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Layer-Resolved Absorption of Light in Arbitrarily Anisotropic Heterostructures

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We present a generalized formalism to describe the optical energy flow and spatially resolved absorption in arbitrarily anisotropic layered structures. The algorithm is capable of treating any number of layers of arbitrarily anisotropic, birefringent, and absorbing media and is implemented in an open access computer program. We derive explicit expressions for the transmitted and absorbed power at any point in the multilayer structure, using the electric field distribution from a 4×4 transfer matrix formalism. As a test ground, we study three nanophotonic device structures featuring unique layer-resolved absorption characteristics, making use of (i) in-plane hyperbolic phonon polaritons, (ii) layer-selective, cavity-enhanced exciton absorption in transition metal dichalcogenide monolayers, and (iii) intersubband-cavity polaritons in quantum wells. Covering such a broad spectral range from the far-infrared to the visible, the case studies demonstrate the generality and wide applicability of our approach.

I. INTRODUCTION

The absorption of light in thin layers of strongly anisotropic materials has received enormous attention since the dawn of two-dimensional (2D) materials and their heterostructures¹. Tremendous progress has been reported using 2D materials for numerous nanophotonic applications such as hybrid graphene-based photodetectors^{2,3}, optoelectronic^{4,5} and photovoltaic^{6,7} devices employing transition metal dichalcogenide (TMDC) monolayers, enhanced light-matter interaction using photonic integration with optical cavities^{8,9}, approaches towards TMDC-based nanolasers^{10,11}, hyperlensing^{12,13} based on hyperbolic polaritons¹⁴, bio-sensing¹⁵, and thermoelectric applications using black phosphorus (BP) monolayers^{16,17}. In light of these thriving developments and the great potential entailed in nanophotonic technology, a robust and consistent theoretical framework for the description of light-matter interaction in layered heterostructures of anisotropic materials is of central importance.

In order to understand, analyze and predict the optical response of multilayer structures, the transfer matrix formalism has proven to be of great utility^{18–20}. In isotropic layered media, a 2×2 transfer matrix fully describes any light-matter interaction, and with knowledge of the local electric and magnetic fields, the optical power flow can be described by the Poynting vector \mathcal{S} ^{21,22}. However, what already proves intricate in isotropic multilayers, becomes even more cumbersome when the materials are uniaxial or even biaxial requiring a 4×4 transfer matrix formalism^{23–25}, as it is the case for many state-of-the-art nanophotonic materials like hexagonal boron nitride (hBN)²⁶, molybdenum trioxide (MoO_3)²⁷, or BP²⁸. In consequence, to the best of our knowledge, previous approaches aiming at the analytical computation of light absorption in anisotropic multilayers are restricted to special cases^{29–32}, whereas a fully generalized formalism applicable to any number of layers of media with arbitrary

permittivity has not been proposed so far.

In this work, we derive explicit expressions for the layer-resolved transmittance and absorption in stratified heterostructures of arbitrarily anisotropic, birefringent, and absorbing media, using the electric field distribution provided by our previous transfer matrix formalism^{25,33}. Our algorithm is numerically stable, yields continuous solutions, and is implemented in an open access computer program^{34,35}, enabling a robust and consistent framework that is capable of treating light of any polarization impinging at any incident angle onto any number of arbitrarily anisotropic, birefringent, and absorbing layers. To demonstrate the capabilities of our algorithm, we present and discuss simulation results for three nanophotonic device structures, featuring several phenomena such as azimuth-dependent hyperbolic phonon polaritons in a MoO_3 / aluminum nitride (AlN) / silicon carbide (SiC) heterostructure, layer-selective exciton absorption of molybdenum disulfide (MoS_2) monolayers in a Fabry-Pérot cavity, and strong light-matter coupling between a cavity mode and an epsilon-near-zero mode in a doped gallium nitride (GaN) multi-quantum well system. Section II summarizes the transfer matrix framework that is used to calculate the electric field distribution and the momenta of the eigenmodes in an anisotropic multilayer system. Based on this theory, section III introduces the calculation of the layer-resolved transmittance and absorption. In section IV, the simulation results are presented.

II. TRANSFER MATRIX FRAMEWORK

The 4×4 transfer matrix formalism comprising the calculation and sorting of the eigenmodes and the treatment of singularities (Section II A), the calculation of reflection and transmission coefficients (Section II B) and of the electric fields (Section II C) is based on our previous work²⁵, and therefore is here only briefly summarized

in order to provide the necessary framework for the calculation of the layer-resolved absorption (Section III).

A. Matrix Formalism

The incident medium is taken to be non-absorptive with isotropic (relative) permittivity ε_{inc} , while all other media can feature absorption and fully anisotropic (relative) permittivity tensors $\bar{\varepsilon}$. Each permittivity tensor $\bar{\varepsilon}_i$ of medium i with principle relative permittivities in the crystal frame ε_x , ε_y , and ε_z can be rotated into the lab frame using a three-dimensional coordinate rotation matrix²⁴ (Eq. 2 in Ref.²⁵). In the following, media with a diagonal permittivity tensor in the lab frame are referred to as non-birefringent, while media with a permittivity tensor that features non-zero off-diagonal elements is called birefringent. Furthermore, all media are assumed to have an isotropic magnetic permeability μ .

The coordinate system in the lab frame is defined such that the multilayer interfaces are parallel to the x - y -plane, while the z -direction points from the incident medium towards the substrate and has its origin at the first interface between incident medium and layer $i = 1$. The layers are indexed from $i = 1$ to $i = N$, and the thickness of each layer is d_i . Furthermore, $i = 0$ refers to the incident medium and $i = N + 1$ to the substrate. The plane of incidence is the x - z -plane, yielding the following wavevector \vec{k}_i in layer i :

$$\vec{k}_i = \frac{\omega}{c}(\xi, 0, q_i), \quad (1)$$

where ω is the circular frequency of the incident light, c is the speed of light in vacuum, $\xi = \sqrt{\varepsilon_{\text{inc}}} \sin(\theta)$ is the in-plane x -component of the wavevector which is conserved throughout the entire multilayer system, θ is the incident angle, and q_i is the dimensionless z -component of the wavevector in layer i .

In any medium, the propagation of an electromagnetic wave is described by exactly four eigenmodes $j = 1, 2, 3, 4$ with different z -components q_{ij} of the wavevector. These four q_{ij} can be obtained for each medium i individually by solving the eigenvalue problem of a characteristic matrix Δ (Eq. 11 in Ref.²⁵), as has been derived originally by Berreman²³. However, for media with highly dispersive permittivities, the four obtained eigenvalues q_{ij} and their related eigenmodes can switch their order as a function of frequency, and thus have to be identified in an unambiguous manner. Following Li *et al.*³⁶, the modes are separated into forward and backward propagating waves according to the sign of q_{ij} (Eq. 12 in Ref.²⁵). We assign the forward propagating (transmitted) waves to be described by q_{i1} and q_{i2} , and the backward propagating (reflected) waves by q_{i3} and q_{i4} . Furthermore, each pair is sorted by the polarization of the corresponding mode, utilizing the electric fields given by the eigenvectors Ψ_{ij} (Eq. 13 in Ref.²⁵). In non-birefringent media, the two modes are separated into p-polarized (q_{i1} and q_{i3})

and s-polarized (q_{i2} and q_{i4}) waves by analyzing the x -component of their electric fields. For birefringent media, on the other hand, the sorting is realized by analyzing the x -component of the Poynting vector $\vec{S}_{ij} = \vec{E}_{ij} \times \vec{H}_{ij}$, and the modes are separated into ordinary (q_{i1} and q_{i3}) and extraordinary (q_{i2} and q_{i4}) waves²⁵.

In the case of non-birefringent media, the four solutions q_{ij} become degenerate, leading to singularities in the formalisms of previous works^{23,24,37}. To resolve this problem, we follow the solution presented by Xu *et al.*³⁸. Using the appropriately sorted q_{ij} , obtained as described above, the eigenvectors $\tilde{\gamma}_{ij}$ of the four eigenmodes in each layer i are:

$$\tilde{\gamma}_{ij} = \begin{pmatrix} \gamma_{ij1} \\ \gamma_{ij2} \\ \gamma_{ij3} \end{pmatrix}, \quad (2)$$

with the values of γ_{ijk} given by Xu *et al.*³⁸ (Eq. 20 in Ref.²⁵), and $k = 1, 2, 3$ being the x , y , and z components of $\tilde{\gamma}_{ij}$. Furthermore, $\tilde{\gamma}_{ij}$ has to be normalized:

$$\tilde{\gamma}_{ij} = \frac{\tilde{\gamma}_{ij}}{|\tilde{\gamma}_{ij}|}. \quad (3)$$

We note that this normalization is essential to ensure a correct calculation of the cross-polarization components of the transfer matrix. The normalized electric field eigenvectors $\tilde{\gamma}_{ij}$, being free from singularities, replace the eigenvectors Ψ_{ij} for all further calculations in the formalism.

