

Excitonic optical absorption in strained monolayer CrSBr

Maurício F. C. Martins Quintela^{1,2,*}, Guilherme J. Inacio^{1,2}, Miguel Sá,² Giovanni Cistaro,³ Alberto M. Ruiz,⁴ José J. Baldoví,⁴ Juan J. Palacios^{1,2,5} and Antonio Picón^{6,†}

¹Condensed Matter Physics Center (IFIMAC), *Universidad Autónoma de Madrid*, E-28049 Madrid, Spain

²Departamento de Física de la Materia Condensada, *Universidad Autónoma de Madrid*, E-28049 Madrid, Spain

³Theory and Simulation of Materials (THEOS), *École Polytechnique Fédérale de Lausanne (EPFL)*, CH-1015 Lausanne, Switzerland

⁴Instituto de Ciencia Molecular, *Universitat de València*, E-46100 Burjassot, Spain

⁵Instituto Nicolás Cabrera (INC), *Universidad Autónoma de Madrid*, E-28049 Madrid, Spain

⁶Instituto de Ciencia de Materiales de Madrid (ICMM-CSIC), E-28049 Madrid, Spain



(Received 15 October 2025; accepted 6 February 2026; published 12 March 2026)

Recently, the isolation of two-dimensional magnetic materials has opened several avenues for possible applications in spintronics. Among these materials, CrSBr has sparked interest due to its relatively high Curie temperature, highly anisotropic lattice structure, and high structural stability. These properties run along with others shared by any atomically thin material such as its outstanding deformation capacity and a strong optical response dominated by excitonic effects. The combination of these properties provides a fairly uncharted playground to explore the interplay between magnetism and optical excitations. Here, we focus our attention on the theoretical optical response of CrSBr under several distinct strain configurations, analyzing the resulting changes to both the excitonic peaks and overall shape of the diagonal components of the linear conductivity tensor.

DOI: [10.1103/8pdd-5md4](https://doi.org/10.1103/8pdd-5md4)

I. INTRODUCTION

Ever since the first isolation of two-dimensional (2D) or atomically thin materials [1], it has been understood that excitons are key to the understanding of the subgap optical response when these materials are semiconducting or insulating [2,3]. Since the number of nonzero unrelated components in the optical response tensors increases as the symmetry decreases, interest has grown in materials with intrinsically or extrinsically broken symmetries, such as the broken vertical symmetry in buckled monolayers [4–8], Janus materials [9–13], biased homobilayers [14–18] and heterobilayers [19,20], or the broken in-plane symmetries created by lattice strain [21–23] or an intrinsic lattice anisotropy, such as the one present in phosphorene [24–27].

In the past few years, since the isolation of the semiconducting 2D magnets CrI₃ [28] and Cr₂Ge₂Te₆ [29] in 2017, it has been an explosion in the discovery of 2D materials with magnetic properties [30]. While CrI₃ [31], Cr₂Ge₂Te₆, and CrBr₃ [32] present a ferromagnetic order out of plane, there are also materials that are in-plane ferromagnets, such as CrCl₃ [33] and CrSBr [34–36]. In particular, CrSBr has a

great potential for spintronics applications in nanoscale devices [37], in which the use of the spin degrees of freedom permits the manipulation and communication of information with extremely low power consumption [28,38–42]. Quantized collective spin excitations, known as magnons, are ideal quasiparticles for encoding spin information and developing spin-wave-based quantum computing concepts [43,44].

CrSBr is a semiconductor whose direct band gap has been reported as $E_g \approx 1.5$ eV and an A-type antiferromagnet, with a magnetic easy axis along the B direction [34–36,45–57] (see Fig. 1). Significantly, CrSBr is a relatively stable material in air [56] for which recent works have shown structural phase transformations [51], correlated magneto-optical [34,52,56] and magnetotransport [49,53,54] properties, and highly anisotropic electron conductivity [54].

