for hybrid modes is lifted, their resonant positions on the frequency scale change a little compared to those of the degenerated modes that existed in the \(\varphi = 0\) case. However, since the rotation of the anisotropy c-axis is maintained in the \(y-z\) plane, noticeable changes are observed in the spectra of the \(x\)-polarized wave. At a certain value of the c-axis tilt angle \((\varphi \approx 50^\circ)\), the resonant frequencies of the EH\(_{11,\delta}\) and HE\(_{11,\delta}\) modes coincide, and with a further increase in \(\varphi\), the resonances rearrange their order on the frequency scale. This mode crossing effect is widely discussed in the context of the implementation of Huygens metasurfaces [17]. Moreover, the quality factor of the EH\(_{11,\delta}\) and HE\(_{11,\delta}\) resonances increases, since the electromagnetic coupling of the corresponding either electric \(p\) or magnetic \(m\) dipole with the field of the incident wave decreases.

Aside from the resonances related to the above-considered hybrid EH\(_{11,\delta}\) and HE\(_{11,\delta}\) modes which possess a good electromagnetic coupling with the field of the normally incident linearly polarized wave, in the frequency band of interest an additional resonance arises in the transmitted spectra of the \(x\)-polarized waves as soon as \(\varphi\) is nonzero. This resonance is related to the manifestation of the TE\(_{01,\delta}\) mode. It appears as an alone-standing lowest frequency resonance whose quality factor decreases with increasing \(\varphi\). This resonance acquires a peak-and-trough (Fano) profile as is typical for the trapped modes excitation [18,19]. While the dip in curves corresponds to the maximum of reflection, the peak corresponds to the maximum of transmission. These extremes approach 0 and 1, respectively, since the material losses in the given metasurface are considered to be negligibly small.

To reveal the origin of changes in the emerging resonances, we plot the patterns of the electric and magnetic fields within the unit cell in three basic projections and show the orientation of the dipole moments \(m\) and \(p\) at the resonator center. These calculations are made for three different values of the c-axis tilt angle \(\varphi\). The results of our calculations are collected in Fig. 3(c). One can see that variation in the material anisotropy leads to a change in the slope of the dipole moment of the corresponding mode, thereby changing the degree of its electromagnetic coupling with the field of the incident wave. This mechanism is fully consistent with the behavior of trapped modes in resonators with artificial anisotropy (perturbed unit cells) [19,29,30] and the corresponding theory [23,31] can be adapted in this case. It is based on the scattering characteristics of a single anisotropic nanoparticle which we discussed in Appendix C.

IV. CONCLUSIONS

We have elucidated the role of material anisotropy in the mechanism of the trapped mode excitation in a metasurface composed of MoS\(_2\) disk-shaped nanoparticles. Our study is based on the analysis of the properties of the three lowest-order modes of cylindrical resonators forming the metasurface. They are the axially symmetric TE\(_{01,\delta}\) mode as well as the non-symmetric hybrid EH\(_{11,\delta}\) and HE\(_{11,\delta}\) modes.

When the anisotropy axis of the MoS\(_2\) composite used for the disk-shaped particles fabrication coincides with the axis of their rotational symmetry, the hybrid EH\(_{11,\delta}\) and HE\(_{11,\delta}\) modes are degenerated, whereas the TE\(_{01,\delta}\) mode behaves like a trapped mode in the metasurface, being a purely real eigenwave. When the anisotropy axis is tilted, the hybrid EH\(_{11,\delta}\) and HE\(_{11,\delta}\) modes are split, and the TE\(_{01,\delta}\) mode transforms into a radiating one, whose quality factor decreases with increasing the anisotropy tilt angle. It is shown how a change in the anisotropy tilt angle affects the orientation of vectors of the electric and magnetic dipole moments of the corresponding modes.

By demonstrating control ability over the high-quality factor trapped modes in MoS\(_2\) metasurfaces by manipulating material anisotropy, we propose a platform for many important applications in light-matter interaction, nonlinear photonics, quantum optics, and spectroscopy.