At each interface, the boundary conditions for electric and magnetic fields allow to connect the fields of the two adjacent layers $i - 1$ and i . Formulated for all four modes simultaneously, the boundary conditions are:

$$\mathbf{A}_{i-1} \vec{E}_{i-1} = \mathbf{A}_i \vec{E}_i, \quad (4)$$

where \mathbf{A}_i is a 4×4 matrix calculated from the eigenvectors γ_{ijk} ³⁸ (Eq. 22 in Ref.²⁵), and \vec{E}_i is a dimensionless 4-component electric field vector containing the amplitudes of the resulting electric fields of all four modes. In the following, we refer to \vec{E}_i as the amplitude vector, and its components are sorted as follows:

$$\vec{E} \equiv \begin{pmatrix} E_{\Rightarrow}^{p/o} \\ E_{\Rightarrow}^{s/e} \\ E_{\Leftarrow}^{p/o} \\ E_{\Leftarrow}^{s/e} \end{pmatrix}, \quad (5)$$

where \Rightarrow (\Leftarrow) stands for the forward propagating, transmitted (backward propagating, reflected) modes, and p, s refers to the p- and s-polarized modes in non-birefringent media, while o, e indicates the ordinary and extraordinary modes in birefringent media. By multiplying \mathbf{A}_{i-1}^{-1} on both sides of Eq. 4, we find the implicit definition of the interface matrix \mathbf{L}_i , which projects the amplitude vector in medium i onto the amplitude vector in medium $i - 1$:

$$\vec{E}_{i-1} = \mathbf{A}_{i-1}^{-1} \mathbf{A}_i \vec{E}_i \equiv \mathbf{L}_i \vec{E}_i. \quad (6)$$

For the transition between two birefringent or between two non-birefringent media, the projection of a wave of one particular polarization in layer i only yields a finite amplitude in layer $i-1$ of the mode of same polarization, i.e. $s/e \leftrightarrow s/e$, and $p/o \leftrightarrow p/o$. For the transition between a birefringent and a non-birefringent medium, on the other hand, the interface matrix \mathbf{L}_i projects a mode of one particular polarization in layer i onto both polarization states in layer $i-1$. This cross-polarized projection occurs because in birefringent media, the in-plane directions of the ordinary and extraordinary eigenmodes are rotated ($\neq n\pi$, $n \in \mathbb{N}_0$) with respect to the directions of the p- and s-polarized eigenmodes in the non-birefringent medium.

The propagation of all four eigenmodes through layer i is described by the propagation matrix \mathbf{P}_i ²⁴:

$$\mathbf{P}_i = \begin{pmatrix} e^{-i\frac{\omega}{c}q_{i1}d_i} & 0 & 0 & 0 \\ 0 & e^{-i\frac{\omega}{c}q_{i2}d_i} & 0 & 0 \\ 0 & 0 & e^{-i\frac{\omega}{c}q_{i3}d_i} & 0 \\ 0 & 0 & 0 & e^{-i\frac{\omega}{c}q_{i4}d_i} \end{pmatrix}, \quad (7)$$

where the rotation of polarization in birefringent media arises due to a phase difference that is accumulated during propagation through the medium, because of different propagation speeds of the ordinary and extraordinary modes ($q_{i1} \neq q_{i2}$ and $q_{i3} \neq q_{i4}$).

The transfer matrix \mathbf{T}_i of a single layer i is defined as:

$$\mathbf{T}_i = \mathbf{A}_i \mathbf{P}_i \mathbf{A}_i^{-1}, \quad (8)$$

and the full transfer matrix $\mathbf{\Gamma}$ of all N layers is

$$\mathbf{\Gamma} = \mathbf{A}_0^{-1} \left(\prod_{i=1}^N \mathbf{T}_i \right) \mathbf{A}_{N+1}, \quad (9)$$

where \mathbf{A}_0^{-1} (\mathbf{A}_{N+1}) ensures the correct mode projection between the multilayer system and the incident medium (substrate).

B. Reflection and Transmission Coefficients

The full transfer matrix $\mathbf{\Gamma}$ projects the amplitude vector in the substrate \vec{E}_{N+1}^+ onto the amplitude vector in the incident medium \vec{E}_0^- :

$$\vec{E}_0^- = \mathbf{\Gamma} \vec{E}_{N+1}^+, \quad (10)$$

where \vec{E}_{i-1}^- and \vec{E}_i^+ denote the fields on both sides of the interface between layer $i-1$ and i , respectively. Following the equations presented by Yeh²⁴, the transmission (t) and reflection (r) coefficients for incident p- or s-polarization can be calculated in terms of the matrix

elements of $\mathbf{\Gamma}$ as follows:

$$r_{pp} = \frac{\Gamma_{31}\Gamma_{22} - \Gamma_{32}\Gamma_{21}}{\Gamma_{11}\Gamma_{22} - \Gamma_{12}\Gamma_{21}} \quad t_{p(p/o)} = \frac{\Gamma_{22}}{\Gamma_{11}\Gamma_{22} - \Gamma_{12}\Gamma_{21}} \quad (11)$$

$$r_{ss} = \frac{\Gamma_{11}\Gamma_{42} - \Gamma_{41}\Gamma_{12}}{\Gamma_{11}\Gamma_{22} - \Gamma_{12}\Gamma_{21}} \quad t_{s(s/e)} = \frac{\Gamma_{11}}{\Gamma_{11}\Gamma_{22} - \Gamma_{12}\Gamma_{21}} \quad (12)$$

$$r_{ps} = \frac{\Gamma_{41}\Gamma_{22} - \Gamma_{42}\Gamma_{21}}{\Gamma_{11}\Gamma_{22} - \Gamma_{12}\Gamma_{21}} \quad t_{p(s/e)} = \frac{-\Gamma_{21}}{\Gamma_{11}\Gamma_{22} - \Gamma_{12}\Gamma_{21}} \quad (13)$$

$$r_{sp} = \frac{\Gamma_{11}\Gamma_{32} - \Gamma_{31}\Gamma_{12}}{\Gamma_{11}\Gamma_{22} - \Gamma_{12}\Gamma_{21}} \quad t_{s(p/o)} = \frac{-\Gamma_{12}}{\Gamma_{11}\Gamma_{22} - \Gamma_{12}\Gamma_{21}}, \quad (14)$$

where the subscripts refer to the incoming and outgoing polarization state, respectively. The transmission coefficients describe the transmitted electric field amplitude into p- and s-polarized states in the case of a non-birefringent substrate, and into the ordinary and extraordinary eigenstates in the case of a birefringent substrate. We note that the indices of $\mathbf{\Gamma}$ differ from the equations reported by Yeh²⁴ in order to account for a different order of the eigenmodes in the amplitude vector (Eq. 5).

C. Electric Field Distribution

Employing the interface and propagation matrices \mathbf{L}_i and \mathbf{P}_i , respectively, an amplitude vector can be projected to any z -point in the multilayer system (please note the published erratum that corrects the calculation of the electric field distribution in our original work³³). However, due to the rotation of polarization in birefringent media and thus the mixing of polarization states, in general, the cases of incident p- and s-polarization have to be treated separately. As a starting point, the transmission coefficients can be utilized to formulate the amplitude vector \vec{E}_{N+1}^+ for either p- or s-polarized incident light in the substrate at the interface with layer N as follows:

$$\begin{aligned} \left(\vec{E}_{N+1}^+ \right)_{p \text{ in}} &= \begin{pmatrix} E_{\Rightarrow}^{p/o} \\ E_{\Rightarrow}^{s/e} \\ E_{\Leftarrow}^{p/o} \\ E_{\Leftarrow}^{s/e} \end{pmatrix} = \begin{pmatrix} t_{p(p/o)} \\ t_{p(s/e)} \\ 0 \\ 0 \end{pmatrix} \\ \left(\vec{E}_{N+1}^+ \right)_{s \text{ in}} &= \begin{pmatrix} E_{\Rightarrow}^{p/o} \\ E_{\Rightarrow}^{s/e} \\ E_{\Leftarrow}^{p/o} \\ E_{\Leftarrow}^{s/e} \end{pmatrix} = \begin{pmatrix} t_{s(p/o)} \\ t_{s(s/e)} \\ 0 \\ 0 \end{pmatrix}, \end{aligned} \quad (15)$$

where the reflected (\Leftarrow) components are set to zero, since no light source is assumed to be on the substrate side of the multilayer system. Furthermore, in order to obtain the electric field amplitudes as a function of z , the propagation through layer i is calculated by means of the

propagation matrix \mathbf{P}_i :

$$\begin{aligned} \vec{E}_i(z) &= \mathbf{P}_i(z) \vec{E}_i^- \\ &= \begin{pmatrix} e^{-i\frac{\omega}{c}q_{i1}z} & 0 & 0 & 0 \\ 0 & e^{-i\frac{\omega}{c}q_{i2}z} & 0 & 0 \\ 0 & 0 & e^{-i\frac{\omega}{c}q_{i3}z} & 0 \\ 0 & 0 & 0 & e^{-i\frac{\omega}{c}q_{i4}z} \end{pmatrix} \vec{E}_i^-, \end{aligned} \quad (16)$$

with $0 < z < d_i$ being the relative z -position in layer i . Starting from \vec{E}_{N+1}^+ , the interface matrices \mathbf{L}_i and propagation matrices \mathbf{P}_i subsequently propagate the amplitude vector towards the incident medium. In the reverse direction, the inverse propagation matrix \mathbf{P}_{N+1}^{-1} allows to calculate the \vec{E} -fields in the substrate. As a result, the four mode amplitudes $E_{\Rightarrow}^{p/o}$, $E_{\Rightarrow}^{s/e}$, $E_{\Leftarrow}^{p/o}$, and $E_{\Leftarrow}^{s/e}$ are obtained as a function of z within each layer.