Two-dimensional materials offer an excellent platform for tuning their properties through strain, which has a pronounced impact on magnonic behavior [58–62]. Strain also significantly influences the optical response of these materials, particularly the characteristics of excitons [63]. Recent research has uncovered strong interactions between excitons and magnon quasiparticles in 2D magnetic systems [64–72], an effect absent in conventional three-dimensional magnets. This effect opens avenues for controlling the magnetic response of 2D semiconducting magnets through light-induced excitations. These findings highlight the need for advanced theoretical frameworks to accurately describe strain effects on excitons in 2D magnetic materials. State-of-the-art theoretical approaches typically rely on the Bethe-Salpeter equation (BSE) to describe excitons and magnons [73,74]. Such methods have been successfully applied to study

*Contact author: mfcquintela@gmail.com

†Contact author: antonio.picon@csic.es

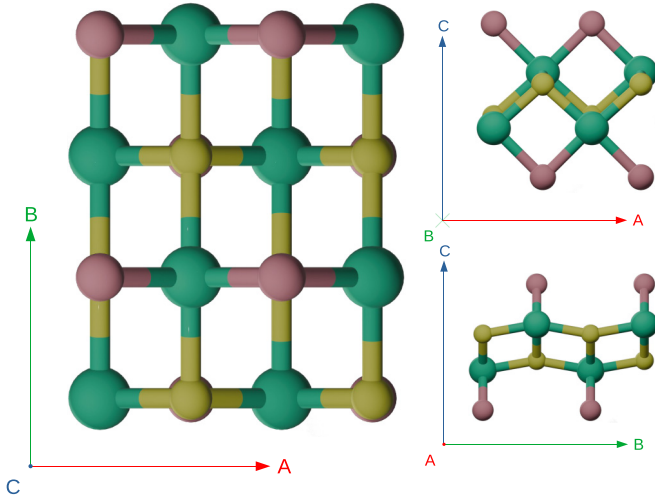


FIG. 1. Top (left) and side views (right) of the unit cell of a single CrSBr layer, where green, yellow, and pink represent the Cr, S, and Br atoms, respectively. In the plots, the A, B, and C directions correspond to x , y , and z axes, respectively.

excitons and optical phenomena in CrSBr, including magneto-optical effects and linear dichroism [36,57]. However, strain effects on CrSBr excitons were not investigated.

In this work, we investigate the impact of strain on the linear optical response of CrSBr. This study represents a first step toward exploring exciton-magnon coupling and understanding strain-induced effects relevant for spintronic applications. We begin in Sec. II by defining the lattice structure of CrSBr, discussing the overall shape of its band structure, and providing a brief overview on the effects of lattice strain in this material. In Sec. III, we outline the methodology that will be considered to obtain the excitonic states, namely, the BSE, together with the necessary modifications to the electrostatic interaction such that the intrinsic anisotropy of the lattice can be properly accounted for. Finally, in Sec. IV, we analyze the effects of strain on the diagonal components of the linear conductivity, together with the response for circularly polarized light.

II. LATTICE STRUCTURE

Monolayer CrSBr is a layered van der Waals antiferromagnet with a rectangular lattice structure [36,60]. It essentially consists of two buckled rectangular planes of CrS fused together, with both surfaces capped by Br atoms. Each atomic site sits at a linear combination of the Bravais vectors:

$$\mathbf{a}_1 = (a, 0, 0), \quad \mathbf{a}_2 = (0, b, 0), \quad (1)$$

where $a \approx 3.59 \text{ \AA}$ and $b \approx 4.81 \text{ \AA}$. As seen in Fig. 1, each unit cell counts with three pairs of Cr, S, and Br located at

$$\begin{aligned} \gamma_1 &= \mathbf{0}, & \gamma_2 &= \frac{\mathbf{a}_1 + \mathbf{a}_2}{2} + h\hat{\mathbf{z}} \quad (\text{Cr}), \\ \sigma_1 &= \frac{\mathbf{a}_1}{2} + d_{\text{Cr-S}}\hat{\mathbf{z}}, & \sigma_2 &= \gamma_2 - \sigma_1 \quad (\text{S}), \\ \beta_1 &= \frac{\mathbf{a}_1}{2} - d_{\text{Cr-Br}}\hat{\mathbf{z}}, & \beta_2 &= \gamma_2 - \beta_1 \quad (\text{Br}), \end{aligned} \quad (2)$$