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Appendix A: MoS$_2$ relative permittivity

Dispersion characteristics of components of the tensor of relative permittivity ($\hat{\epsilon} = \epsilon' + i\epsilon''$) of MoS$_2$ material are shown in Fig. 4. Since in our work, we focus on the spectral range within the third telecommunication window ($\lambda \in [1500, 1600]$ nm), where negligibly weak dispersion exists (see the spectral region marked gray), we adopt $\epsilon'_\parallel = 16.6$, $\epsilon'_{\perp} = 6.3$, $\epsilon''_{\parallel} = \epsilon''_{\perp} = 0.0$ in all considered region.

Appendix B: Lowest-order modes of an anisotropic nanowire

For reference, here we present dispersion features of three lowest-order modes (TE$_{01}$, EH$_{11}$, and HE$_{11}$) of an anisotropic nanowire. The nanowire is made of a nonmagnetic material (MoS$_2$) with tensor-valued relative permittivity $\hat{\epsilon}$. The nanowire is disposed of in a surrounding medium with permittivity $\epsilon_0$. The radius of the nanowire is $a$. The symmetry axis of the nanowire coincides with the $z$-axis of the Cartesian coordinate system [see the inset in Fig. 4(a)].

The optic $c$-axis of the uniaxial crystalline MoS$_2$ core of the nanowire is tilted in the $y$-$z$-plane and makes an angle $\varphi$ with the $z$-axis. The full relative permittivity tensor of the nanowire core $\hat{\epsilon}(\varphi)$ can be evaluated by using the rotation matrix

$$
\hat{R}(\varphi) = \hat{\epsilon}_{|\varphi=0}\cdot \hat{R}^T = \begin{pmatrix}
\epsilon_{xx} & 0 & \epsilon_{yy} \cos^2 \varphi + \epsilon_{zz} \sin^2 \varphi \\
0 & \epsilon_{yy} \sin \varphi \cos \varphi - \epsilon_{zz} \sin \varphi \cos \varphi & 0 \\
\epsilon_{yy} \sin \varphi \cos \varphi + \epsilon_{zz} \sin \varphi \cos \varphi & 0 & \epsilon_{zz} \cos^2 \varphi + \epsilon_{yy} \sin^2 \varphi
\end{pmatrix},
$$

where $\hat{\epsilon}_{|\varphi=0} = \{\epsilon_{xx}, \epsilon_{yy}, \epsilon_{zz}\} = \{\epsilon_{\parallel}, \epsilon_{\perp}, \epsilon_{\perp}\}$ and superscript $T$ denotes the matrix transposition.

As follows from Eq. \ref{B2}, permittivity of the nanowire can be defined in the diagonal form as $\hat{\epsilon}_{|\varphi=90^\circ} = \{\epsilon_{\parallel}, \epsilon_{\parallel}, \epsilon_{\perp}\}$ in two special cases when the $c$-axis is directed along the $z$-axis and the $y$-axis, respectively. For the rest range $\varphi \in (0^\circ, 90^\circ)$, the tensor $\hat{\epsilon}(\varphi)$ has nonzero off-diagonal components.

When the directions of the $c$-axis and the $z$-axis coincide, there is an analytical solution for the nanowire modes \ref{B2}. Generally, such an anisotropic nanowire supports an infinite set of the axially symmetric TE$_{mn}$ and TM$_{mn}$ modes as well as the non-symmetric hybrid EH$_{mn}$ and HE$_{mn}$ modes, whose dispersion equation can be expressed as

$$
\begin{align*}
\left[\epsilon_0 K'_m(\gamma a) + \sqrt{\epsilon_{\parallel}} J_m(p \kappa a)\right]
+ \frac{1}{\gamma a} K'_m(\gamma a)
= \left(\frac{m \beta}{k_0}\right)^2 \left[\frac{1}{(\gamma a)^2} + \frac{1}{(\kappa a)^2}\right]^2,
\end{align*}
$$

where, $k_0$ is the wavenumber in free space, $m$ and $n$ are the integer values known as the azimuthal and radial indices, respectively, $\beta$ is the longitudinal propagation constant, $p = \sqrt{\epsilon_{\parallel}/\epsilon_{\perp}}$ is the anisotropy parameter, $\kappa = \sqrt{k_0^2 \epsilon_{\parallel} - \beta^2}$ and $\gamma = \sqrt{\beta^2 - k_0^2 \epsilon_{0}}$ are the transverse propagation constants inside and outside the nanowire, respectively, $J_m(\cdot)$ and $K_m(\cdot)$ are the Bessel function of the first kind and the modified Bessel function of the second kind, and $J'_m(\cdot)$ and $K'_m(\cdot)$ are their derivatives with respect to the function argument.