In order to obtain the three-components \mathcal{E}_x , \mathcal{E}_y , and \mathcal{E}_z of the electric field for each of the four modes j , the four mode amplitudes have to be multiplied with their respective eigenmode vector $\vec{\gamma}_{ij}$ (Eq. 3). This yields for the electric fields $\vec{\mathcal{E}}$ of the four modes for each layer i , as a function of z , and for either p- or s-polarized incident light:

$$\begin{aligned} \left(\vec{\mathcal{E}}_{\Rightarrow}^{p/o}\right)_{p/s \text{ in}} &= \left(E_{\Rightarrow}^{p/o}\right)_{p/s \text{ in}} \begin{pmatrix} \hat{\gamma}_{i11} \\ \hat{\gamma}_{i12} \\ \hat{\gamma}_{i13} \end{pmatrix}, \quad j = 1 \\ \left(\vec{\mathcal{E}}_{\Rightarrow}^{s/e}\right)_{p/s \text{ in}} &= \left(E_{\Rightarrow}^{s/e}\right)_{p/s \text{ in}} \begin{pmatrix} \hat{\gamma}_{i21} \\ \hat{\gamma}_{i22} \\ \hat{\gamma}_{i23} \end{pmatrix}, \quad j = 2 \\ \left(\vec{\mathcal{E}}_{\Leftarrow}^{p/o}\right)_{p/s \text{ in}} &= \left(E_{\Leftarrow}^{p/o}\right)_{p/s \text{ in}} \begin{pmatrix} \hat{\gamma}_{i31} \\ \hat{\gamma}_{i32} \\ \hat{\gamma}_{i33} \end{pmatrix}, \quad j = 3 \\ \left(\vec{\mathcal{E}}_{\Leftarrow}^{s/e}\right)_{p/s \text{ in}} &= \left(E_{\Leftarrow}^{s/e}\right)_{p/s \text{ in}} \begin{pmatrix} \hat{\gamma}_{i41} \\ \hat{\gamma}_{i42} \\ \hat{\gamma}_{i43} \end{pmatrix}, \quad j = 4, \end{aligned} \quad (17)$$

where we have omitted the index i and the z dependence for the sake of readability. The full electric field $\vec{\mathcal{E}}_i(z)$ for either p- or s-polarized incident light in layer i at point z is given by the sum of all four electric field vectors:

$$\vec{\mathcal{E}}_i(z) = \vec{\mathcal{E}}_{\Rightarrow,i}^{p/o}(z) + \vec{\mathcal{E}}_{\Rightarrow,i}^{s/e}(z) + \vec{\mathcal{E}}_{\Leftarrow,i}^{p/o}(z) + \vec{\mathcal{E}}_{\Leftarrow,i}^{s/e}(z). \quad (18)$$

The in-plane components of the sum, \mathcal{E}_x and \mathcal{E}_y , are continuous throughout the entire multilayer structure, as it is required by Maxwells boundary conditions.

III. LAYER-RESOLVED TRANSMITTANCE AND ABSORPTION

The total reflectance \mathcal{R} of the multilayer system for a given ingoing and outgoing polarization a and b , respectively, can be readily calculated from the corresponding

reflection coefficient (Eqs. 11-14):

$$\mathcal{R}^{ab} = |r_{ab}|^2, \quad a, b = p, s. \quad (19)$$

The transmittance \mathcal{T} , which is the transmitted power into the substrate, on the other hand, in general is not given by the electric field intensity $\mathcal{T} \neq |t|^2$ (except for the special case if the substrate is vacuum, $\varepsilon = 1$). Instead, \mathcal{T} can be calculated from the time-averaged Poynting vector $\vec{\mathcal{S}}^{39-41}$, which describes the direction and magnitude of the energy flux of an electromagnetic wave at any point z in the structure:

$$\vec{\mathcal{S}}_i(z) = \frac{1}{2} \text{Re} \left[\vec{\mathcal{E}}_i(z) \times \vec{\mathcal{H}}_i^*(z) \right]. \quad (20)$$

The full electric field $\vec{\mathcal{E}}$ (for incident polarization a) as a function of z in each layer i was calculated in the previous section (Eq. 18), and the full magnetic field $\vec{\mathcal{H}}$ is obtained as follows using Maxwells equations:

$$\begin{aligned} \vec{\mathcal{H}}_i(z) &= \frac{1}{\omega\mu_i} \left(\vec{k}_{i1} \times \vec{\mathcal{E}}_{\Rightarrow,i}^{p/o}(z) + \vec{k}_{i2} \times \vec{\mathcal{E}}_{\Rightarrow,i}^{s/e}(z) \right. \\ &\quad \left. + \vec{k}_{i3} \times \vec{\mathcal{E}}_{\Leftarrow,i}^{p/o}(z) + \vec{k}_{i4} \times \vec{\mathcal{E}}_{\Leftarrow,i}^{s/e}(z) \right), \end{aligned} \quad (21)$$

where \vec{k}_{ij} are the wavevectors in layer i of the four modes j , see Eq. 1. Because $\vec{\mathcal{E}}$ and $\vec{\mathcal{H}}$ are known in each layer i and as a function of z from the transfer matrix formalism, the Poynting vector can be evaluated likewise yielding $\vec{\mathcal{S}}_i(z)$, which will be used in the following to calculate the transmittance and absorption at any point z in the multilayer system.

It is important to note that while $\vec{\mathcal{E}}$ and $\vec{\mathcal{H}}$ can be calculated for each of the four modes j individually, this mode separation in general – specifically, in the case of birefringent media – is not possible for the Poynting vector $\vec{\mathcal{S}}$. In other words, in birefringent media, the sum of the Poynting vectors of the four modes is not equal to the Poynting vector calculated from the total fields $\vec{\mathcal{E}}$ (Eq. 18) and $\vec{\mathcal{H}}$ (Eq. 21). The difference arises because in birefringent media, $\vec{\mathcal{E}} \not\propto \vec{\mathcal{H}}$. Therefore, the cross products $\vec{\mathcal{E}} \times \vec{\mathcal{H}}$ between different modes j are no longer zero. For the correct calculation of the Poynting vector in birefringent media, it is thus necessary to calculate the cross product of the total fields $\vec{\mathcal{E}}$ and $\vec{\mathcal{H}}$, as shown in Eq. 20. Interestingly, this means that the energy flux in birefringent media cannot be split up into the ordinary and extraordinary eigenmodes, but has to be considered as a single quantity. In the following, we therefore discuss the transmittance and absorption for s- or p-polarized incident light without differentiating between the eigenmodes anymore.