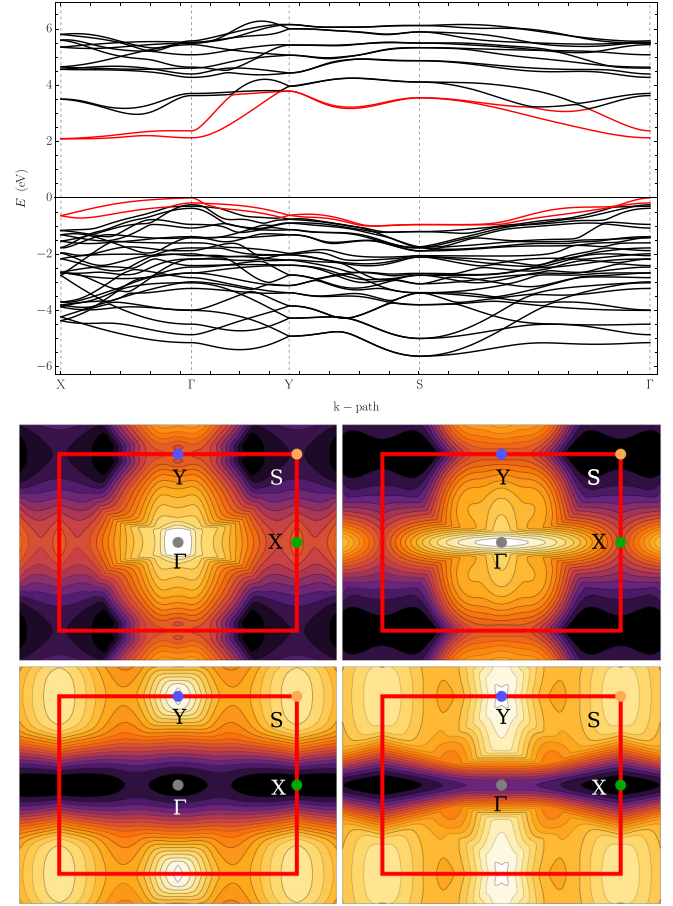


FIG. 2. Top: Band structure of CrSBr along the $X-\Gamma-Y-S-\Gamma$ path in the first Brillouin zone. Red bands were directly utilized for the BSE calculations in this work. Bottom: Contour plots of highlighted bands (increasing in energy from top left to bottom right) in the FBZ (red rectangle). Gray, green, blue, and orange points represent the high-symmetry Γ , X, Y, and S points, respectively.

where $h \approx 2.08 \text{ \AA}$ is the difference in height between the two Chromium atoms, $d_{\text{Cr-S}} \approx 1.61 \text{ \AA}$ and $d_{\text{Cr-Br}} \approx 1.77 \text{ \AA}$. In this notation, γ_2 is located in the middle of the unit cell, $\sigma_{1/2}$ halfway along $\mathbf{a}_{1/2} \pm d_{\text{Cr-S}}\hat{\mathbf{z}}$, respectively, and $\beta_{1/2}$ vertically shifted from $\sigma_{1/2}$ by $\mp(d_{\text{Cr-S}} + d_{\text{Cr-Br}})\hat{\mathbf{z}}$, respectively.

The high-symmetry points of the rectangular lattice have coordinates

$$\begin{aligned} \Gamma &= [0, 0], & \mathbf{X} &= [1/2, 0], \\ \mathbf{Y} &= [0, 1/2], & \mathbf{S} &= [1/2, 1/2], \end{aligned} \quad (3)$$

in the basis of the reciprocal lattice vectors $\mathbf{b}_1$ and $\mathbf{b}_2$. These points are represented in Fig. 2 by the gray, green, blue, and orange points, respectively.