A formal substitution of $m = 0$ into Eq. \ref{B3} yields us two separate dispersion equations related to the transverse magnetic TM$_{0n}$ and transverse electric TE$_{0n}$ modes (see, the first and second multiplier on the left side of the dispersion equation \ref{B3}, respectively), similarly to the case of a nanowire with an isotropic core \ref{B4}.

In the general case of a uniaxial crystal core when the $c$-axis does not coincide with the $z$-axis, the propagation constants and field components can be determined numerically \ref{B5}. The calculated effective mode index $\tilde{\beta} = \beta/k_0$ and the electric field patterns of the lowest-order TE$_{01}$, EH$_{11}^x$, and HE$_{11}^y$ modes propagated in the
FIG. 5. (a)-(c) Dispersion curves of the axially symmetric TE\textsubscript{01} and non-symmetric hybrid HE\textsubscript{x,y}\textsuperscript{11} modes of the cylindrical MoS\textsubscript{2} nanowire at different values of the c-axis tilt angle \(\varphi\): (a) \(\varphi = 0^\circ\), (b) \(\varphi = 45^\circ\), and (c) \(\varphi = 90^\circ\). The circles in panel (a) correspond to the analytical solution given by Eq. (B3). (d) The effective mode index \(\tilde{\beta}\) of the TE\textsubscript{01}, HE\textsubscript{x,y}\textsuperscript{11} and EH\textsubscript{x,y}\textsuperscript{11} modes versus the c-axis tilt angle \(\varphi\) at the fixed frequency \(f = 200.0\) THz. (e) Simulated electric field intensities \(|E|\) of the nanowire modes corresponding to panels (a), (b), and (c). A schematic of the MoS\textsubscript{2} nanowire is shown in the inset of panel (a). The red arrow represents the c-axis direction in the nanowire core. The nanowire radius is \(a = 258\) nm, and components of the tensor of relative permittivity are: \(\varepsilon_\parallel = 16.6\) and \(\varepsilon_\perp = 6.24\).
MoS$_2$ nanowire are presented in Fig. 5 for different values of the c-axis tilt angle $\varphi$. In particular, when the c-axis is directed along the z-axis, the results of our simulation are checked against those obtained from the analytical solution given by Eq. (B3).

From Figs. 5(a), 5(b), 5(c), one can conclude that when $\varphi \in (0^\circ, 90^\circ)$, the dispersion characteristic of the TE$_{01}$ mode does not depend on the transverse polarization, that is, this mode does not split into the $x$-polarized (TE$_{01x}$) and $y$-polarized (TE$_{01y}$) components (see, also Refs. [28, 39]). Nevertheless, when $\varphi \neq 0^\circ$, the axial symmetry of the electric field of the TE$_{01}$ mode becomes violated, as shown in Fig. 5(e).

In turn, the dispersion characteristics of hybrid modes are more complex. Figure 5(a) shows that at $\varphi = 0^\circ$, no modal birefringence phenomenon exists, it means that the hybrid HE$_{01}^{x,y}$ and EH$_{11}^{x,y}$ modes are degenerated as shown in Fig. 5(e), which is typical for uniaxial nanowires [28, 39].

In the range $\varphi \in (0^\circ, 90^\circ)$, the dispersion characteristics of hybrid HE$_{11}^{x,y}$ and EH$_{11}^{x,y}$ modes depend on the transverse polarization orientations, which leads to degeneracy lifting as presented in Fig. 5(e). Thus, the different polarizations of HE$_{11}^{x}$ (EH$_{11}^{x}$) and HE$_{11}^{y}$ (EH$_{11}^{y}$) modes have different dispersion relations and propagate like different modes, as shown in Figs. 5(b) and 5(c). For the chosen parameters of anisotropy, the effect of the c-axis orientation is much stronger for the $y$-polarized modes compared to the $x$-polarized ones due to the fact that $\varepsilon_{yy}(\varphi) \in [\varepsilon_{\perp}, \varepsilon_{||}]$ while $\varepsilon_{xx}(\varphi) = \varepsilon_{||}$ [see, for clarity, Eq. (B2)]. A similar feature has been reported previously for an anisotropic rectangular waveguide [39]. Besides, Fig. 5(d) indicates that difference between the $x$-polarized and $y$-polarized modes increases as the c-axis tilt angle $\varphi$ rises, and the difference between HE$_{11}^{x}$ and EH$_{11}^{y}$ is smaller than the difference between the HE$_{11}^{y}$ and HE$_{11}^{x}$ modes.