An exception is the incident medium, which is set to be isotropic. Here, the Poynting vector can be calculated for each mode individually, and for the purpose of normalizing the transmitted power, we calculate the Poynting vector of the incident light $\vec{\mathcal{S}}_{\text{inc}}$ (in layer $i = 0$ at position

$z = 0$) for either p- or s-polarization as follows:

$$\begin{aligned}\bar{\mathcal{S}}_{\text{inc}}^p &= \frac{1}{2} \text{Re} \left[\bar{\mathcal{E}}_{\Rightarrow,0}^p(0) \times \left(\vec{k}_{01} \times \bar{\mathcal{E}}_{\Rightarrow,0}^p(0) \right)^* \right] \\ \bar{\mathcal{S}}_{\text{inc}}^s &= \frac{1}{2} \text{Re} \left[\bar{\mathcal{E}}_{\Rightarrow,0}^s(0) \times \left(\vec{k}_{02} \times \bar{\mathcal{E}}_{\Rightarrow,0}^s(0) \right)^* \right].\end{aligned}\quad (22)$$

In a stratified multilayer system, the transmitted energy is given by the z -component of the Poynting vector. Thus, we note that alternatively to Eq. 19, the reflectance \mathcal{R} can be calculated from the Poynting vector:

$$\mathcal{R}^{ab} = \frac{-\mathcal{S}_{\text{refl},z}^b}{\mathcal{S}_{\text{inc},z}^a}, \quad (23)$$

where the minus sign accounts for the negative z -direction of the reflected light. $\mathcal{S}_{\text{refl},z}^b$ is the z -component of the Poynting vector of the reflected light of polarization $b = p, s$ (in layer $i = 0$ at position $z = 0$) given by:

$$\begin{aligned}\bar{\mathcal{S}}_{\text{refl}}^p &= \frac{1}{2} \text{Re} \left[\bar{\mathcal{E}}_{\Leftarrow,0}^p(0) \times \left(\vec{k}_{03} \times \bar{\mathcal{E}}_{\Leftarrow,0}^p(0) \right)^* \right] \\ \bar{\mathcal{S}}_{\text{refl}}^s &= \frac{1}{2} \text{Re} \left[\bar{\mathcal{E}}_{\Leftarrow,0}^s(0) \times \left(\vec{k}_{04} \times \bar{\mathcal{E}}_{\Leftarrow,0}^s(0) \right)^* \right].\end{aligned}\quad (24)$$

As discussed above, for anisotropic media, a separation of the energy flow into the different eigenmodes of polarization b is not generally possible. Therefore, all following equations calculate the total transmittance or absorption for the respective incident polarization a .

The transmittance \mathcal{T} into the substrate $i = N + 1$ at the interface with layer N for incident light of polarization a is given by:

$$\mathcal{T}^a = \frac{\mathcal{S}_{N+1,z}^a(D)}{\mathcal{S}_{\text{inc},z}^a}, \quad (25)$$

where $D = \sum_{i=1}^N d_i$ is the thickness of the multilayer system. The full z -dependence of the transmittance can be evaluated by using the z -component of the Poynting vector $\mathcal{S}_{i,z}(z)$ at a certain z -position in layer i :

$$\mathcal{T}_i^a(z) = \frac{\mathcal{S}_{i,z}^a(z)}{\mathcal{S}_{\text{inc},z}^a}. \quad (26)$$

With this, the absorption \mathcal{A} of the entire multilayer system, that is up to the last interface between layer N and the substrate, is given by

$$\mathcal{A}^a = 1 - \mathcal{R}^a - \mathcal{T}^a, \quad (27)$$

and the z -resolved absorption $\mathcal{A}_i(z)$ in each layer i is

$$\mathcal{A}_i^a(z) = 1 - \mathcal{R}^a - \mathcal{T}_i^a(z), \quad (28)$$

where $\mathcal{R}^a = \mathcal{R}^{ap} + \mathcal{R}^{as}$ is the total reflectance. Note that Eq. 28 describes the total absorption starting from $z = 0$ at the first interface up to the specified position z

in layer i . The layer- i -resolved absorption, on the other hand, is given by:

$$\begin{aligned}\mathcal{A}_i^a &= \mathcal{T}_i^a(d_{1..i-1}) - \mathcal{T}_i^a(d_{1..i-1} + d_i) \\ &= \mathcal{A}_i^a(d_{1..i-1} + d_i) - \mathcal{A}_i^a(d_{1..i-1}),\end{aligned}\quad (29)$$

where $d_{1..i-1} = \sum_{i=1}^{i-1} d_i$ is the thickness of all layers through which the incident light has propagated before reaching the layer i .

Before we study three nanophotonic device structures in the following section, we calculate the layer-resolved absorption for two simple test structures in Fig. 1. The first is a typical TMDC heterostructure, comprising monolayers of tungsten diselenide (WSe₂), MoS₂, and tungsten disulfide (WS₂) sandwiched between hBN monolayers (sketched in Fig. 1a), where each TMDC monolayer features individual exciton absorption lines. In Fig. 1b, the reflection and transmittance of the entire structure is plotted, and Fig. 1c shows the absorption spectra of each TMDC monolayer. The total absorption (gray line in Fig. 1c) obtained from the reflectance and transmittance spectra (Eq. 27) exhibits three indistinguishable absorption features, whereas the layer-resolved absorption calculations unravel the absorption spectrum, allowing to identify the contribution of each TMDC monolayer.

In Fig. 1d-f, we show the absorption in a polar dielectric heterostructure of SiC, AlN, and GaN thin films on a Si substrate probed at infrared (IR) frequencies. Polar dielectric crystals feature an IR-active transverse optical (TO) phonon mode, where light is predominantly absorbed, whereas the longitudinal optical (LO) phonon mode is not IR-active and thus featureless in a bulk crystal. Thin films, on the other hand, support the so called Berreman mode in proximity to the LO frequency, leading to a strong absorption feature at oblique incidence^{43–46}. Thus, the reflectance and transmittance spectra (Fig. 1e) of the polar dielectric heterostructure are of complicated shape, exhibiting six different features arising from the three different polar crystal thin films. The layer-resolved absorption calculations split these features into three spectra with two absorption peaks each (Fig. 1f), allowing to identify the respective polar crystal thin film that leads to the absorption at its respective TO and LO frequencies.

IV. SIMULATIONS OF NANOPHOTONIC DEVICES

The transfer matrix formalism and the calculation of the layer-resolved absorption and transmittance presented in the previous section can be applied for any wavelength and any number of layers, consisting of birefringent or non-birefringent media described by an arbitrary permittivity tensor $\bar{\epsilon}_i$. As case studies, in this section we describe three selected nanophotonic device structures. The first example discusses the hyperbolic

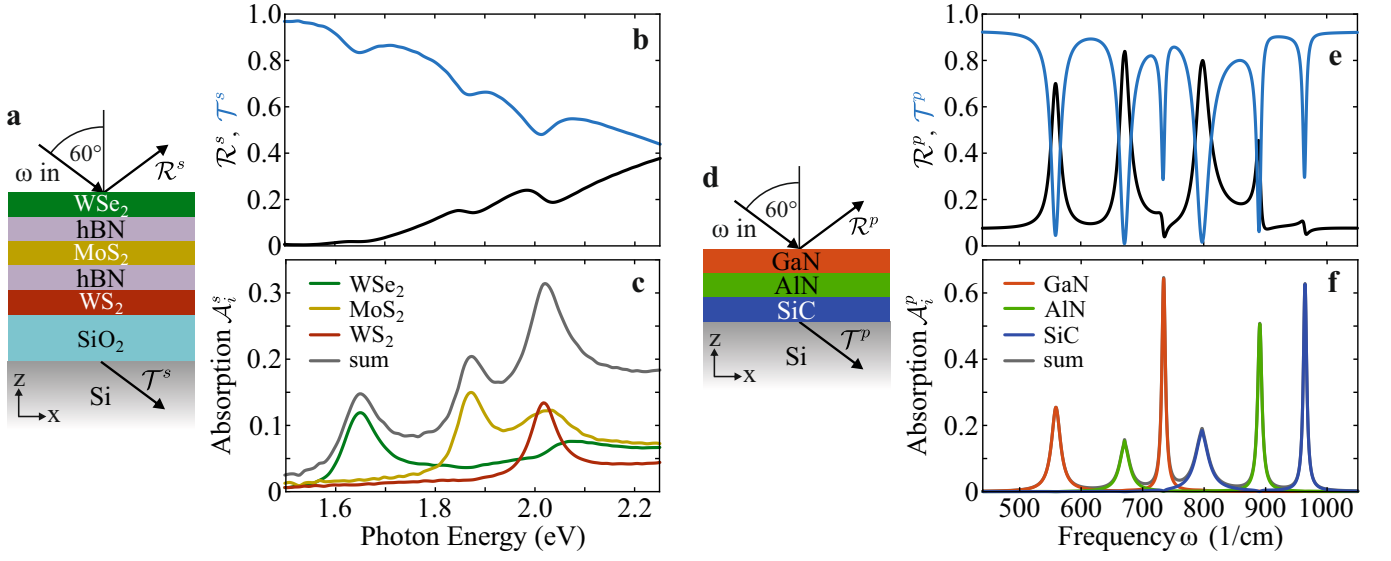


FIG. 1: **Layer-resolved absorption calculations of two simple test structures.** **a** Sketch of the TMDC heterostructure comprising monolayers of WSe₂, MoS₂, and WS₂⁴² separated by hBN monolayers on a 140 nm thick SiO₂ film on a Si substrate. **b** Reflectance (black line) and transmittance (blue line) spectra of the system at visible wavelengths and at an incident angle of 60° for s-polarized incident light. **c** Layer-resolved absorption spectra of the TMDC monolayers (colored lines), revealing their respective contribution to the overall absorption spectrum (gray line). **d** Sketch of the polar dielectric heterostructure comprising 100 nm thin GaN, AlN, and SiC films on a Si substrate. **e** Reflectance and transmittance spectra and **f** layer-resolved absorption spectra of the second system, enabling identification of the absorbing layer for each of the six absorption lines.

phonon polaritons arising in a MoO₃ / AlN / SiC system excited evanescently at far-IR wavelengths, highlighting the potential of the formalism for nanophotonic studies in stratified media. The second example describes the freespace response in the visible of a van der Waals heterostructure of monolayers of MoS₂ embedded in a hBN matrix, featuring layer-selective absorption of the MoS₂ excitons. Finally, the third example calculates the mid-IR absorption of strongly coupled modes formed from intersubband plasmons in multi-quantum wells embedded in an optical cavity.