For our calculations, we consider a tight-binding-like Hamiltonian written in a basis of maximally localized Wannier functions [75,76], as obtained and discussed in Ref. [60], where the preferential magnetization direction was set along the y axis. The Wannierization was performed on collinear DFT + U calculations, where U is the on-site Coulomb repulsion. The exchange-correlation energy was described by the generalized gradient approximation and the

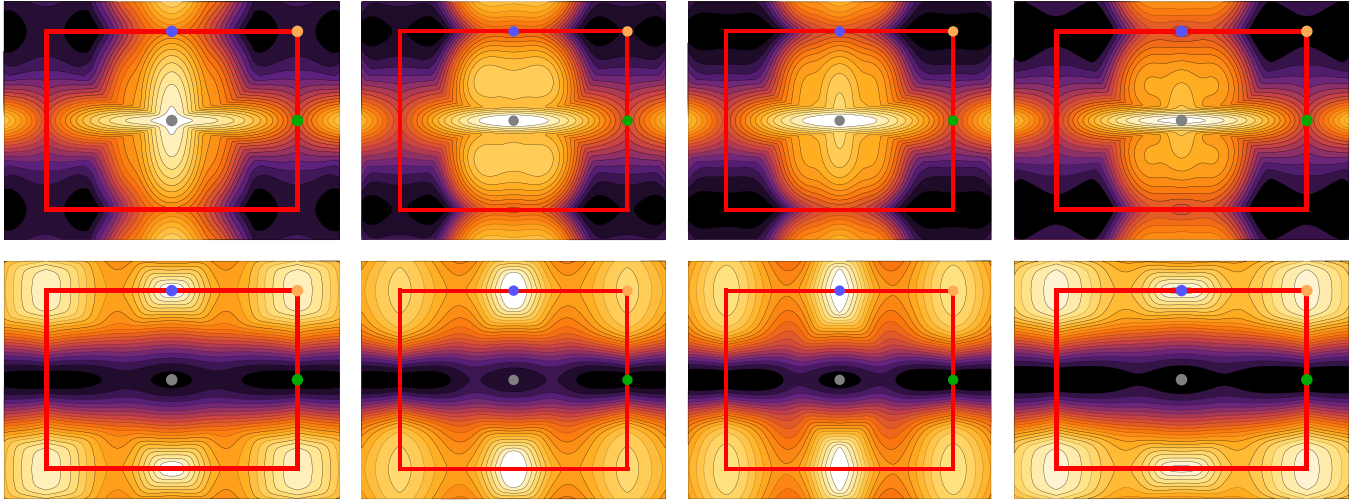


FIG. 3. Contour plots of the two bands closest to the Fermi level (valence top, conduction bottom) in the FBZ (red rectangle) for strain configurations 95% A, 105% A, 95% B, 105% B (left to right, respectively).

Perdew-Burke-Ernzerhof functional. The band structure of this Hamiltonian is portrayed in Fig. 2, where a scissor cut has been applied to match the direct band gap with other theoretical works at $E_g = 2.1$ eV [36,57]. The top panel shows the energy following a path in k space along the high-symmetry points of the material [see Eq. (3)]. We note the extremely flat dispersion of the first two conduction bands along the ΓX direction, in contrast to the much steeper dispersion along Γ and Y , where the lowest conduction band rises from approximately 2 and 4 eV between the Γ and Y points. As discussed below, this anisotropy in the energy dispersion leads to a quasi-one-dimensional (1D) exciton wave function for the lowest-energy states. To illustrate this, we plot the energy dispersion as a function of k_x and k_y . The bottom panel portrays the contour plots of the two highest valence bands and two lowest conduction bands in the FBZ. As these states are included in the BSE calculations, we ensured convergence by using $N_k = 90^2$ k points in the Brillouin zone. With this sampling, the excitonic energies remain stable within less than 1%.

Strain

The strain configuration will be described by its effects on the $\mathbf{a}_{1/2}$ vectors. Recalling the definition of the primitive vectors given by Eq. (1), we will identify the strain as A or B strain as it will directly affect the a and b lengths in Eq. (1). Therefore, besides the unstrained system, we will also consider compression (95% strain) and extension (105% strain) of the material along both A and B directions. Recent experiments show strains up to 4% in thin bulk CrSBr [77]. The effects of strain on the first valence and conduction bands are presented in Fig. 3. For each strain configuration, DFT + U calculations followed by Wannierization were performed. Note that the lowest-energy region of the conduction band, which is like a cylindrical-shape valley along the ΓX direction, is modified by the strain configuration. As we will see in the following sections, this will have clear implications on exciton wave functions and, consequently, in the optical response of the