Appendix C: Scattering cross-section of an anisotropic nanoparticle

For numerical simulations of the single particle scattering cross-section and the particle electric and magnetic dipole moments, we use the discrete dipole approximation (DDA) and the decomposed discrete dipole approximation (DDDA) methods [14]. The main idea of the DDA method consists in the replacement of the scattering object by a cubic lattice of electric point dipoles with known polarizability tensor $\hat{\alpha}_p$. The corresponding dipole moment $\mathbf{d}_i$ induced in each lattice point $i$ (with the radius vector $\mathbf{r}_i$) is found by solving coupled dipole equations:

$$
\mathbf{d}_i = \hat{\alpha}_p \mathbf{E}_i^0 + \hat{\alpha}_p \frac{k_0}{\varepsilon_0} \sum_{j \neq i} N \hat{G}_{ij} \mathbf{d}_j, \quad i = 1...N,
$$

where $\mathbf{E}_i^0$ is the electric field of the incident wave at the point $\mathbf{r}_i$, $k_0$ is the wavenumber in a vacuum, $\varepsilon_0$ is the vacuum dielectric constant, $\hat{G}_{ij} = \hat{G}(\mathbf{r}_i, \mathbf{r}_j)$ is the Green tensor of the system without the particle, $N$ is the number of dipoles replacing the particle after the discretization procedure. For a MoS$_2$ particle (disk), when the c-axis of anisotropy is directed along the z-axis in the chosen Cartesian coordinate frame ($\varphi = 0^\circ$), the permittivity tensor is written as

$$
\hat{\varepsilon} = \begin{pmatrix}
\varepsilon_{||} & 0 & 0 \\
0 & \varepsilon_{\perp} & 0 \\
0 & 0 & \varepsilon_{\perp}
\end{pmatrix},
$$

and the polarizability tensor can be taken as

$$
\hat{\alpha}_p \simeq 3\varepsilon_0 \varepsilon_s V_p \begin{pmatrix}
\frac{\varepsilon_{\perp} - \varepsilon_s}{\varepsilon_{||} + 2\varepsilon_s} & 0 & 0 \\
0 & \frac{\varepsilon_{\perp} - \varepsilon_s}{\varepsilon_{||} + 2\varepsilon_s} & 0 \\
0 & 0 & \frac{\varepsilon_{\perp} - \varepsilon_s}{\varepsilon_{||} + 2\varepsilon_s}
\end{pmatrix}.
$$
where \(V_p\) is the volume of the discretization cell, \(\varepsilon_s\) is the relative permittivity of the surrounding medium. Here we assume that the particle is localized in a vacuum or in the air where \(\varepsilon_s = 1\). After the solution of Eqs. (C1) and choosing the origin of the Cartesian coordinate system in the center of mass of the particle, the scattered electric field \(\mathbf{E}^{\text{scat}}\) in the far-field zone and the spherical coordinates are written as

\[
\mathbf{E}^{\text{scat}}_{\phi}(r, \phi, \theta) = \frac{k_0^2 e^{ik \cdot r}}{4\pi \varepsilon_0 r} \sum_{j=1}^{N} e^{-ik \cdot (\mathbf{n} \cdot \mathbf{r}_j)} \left( d_y^j \cos \phi \right. \\
\left. - d_z^j \sin \phi \right),
\]

\[
\mathbf{E}^{\text{scat}}_{\theta}(r, \phi, \theta) = \frac{k_0^2 e^{ik \cdot r}}{4\pi \varepsilon_0 r} \sum_{j=1}^{N} e^{-ik \cdot (\mathbf{n} \cdot \mathbf{r}_j)} \left( d_z^j \cos \phi \cos \theta \right. \\
\left. + d_y^j \sin \phi \cos \theta - d_z^j \sin \theta \right),
\]

where \(k_s = k_0 \sqrt{\varepsilon_s}\), \(\mathbf{n} = (\sin \theta \cos \phi, \sin \theta \sin \phi, \cos \theta)\) is the unit vector directed to the observation point with spherical coordinate \((r, \phi, \theta)\), \(r\) is the distance to the observation point, \(\phi\) and \(\theta\) are the azimuthal and polar angles, respectively.