A. Hyperbolic Phonon Polaritons in MoO₃/AlN/SiC

Polar crystals such as MoO₃, AlN, and SiC support surface phonon polaritons (SPhP) at frequencies inside their reststrahlen region between the TO and LO phonon frequencies⁴⁸. On smooth surfaces, SPhPs can be excited via prism coupling in the Otto geometry^{49,50} as illustrated in Fig. 2a, where the air gap width d_{gap} governs the excitation efficiency and the incident angle θ defines the in-plane momentum of the launched SPhP⁵¹. The system we investigate here is a multilayer heterostructure comprising an MoO₃ and AlN film on a SiC substrate. Employing the presented transfer matrix formalism, the layer-resolved absorption \mathcal{A}_i of such a structure can be calculated as a function of incident angle θ , incident fre-

quency ω , layer thicknesses d_i , and azimuthal angle Φ of the sample.

The absorption in the MoO₃, AlN, and SiC layers as a function of ω and Φ and for fixed θ and d_i is shown in Fig. 2d-f. The reflectance of the entire system is plotted in Fig. 2c. As required by energy conservation, the sum of the absorbed power in the three polar crystals equals the attenuated power visible as absorption dips in the reflectance. However, while the reflectance only yields the total absorption, the layer-resolved calculations allow to identify the exact position of a power drain in a multilayer system.

In particular, the MoO₃/AlN/SiC heterostructure features several sharp absorption lines at 660, 800, 920, and 980 cm⁻¹ that are mostly independent of Φ , and one prominent absorption line that strongly varies with Φ , indicating that the latter depends on in-plane anisotropy ($\epsilon_x \neq \epsilon_y$) while the former do not. In the multilayer sample, only the MoO₃ layer exhibits in-plane anisotropy, while AlN and SiC are c-cut uniaxial crystals (principle relative permittivities ϵ_x , ϵ_y , and ϵ_z are shown in Fig. 2b). Indeed, the Φ -dependent feature is mostly absorbed in the MoO₃ layer. This feature is the hyperbolic phonon polariton (hPhP) supported by the air/MoO₃ interface arising in the in-plane reststrahlen bands of MoO₃. Its tunability in frequency arises from the large in-plane anisotropy of MoO₃, which leads to a Φ -dependent effective permittivity sensed by the hPhP upon azimuthal rotation.

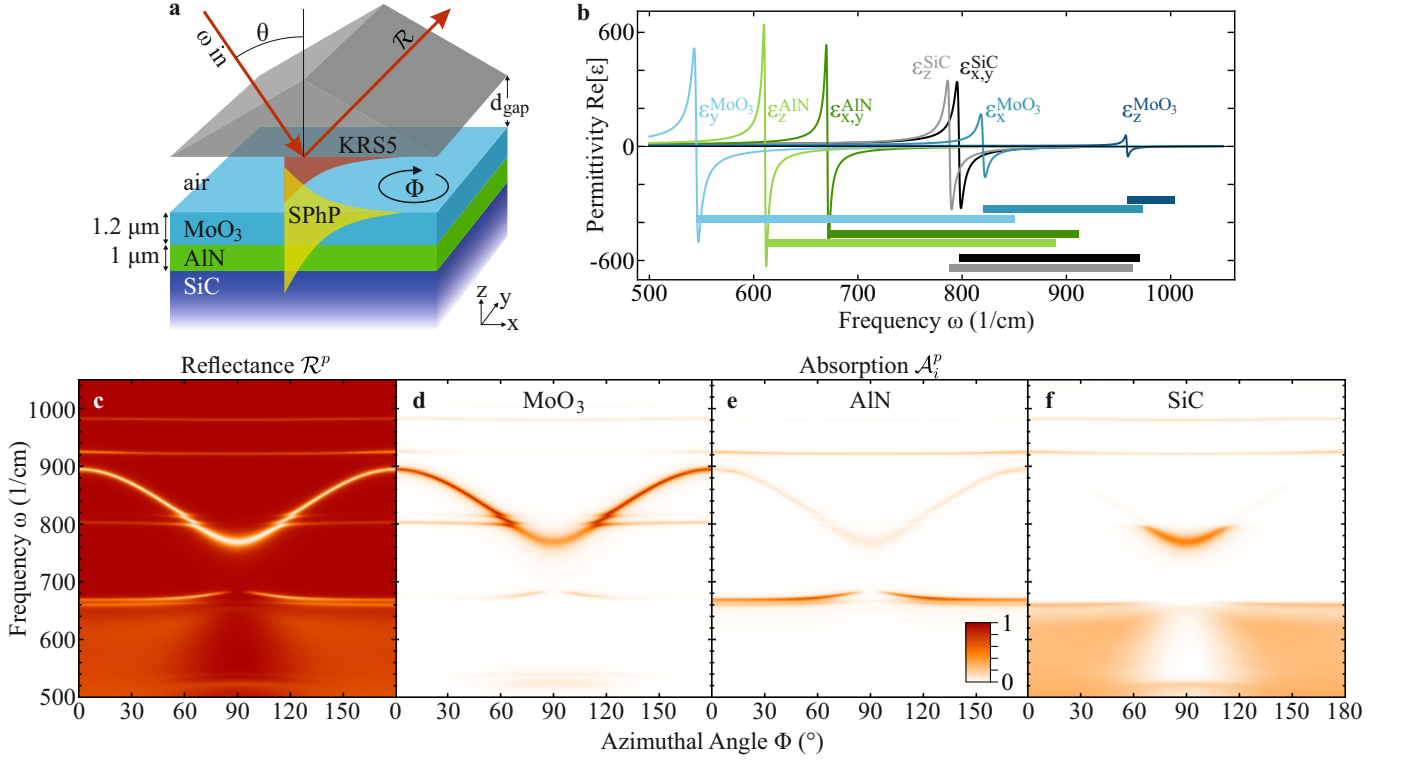


FIG. 2: Azimuthal dependence of the layer-resolved absorption in a $\text{MoO}_3/\text{AlN}/\text{SiC}$ heterostructure.

a Prism coupling setup in the Otto geometry for the evanescent excitation of phonon polaritons in a 1200 nm MoO_3 / 1000 nm AlN / SiC substrate multilayer sample with p-polarized incident light. The incident angle is fixed to $\theta = 28^\circ$ and the air gap to $d_{\text{gap}} = 8 \mu\text{m}$. **b** Real value of the principle relative permittivities ϵ_x , ϵ_y , and ϵ_z of uniaxial SiC and AlN and biaxial MoO_3 . Their respective reststrahlen bands located between the corresponding TO and LO phonon frequencies are indicated by the horizontal color bars. **c** Reflectance \mathcal{R}^p of the entire system as a function of incident frequency ω and azimuthal angle of the sample Φ . **d-f** Absorptions \mathcal{A}_i^p (Eq. 29) of the MoO_3 , AlN , and SiC layers as a function of ω and Φ .

Notably, below the SiC TO frequencies ($\sim 800 \text{ cm}^{-1}$), a significant part of the hPhP leaks into the SiC substrate, while above $\omega_{\text{TO}}^{\text{SiC}}$ the mode is mostly confined to the MoO_3 layer. The high confinement above $\omega_{\text{TO}}^{\text{SiC}}$ occurs because of the negative permittivity in the SiC reststrahlen band, while below $\omega_{\text{TO}}^{\text{SiC}}$, the mode can penetrate the substrate. Interestingly, this mode penetration happens across the AlN layer, where only a small part of the mode is absorbed. Since AlN features its reststrahlen bands across the entire frequency range of the hPhP supported by the MoO_3 , and thus evanescently attenuates all modes, the hPhP appears to tunnel through the AlN layer to be absorbed by the SiC substrate.

The multilayer system presented here only scratches the surface of various possible material configurations and compositions that can potentially be employed for tailoring surface and interface polariton resonances^{20,52–57}. In particular the emerging field of volume-confined hyperbolic polaritons^{14,20,58,59}, enabled by the anisotropic permittivity of the supporting media, holds great potential for future nanophotonic applications, such as subdiffraction imaging and hyperlensing^{12,13}. Providing the full layer-resolved ab-

sorption, our algorithm paves the way to predict and study hyperbolic polariton modes in any anisotropic stratified heterostructure.