material. More pronounced is the effect of strain on the valence band. The highest-energy region is like a cylindrical-shape mountain along the ΓX direction, and the compression along the A direction clearly affects the energy between the ΓY direction. Furthermore, the lowest conduction band remains largely unchanged across all strain configurations, becoming noticeably flatter along the ΓX direction near the band gap under compression along the A axis and stretching along the B axis. In contrast, the highest valence band develops a more “plus-shaped” dispersion around Γ when compressed along the A axis. Furthermore, stretching along the B axis significantly reduces the extent of the flat region near the gap. This modification enhances the localization of exciton wave functions along the same axis, as detailed in Appendix B, and strongly influences exciton energies, as discussed in the following sections.

III. BETHE-SALPETER EQUATION

The excitation of a valence band electron onto the conduction band of a material, leaving behind a hole in the valence band, can lead to the formation of bound states. Those states are bound via the Coulomb interaction of the electron-hole pair and their energy lies within the band gap of the system. Using valence (v) and conduction (c) single-particle states, we expand exciton states of zero center of mass momentum ($\mathbf{Q} = 0$) in a basis of free electron-hole pairs as

$$|X_N\rangle = \sum_{v\mathbf{c}\mathbf{k}} A_{v\mathbf{c}\mathbf{k}}^{(N)} c_{\mathbf{c}\mathbf{k}}^\dagger c_{v\mathbf{k}} |0\rangle, \quad (4)$$

where $|0\rangle$ is the ground state, identified as the Fermi sea, $A_{v\mathbf{c}\mathbf{k}}^{(N)}$ are the coefficients in the expansion of the excitonic states in terms of electron-hole excitations, and N is a generic quantum number that describes the excitonic state. Following from Esteve-Paredes *et al.* [78], exciton states are found by

solving the BSE [79] in the Tamm-Dancoff approximation as

$$E^{(N)} A_{v\mathbf{k}}^{(N)} = (E_{c\mathbf{k}} - E_{v\mathbf{k}}) A_{v\mathbf{k}}^{(N)} + \sum_{v'\mathbf{k}'} \langle v\mathbf{k} | K_{eh} | v'\mathbf{k}' \rangle A_{v'\mathbf{k}'}^{(N)}, \quad (5)$$

where $E_{c/v\mathbf{k}}$ are the conduction/valence electronic bands and K_{eh} is the electron-hole interaction kernel. Following the numerical implementation of the BSE in the XATU code [80], the interaction kernel reads $K_{eh} = -(D - X)$, where D is the direct term, given by

$$D_{vcv'\mathbf{k}'}(\mathbf{k}, \mathbf{k}') = \int \psi_{c\mathbf{k}}^*(\mathbf{r}) \psi_{v'\mathbf{k}'}^*(\mathbf{r}') W(\mathbf{r}, \mathbf{r}') \psi_{c'\mathbf{k}'}(\mathbf{r}) \psi_{v\mathbf{k}}(\mathbf{r}'), \quad (6)$$

and X is the exchange term (obtained by interchanging $c'\mathbf{k}'$ and $v\mathbf{k}$). The $W(\mathbf{r}, \mathbf{r}')$ represents the screened Coulomb interaction between two charged particles, which will be treated in the static limit as we detail in the following section.

Screened Coulomb interaction

When solving the BSE for excitons in 2D materials [18,78,80–82], the electrostatic interaction modeled by the Rytova-Keldysh (RK) potential [83,84] may represent a good description. The RK potential is derived from the Poisson's equation, in which the charge from the induced polarization in response to an external electric field is only contained in a 2D plane. In real space, this potential is given by

$$W_{RK}(\mathbf{r}, \mathbf{r}') = -\frac{\hbar c \alpha}{\epsilon_r} \frac{\pi}{2r_0} \left[H_0\left(\frac{|\mathbf{r} - \mathbf{r}'|}{r_0}\right) - Y_0\left(\frac{|\mathbf{r} - \mathbf{r}'|}{r_0}\right) \right], \quad (7)$$