The scattering cross-section \(\sigma_{\text{scat}}\) is calculated as

\[
\sigma_{\text{scat}} = \frac{1}{|\mathbf{E}_0|^2} \int_{\Omega} \left( |\mathbf{E}^{\text{scat}}_{\phi}|^2 + |\mathbf{E}^{\text{scat}}_{\theta}|^2 \right) r^2 d\Omega,
\]

where \(\Omega\) and \(d\Omega = \sin \theta d\phi d\theta\) is the full solid angle and its differential.

In the DDDA, a discrete representation of the induced polarization inside the particle is obtained as

\[
\mathbf{P}(\mathbf{r}) = \sum_{j=1}^{N} \mathbf{d}^j \delta(\mathbf{r} - \mathbf{r}_j),
\]

where \(\delta(\mathbf{r} - \mathbf{r}_j)\) is the Dirac delta function.

Using the relation \(\mathbf{j} = -i\omega \mathbf{P}\), where \(\omega\) is the field angular frequency, between the induced polarization \(\mathbf{P}\) and the induced electric current density \(\mathbf{j}\) and Eq. (C6), the multipole moments of the particle can be calculated by applying the expressions from Ref. [40]. In this approach the multipole decomposition of the scattering cross-section is

\[
\sigma_{\text{scat}} \simeq \frac{k_0^4}{6\pi \varepsilon_0 |\mathbf{E}_0|^2} |\mathbf{p}|^2 + \frac{k_0^4 \varepsilon_s \mu_0}{6\pi \varepsilon_0 |\mathbf{E}_0|^2} |\mathbf{m}|^2 \\
+ \frac{k_0^4 \varepsilon_s |Q_{\alpha\beta}|^2}{720\pi \varepsilon_0 |\mathbf{E}_0|^2} + \frac{k_0^6 \varepsilon_s \mu_0}{80\pi \varepsilon_0 |\mathbf{E}_0|^2} \sum_{\alpha\beta} |M_{\alpha\beta}|^2,
\]

where \(\mu_0\) is vacuum permeability, \(\mathbf{p}\) and \(\mathbf{m}\) are the electric and magnetic dipole moments, \(Q\) and \(M\) are the electric and magnetic quadrupole moments of the particle.

Note that from the practical point of view, it is convenient to rotate the disk under the fixed polarizability tensor \((C3)\) in the numerical simulation in order to change the anisotropic properties of the disk.

The results of our modeling of the cross-section characteristics of a single particle for several different values of the \(c\)-axis tilt angle \(\varphi\) are shown in Fig. 5. First, one can see that the resonant response of the disk depends on both orientations of the MoS\(_2\) layers and irradiation conditions. Second, in the chosen frequency range, the resonant features are associated only with the resonant excitation of either the electric (ED) or magnetic (MD) dipole moments of the particle. Importantly, in the range, \(\varphi \in (0, 90^\circ)\), the material anisotropy of the disk leads to the resonant excitation of the longitudinal (directed along the wave vector \(\mathbf{k}\) of the incident wave) components of the ED and MD dipole moments (Fig. 7). The excitation of \(p_z\) (\(m_z\)) component is realized for the \(y\)-polarized \((x\)-polarized\) waves, respectively, and spec-

![FIG. 7. Variation of the magnitude of the z component of the electric \(p\) and magnetic \(m\) dipole moments for several values of the \(c\)-axis tilt angle \(\varphi\) for the frontal irradiation of the disk by the (a) \(x\)-polarized and (b) \(y\)-polarized wave. Parameters of the disk are the same as in Fig. 5.](image_url)
tral positions of their extremes are completely correlated with the resonant features of the transmission spectra of the MoS$_2$ metasurface presented in Figs. 3(a) and 3(b), respectively. This demonstrates that the discussed resonant states of the anisotropic metasurface are basically influenced by the anisotropy and modes of an individual dielectric resonator rather than by the electromagnetic coupling between them.
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