B. Layer-selective absorption of MoS_2 excitons in a Fabry-Pérot cavity

TMDC monolayers such as MoS_2 feature strong exciton resonances at visible frequencies^{42,47}. By inserting these monolayers into van der Waals heterostructures forming a Fabry-Pérot cavity, the light-matter interaction enabled by the TMDC exciton can be strongly enhanced⁶⁰. Here, we embed two MoS_2 monolayers into a $d_c = 1.9 - 2.4 \mu\text{m}$ thick hBN cavity with a SiO_2 back-reflector on a Si substrate⁶¹, as sketched in Fig. 3a. Employing the presented formalism, the absorption \mathcal{A}_i in the two MoS_2 monolayers as a function of photon energy and cavity thickness d_c can be calculated.

In the photon energy range of $1.7 - 2.2 \text{ eV}$, MoS_2 features two excitons (A and B) at ~ 1.9 and $\sim 2.1 \text{ eV}$. These excitons are apparent as resonance peaks in the isotropic relative permittivity plotted in Fig. 3b and re-

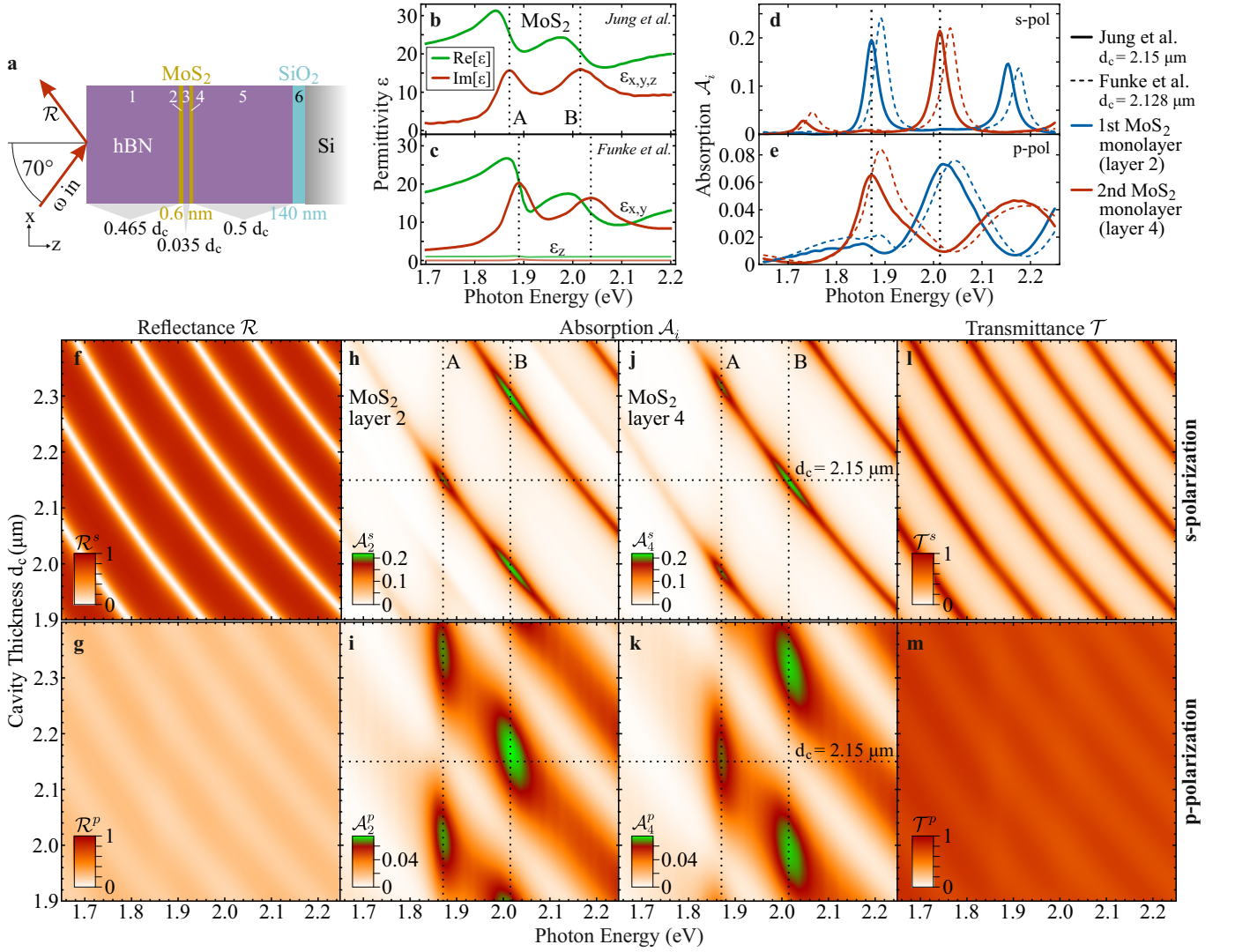


FIG. 3: Cavity-enhanced exciton absorption in MoS₂ monolayers. **a** Structure of the Fabry-Pérot cavity. A 140 nm thin SiO₂ film on the Si substrate serves as a back-reflector, while the cavity with variable thickness $d_c = 1.9 - 2.4 \mu\text{m}$ is made of three layers of hBN of relative thicknesses $0.465 d_c$, $0.035 d_c$, and $0.5 d_c$, separated by two 0.6 nm thin MoS₂ monolayers. **b** Real and imaginary values of the isotropic relative permittivity of MoS₂⁴². All calculations are based on this permittivity, except the dashed lines in subfigures d and e. **c** Anisotropic relative permittivity of MoS₂⁴⁷. **d** Absorption spectra of the two MoS₂ monolayers for s-polarized incident light, for a cavity thickness of $d_c = 2.15 \mu\text{m}$ ($d_c = 2.128 \mu\text{m}$) optimized for layer-selective absorption of the two MoS₂ excitons, calculated with the MoS₂ permittivities of Jung *et al.* (Funke *et al.*). **e** Analogous calculations as in subfigure d but for p-polarized incident light. **f,g** Reflectance \mathcal{R}^s and \mathcal{R}^p for s- and p-polarized incident light, respectively. **h,i** and **j,k** Absorption \mathcal{A}_i^s and \mathcal{A}_i^p of the two MoS₂ monolayers, respectively. **l,m** Transmitted power \mathcal{T}^s and \mathcal{T}^p into the Si substrate, respectively. The maps of \mathcal{R} , \mathcal{A} , and \mathcal{T} are all plotted as a function of the incident photon energy and the cavity thickness d_c .

sulting in peaks in an absorption spectrum. However, the Fabry-Pérot cavity creates a static modulation of the electric field enhancement with peaks and nodes as a function of z position, and thus the resulting absorption in a MoS₂ monolayer not only depends on the photon energy, but also sensitively depends on the z position of the MoS₂ monolayer in the cavity. Taking advantage of this field modulation, we place one MoS₂ monolayer (layer 4)

at the center of the cavity where the cavity modes alternate between node and peak with maximal amplitude, and the other MoS₂ monolayer (layer 2) in close proximity where the cavity features a node when there is a peak in the center, and vice versa.

The cavity modes yield the periodic modulation in photon energy and cavity thickness d_c that can be seen in the reflectance (transmittance) maps shown in Fig. 3f

and g (l and m), for incoming s- and p-polarized light, respectively. The different modulation contrast for \mathcal{R}^s and \mathcal{R}^p (\mathcal{T}^s and \mathcal{T}^p) arises from the large incident angle of $\theta = 70^\circ$, which was chosen to optimize the absorption \mathcal{A}^s in the MoS₂ monolayers for s-polarized incident light. For smaller incident angles, the differences for s- and p-polarization decrease, but with a reduction in the absorption \mathcal{A}^s .

In Fig. 3h,i (j,k) the absorption for s- and p-polarized incident light in the first MoS₂ monolayer, $\mathcal{A}_2^{s,p}$ (second MoS₂ monolayer, $\mathcal{A}_4^{s,p}$), is shown. Due to the choice of the z positions of the two MoS₂ monolayers, each film is sensitive to only every second cavity mode, where layer 2 (first MoS₂ monolayer) absorbs those modes that are not absorbed by layer 4 (second MoS₂ monolayer). Additionally to the absorption modulation imposed by the cavity, the A and B excitons of MoS₂ yield two absorption features at their respective energies, marked by dotted vertical lines in Fig. 3h-k. For the optimized case of s-polarized incident light, the MoS₂ monolayers reach cavity-enhanced absorption values of up to 20% at both exciton energies. At a cavity thickness of $d_c = 2.15 \mu\text{m}$ for s-polarization, layer 2 only absorbs at the energy of exciton A, while in layer 4, absorption only occurs at the energy of exciton B. This layer-selective absorption is further illustrated in the absorption spectra (solid lines) for a fixed cavity thickness of $d_c = 2.15 \mu\text{m}$ shown in Fig. 3d and e for s- and p-polarized light, respectively. For both polarizations, a high contrast between the two layers at each exciton absorption line is achieved, yielding efficient layer-selectivity.