where $H_0(x)$ is the zeroth-order Struve function, $Y_0(x)$ is the zeroth-order Bessel function of the second kind, r_0 is a material-specific screening length [85], and ϵ_r is the average dielectric constant of the medium surrounding the monolayer. This value is set at $\epsilon_r = 1$, corresponding to a freely suspended monolayer. While most frequently studied materials, such as hexagonal Boron-Nitride (hBN) [86], transition metal dichalcogenides (TMDCs) [85,87,88], and biased bilayer systems [89,90], are well modeled by an isotropic screening length, the high intrinsic anisotropy of CrSBr (see Fig. 1, for instance) demands that we consider a more general form of screening. From the large anisotropy of the bands, as it can be observed in Fig. 2, we will consider different screening lengths along the x and y directions.

Explicitly, the anisotropic Rytova-Keldysh potential will read as

$$W_{RK}(\mathbf{r}, \mathbf{r}') = -\frac{\hbar c \alpha}{\epsilon_r} \frac{\pi}{r_0^x + r_0^y} [H_0(\rho) - Y_0(\rho)], \quad (8)$$

where the r_0 term usually outside of the Bessel and Struve functions is now taken as the average of the screening lengths along the x (r_0^x) and the y (r_0^y) direction. Here,

$$\rho = \sqrt{\left(\frac{x - x'}{r_0^x}\right)^2 + \left(\frac{y - y'}{r_0^y}\right)^2 + \left(\frac{z - z'}{r_0^z}\right)^2}, \quad (9)$$

where the z component is explicitly included due to the complex lattice structure and r_0^z is also taken as the average of the

x and y components. While the material is still an atomically thin layer and, therefore, finite in the z direction, it is important to define a “vertical screening length” as we will have distinct z, z' positions for many of the atomic sites. Regarding the values of r_0^x and r_0^y , these can be obtained by doing a linear fit of the dielectric function of the material (as obtained via density functional theory (DFT) calculations) near $q = 0$. Considering previous calculations of the dielectric function for monolayer CrSBr [57], a linear fit near $q = 0$ along both q_x and q_y directions gives

$$r_0^x = 26.3894 \text{ \AA}, \quad r_0^y = 65.3451 \text{ \AA}. \quad (10)$$

Note the significant difference of the screen parameter depending on the direction. This presents an “anisotropy ratio” of $r_0^y/r_0^x \approx 2.476$, in good agreement with other computed results presented in Ref. [36].

Knowing the specific form of the anisotropic Rytova-Keldysh potential, we can now proceed to compute the excitonic wave functions. While the large anisotropy means angular momentum is not a good quantum number in this system, we can still label the excitonic states by their energy ordering. In Fig. 4, we plot the exciton wave functions for the lowest-energy state ($n = 1$), which is optically dark, together with the first four optically bright states ($n = 7, 14, 19, 26$), defined as $|\psi_{\mathbf{k}}^{(n)}|^2 = \sum_{v,c} |A_{v\mathbf{k}}^{(n)}|^2$. Although it will be discussed in the following section, the states are presented with a snippet of the subgap optical conductivity for easier visualization, with solid and dot-dashed lines highlighting the spectral location of the optically bright and dark states, respectively. We only represent the first eight optically dark states ($n = 1$ state highlighted in blue for easier identification). Note that 7-exciton and 26-exciton strongly contribute to the optical conductivity, and while 7-exciton is quite spread in the k_y direction, i.e., it behaves as a 1D exciton, the 26-exciton starts to have some spread along the k_x direction. We note that the optical activity of excitons can be understood from the $\mathbf{k}$ distribution of the exciton dipole matrix elements (see more details in Appendix C).

While there is a resemblance of the found excitonic states with previous calculations in Ref. [57], there are important differences, particularly in the energies. This can be easily understood by analyzing the used bands structure, which significantly differ. As a consequence, the resulting Wannier Hamiltonian will be quite distinct and, therefore, the excitonic states resulting from solving the BSE in the two systems are difficult to compare.