Finally, we compare these results obtained for an isotropic permittivity model⁴² with the same calculations performed for an anisotropic model of MoS₂⁴⁷. In Fig. 3c, the in-plane ($\varepsilon_{x,y}$) and out-of-plane (ε_z) permittivity values taken from Funke *et al.*⁴⁷ are plotted. While $\varepsilon_{x,y}$ are qualitatively the same as the values from Jung *et al.*⁴² (Fig. 3b), ε_z differs strongly, taking the almost constant value of $\varepsilon_z = 1 + 0i$. Even though the difference in ε_z is substantial, the absorption spectra shown in Fig. 3d,e (dashed lines) are qualitatively identical to the spectra calculated from an isotropic permittivity model (solid lines). This confirms that spectroscopic measurements of TMDC monolayers are mostly insensitive to their out-of-plane permittivity⁴², with the exception of cases where ε_z features a zero-crossing, the so-called epsilon-near-zero (ENZ) frequency, giving rise to drastic optical responses such as enhanced higher-harmonic generation^{45,62,63}. However, this is not the case for MoS₂, and therefore the spectra are almost identical.

In this example, the layer-resolved absorption calculations from our algorithm provide the essential information for simulating the layer-selective exciton absorption and optimizing the system parameters. In the thriving field of 2D nanophotonics featuring TMDC van der Waals heterostructures, where structures are optimized for maximal light harvesting^{6,7}, optoelectronic devices^{4,5} or nanolasers^{10,11}, such layer-resolved absorption calcu-

lations promise to be of essential importance. Due to the generality of the presented algorithm, the light-matter interaction in any 2D heterostructure can be readily investigated, highlighting the broad applicability of our approach.

C. Strong Coupling in a Multi Quantum Well - Cavity System

Doped semiconductor quantum wells (QWs) support transitions between consecutive quantum-confined electronic levels, called intraband or inter-subband (ISB) transitions. Contrary to interband transitions, ISB transitions do not only depend on the bandgap properties of the semiconductor, but also on the electronic confinement inside the QWs, and thus offer a great frequency tunability by changing the width, but also the doping level inside the QW. They play a major role in semiconductor optic devices operating in the IR where semiconducting materials with a suitable bandgap are lacking, and are the building block of quantum well IR photodetectors⁶⁴ and quantum cascade lasers⁶⁵. They also offer a practical platform to study the optical properties of dense confined electron gases⁶⁶, which notably lead to the demonstration of the strong^{67,68} and ultra-strong light-matter coupling regimes^{69,70}. It is remarkable that such fundamental electrodynamical phenomena are directly observable on semiconductor devices⁷¹⁻⁷³. One peculiar aspect of these ISB transitions is that they only couple to the component of the electric field along the confinement direction of the QW structure. Hence, the optical properties of a doped QW can be described by an effective permittivity tensor with different in-plane ($\varepsilon_{x,y}$) and out-of-plane (ε_z) values, which has been realized by several permittivity models⁷⁴⁻⁷⁷. The description of light propagation in stratified anisotropic media containing such QWs requires a complex formalism, such as the transfer matrix method the here presented algorithm builds on²⁵.

We focus here on an existent experimental configuration to further demonstrate the potential of our formalism for the case of strong light-matter coupling between a cavity mode and a collective intersubband excitation in a multi-quantum well (MQW) superlattice. The system is composed of a GaN cavity formed by a 500 nm thick, Si-doped GaN slab and a Au mirror, as sketched on the top of Fig. 4. The doped GaN layer is modeled using the Drude model, and acts as a low-index mirror. The two mirrors are separated by a 1 μm thick GaN spacer, forming an empty cavity. The system sustains a guided transverse magnetic (TM) mode, where the electric field is confined mostly between the two mirrors and its out-of-plane component is maximal near the Au mirror. This guided mode can be probed in a reflectance experiment, as discussed in the following. In order to probe large internal angles of incidence experimentally, the sample has to be prepared in a prism shape, for example by cleaving the incident GaN layer facets. The calculated p-polarized

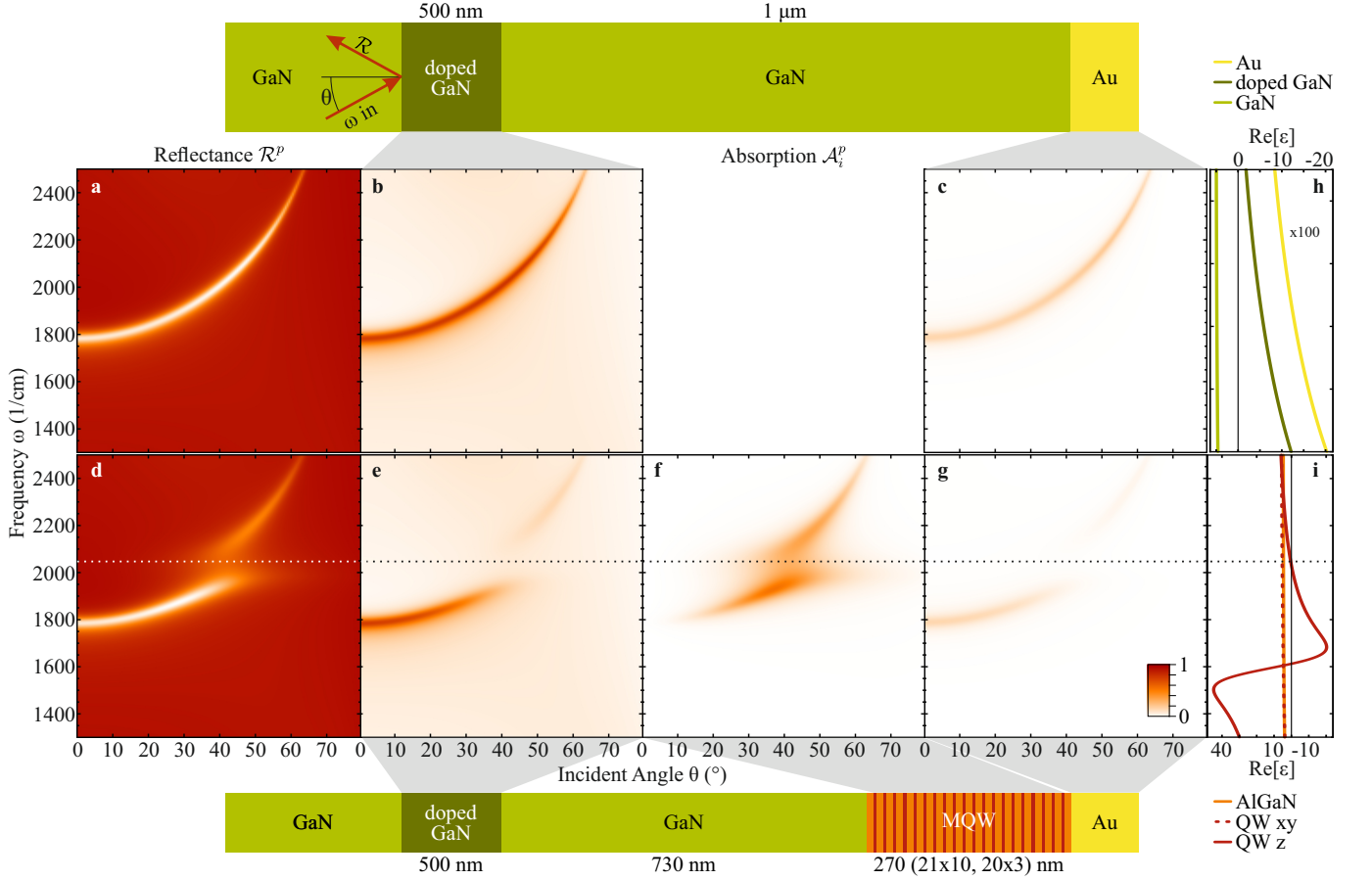


FIG. 4: **Strong coupling between an ENZ mode in a MQW superlattice and a cavity mode.** A 1 μm thick GaN cavity is formed between a Au mirror and a 500 nm thick doped GaN slab on a GaN substrate (top sketch). The doped GaN slab acts as a low-index mirror. **a** Simulated reflectance \mathcal{R}^p of the cavity mode showing its dispersion relation as a function of the angle of incidence θ inside the GaN substrate. **b,c** Layer-resolved absorption \mathcal{A}^p inside the doped GaN slab and in the Au mirror, respectively. **d** Calculated reflectance \mathcal{R}^p of the 1 μm thick cavity partially filled with a doped GaN/AlGaIn MQW superlattice (see bottom sketch), featuring an electronic excitation at $\sim 2030 \text{ cm}^{-1}$ (white dotted line). The strong light-matter coupling between the cavity mode and QW resonance leads to an avoided crossing and the emergence of two polariton branches. **e-g** Layer-resolved absorption \mathcal{A}^p inside the doped GaN mirror, the superlattice and the Au mirror, respectively. **h** Real part of the permittivity of the isotropic layers forming the cavity. **i** Real part of the different components of the permittivity tensor of the doped GaN QW and of the AlGaIn barrier, showing the ENZ mode frequency of the QW at $\sim 2030 \text{ cm}^{-1}$.

reflectance \mathcal{R}^p is shown in Fig. 4a, evidencing the dispersion relation of the cavity mode with varying incidence angle inside the GaN substrate. The layer-resolved absorption spectra as a function of the angle of incidence for this system are reported in Fig. 4b,c and reveal that absorption occurs mostly in the doped GaN mirror. Notably, for an internal incidence angle of 48° at the guided mode frequency, all the light is dissipated in the mirrors, leading to a minimum of zero reflectance in Fig. 4a.

We now turn to the system's response when the cavity is partially filled with a MQW structure (Fig. 4d-g). The superlattice is composed of twenty repetitions of a 3 nm thick GaN QW, Si-doped with a concentration of $2 \times 10^{13} \text{ cm}^{-2}$ and twenty-one loss-less 10 nm thick $\text{Al}_{0.26}\text{Ga}_{0.74}\text{N}$ barriers. Since the guided mode is

a TM mode, it naturally provides a component of the electric field along the z -direction for non-zero angles of incidence, which fulfills the ISB transition selection rule. In order to maximize the coupling between the ISB transition in the MQW and the cavity mode, the superlattice is placed where the z -component of the electric field is the largest, that is just below the Au mirror, as shown at the bottom of Fig. 4. The QW dielectric tensor is modeled using a semi-classical approach⁷⁵. We selected the QW dimension and doping level in a way that it sustains a strong, collective electronic excitation known as an intersubband plasmon⁶⁶. The components of the real part of the dielectric permittivity tensor of all the layers are presented in Fig. 4h,i. Note that while the ISB transition in the quantum well has a resonance frequency

of $\sim 1600 \text{ cm}^{-1}$, the Coulomb interaction between the QW electrons results in an ENZ mode at $\sim 2030 \text{ cm}^{-1}$, marked by the dotted line in Fig. 4i. The ENZ mode dominates the optical response of the QWs.

We show in Fig. 4d the calculated reflectance \mathcal{R}^P of the cavity containing the MQW. The white dotted line shows the ENZ frequency. A clear anti-crossing can be seen between the cavity mode and the ENZ resonance, which is characteristic of the strong light-matter coupling regime, resulting in two polariton branches. The minimal separation between the two branches amounts to a vacuum Rabi splitting $2\Omega_R = 200 \text{ cm}^{-1}$. The layer-resolved absorption spectra as a function of the angle of incidence are shown in Fig. 4e-g for the GaN mirror, the MQW superlattice, and the Au mirror, respectively. When the cavity mode is far detuned from the ENZ frequency, the absorption occurs mostly in the two mirrors, and especially in the GaN mirror, as for the empty cavity case. The situation changes dramatically when the cavity mode is tuned near the ENZ frequency. The absorption then mostly occurs in the MQW. It is however important to note that the absorption is maximal at the frequencies of the two polaritons and not at the ENZ frequency, as it would occur in the case of a weak coupling between the cavity mode and the QW resonance. For an internal incidence angle of 48° , the maximum absorption inside the MQW stack is now 0.5 at each of the frequencies of the two polaritons.

The algorithm presented here thus allows to directly calculate the light absorption in the complex case of a doped MQW superlattice strongly coupled to a cavity mode. In addition to the known features, such as the avoided crossing in the angle-dependent reflectance spectrum, we can directly calculate the absorption inside the MQW active region, which can be usefully linked to the detected photocurrent in the perspective of using such structures in photodetector devices^{67,71,73}.

V. DISCUSSION

We have presented three nanophotonic devices based on anisotropic multilayer structures made from metals, polar dielectrics, and TMDC monolayers, covering incident wavelengths from the far-IR up to the visible. Our formalism allows to calculate the transmittance and absorption in any layer, giving unprecedented insight into the physics of light propagation in anisotropic, and even birefringent, stratified systems.

In recent years, the field of nanophotonics has intensely investigated the optical response of 2D heterostructures. A particularly thriving subject has been polaritonic excitations, which can be supported by a broad variety of systems including slabs of metals, doped semiconductors, polar dielectrics, 2D materials such as TMDC monolayers and their stratified heterostructures^{17,54,78}. Key features of polaritons for nanophotonic technologies are their high spatial confinement and field enhancement, which are

driven by the particular design of the multilayer materials, stacking order, and layer thicknesses. Potential applications of such systems range from sensing^{79,80} and solar cells⁸¹, over optoelectronic devices³ and beam manipulation via metamaterials⁸², to waveguiding^{56,83}, and ultrafast optical components^{45,84}. However, due to the lack of a general formalism, the optical response of these polaritonic multilayer systems is often either approximated by effective, isotropic permittivity models⁸⁵⁻⁸⁷, or described by specifically derived formulas²⁹⁻³². Our generalized formalism allows for a precise, layer-resolved study that includes any isotropic, anisotropic or even birefringent response of any number of layers, and thus holds great potential for the prediction and analysis of polariton modes in stratified heterostructures.

This is especially relevant for systems where one or more materials feature anisotropic permittivity with spectral regions of hyperbolicity where the principle real permittivities have opposite signs, such as hBN or MoO₃. Recently, these hyperbolic materials have attracted increasing interest^{14,20,58,59} due to the existence of hyperbolic polaritons, featuring novel properties for nanophotonic applications such as subdiffraction imaging and hyperlensing^{12,13}. Because of the strong anisotropy of these systems, an effective permittivity approach is not purposeful. Here, our formalism provides the essential theoretical framework that is necessary to model, predict and analyze the optical response of such hyperbolic heterostructures, as we have discussed exemplarily for a MoO₃/AlN/SiC system (Fig. 2). Providing the full layer-resolved information about the field distribution and power flow of the excited polaritons, our method allows to readily and concisely model and study hyperbolic polariton modes in any anisotropic stratified heterostructure.

Furthermore, the layer-resolved absorption formalism provides a description for designing optoelectronic devices such as detectors, for which the photoresponse is linked to the light absorption solely in the active region of the device. In the case of the MQW system, optimizing the overall light absorption by minimizing both the reflectance and transmittance of the system would not be sufficient to model the performances of a photodetector in the strong light-matter coupling regime^{71,73}. Unfortunately, these are the only quantities that can be probed in a reflectance experiment. Calculating the layer-resolved absorption in the structure allows to optimize the cavity and MQW design, aiming at minimizing the light absorption in the cavity mirrors while maximizing the absorption in the MQW. This is well exemplified in Fig 4 e,f where we can see that the light is preferably dissipated in either the doped GaN mirror or the MQW superlattice depending on the detuning between the cavity mode and the QW resonance. This behavior cannot be deduced only from the reflectance measurement simulated in Fig. 4d. Fitting experimental reflectance data using our formalism²⁵ would allow to retrieve the amount of light dissipated inside the active region only from the

experimentally observable quantities, and to estimate figures of merit such as the quantum efficiency of the device. The present method thus provides a convenient way to model and optimize complex, optically anisotropic heterostructures for optoelectronic devices.

VI. CONCLUSION

In this work, we have derived explicit expressions for the calculation of the layer-resolved transmittance and absorption of light propagating in arbitrarily anisotropic, birefringent, and absorbing multilayer media. The algorithm relies on the electric field distribution computed from a 4×4 transfer matrix formalism^{25,33}, yielding a robust and consistent framework for light-matter interaction in stratified systems of arbitrary permittivity, which is implemented in an open access computer program^{34,35}. As case studies, we applied the algorithm to simulations of three nanophotonic device structures

featuring hyperbolic phonon polaritons in a polar dielectric heterostructure, MoS₂ excitons in a Fabry-Pérot cavity, and ENZ resonances in a cavity-coupled multi-quantum-well, where we observed azimuth-dependent hyperbolic polariton tunneling, layer-selective exciton absorption, and strong coupling between ENZ and cavity modes. Allowing for a detailed analysis of the layer-resolved electric field distribution, transmittance, and absorption of light in any multilayer system, our algorithm holds great potential for the prediction of nanophotonic light-matter interactions in arbitrarily anisotropic stratified heterostructures.

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