IV. STRAIN EFFECTS ON THE LINEAR OPTICAL RESPONSE

Having examined both the Bethe-Salpeter equation and the role of anisotropy in the electrostatic electron-hole interaction, we now turn to the influence of strain on the linear optical response of CrSBr.

To understand the impact of strain on the linear optical response of the 2D magnetic material, it is instructive to examine the optical response in the absence of electron-hole interactions, i.e., within the independent particle approximation (IPA). The IPA calculations allow us to isolate the primary changes in optical conductivity arising from

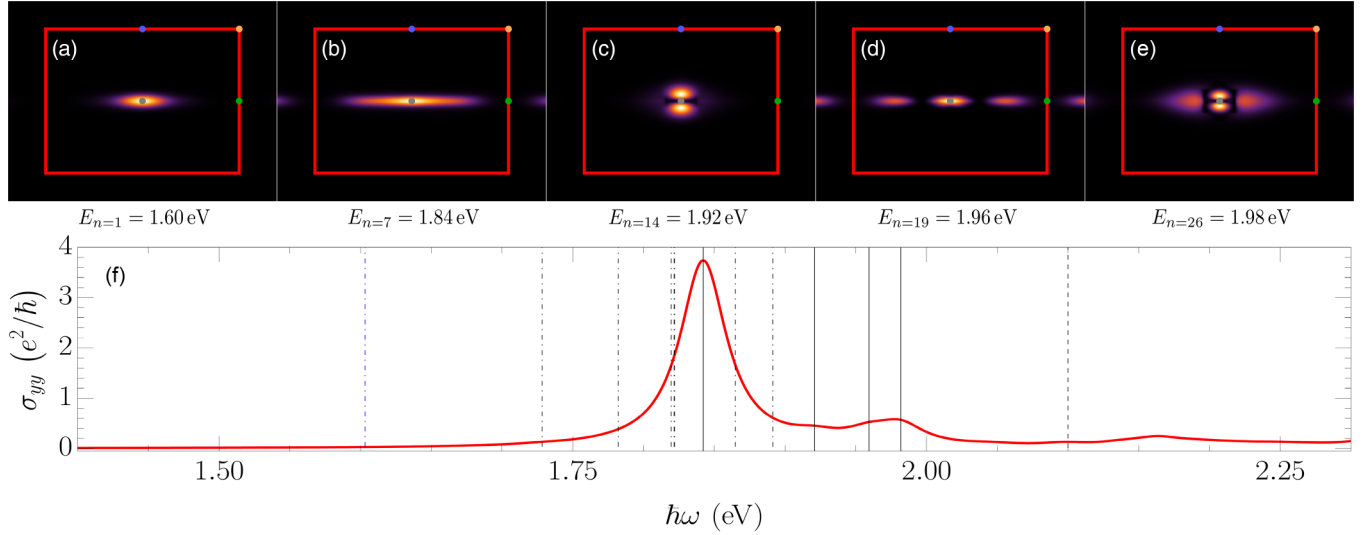


FIG. 4. Wave functions of the $n = 1$ (optically dark), $n = 7$, $n = 14$, $n = 19$, and $n = 26$ exciton states plotted in the FBZ [top panels (a)–(e)], together with the subgap region of the optical conductivity (bottom panel). In the bottom panel, vertical dashed line at $\hbar\omega = 2.1$ eV corresponds to the band gap at the Γ point for the unstrained system, solid vertical lines correspond to the optically bright states, and dot-dashed lines correspond to optically dark states until $n = 7$ (blue dot-dashed line highlights the lowest-energy exciton state, $n = 1$).

modifications in the energy band dispersion. This, in turn, provides an initial information to further analyze and disentangle the excitonic effects under strain. Accordingly, we compute the linear optical response at both the IPA level and with full excitonic interactions.

The excitonic optical conductivity is computed directly from the eigenstates of the Bethe-Salpeter equation as

$$\frac{\sigma_{\alpha\beta}(\omega)}{\sigma_0} = \frac{-i}{2\pi^3} \sum_n \left[\frac{E_n X_{0n}^\alpha X_{n0}^\beta}{E_n - \hbar\omega} - (\omega \rightarrow -\omega)^* \right], \quad (11)$$

where $\sigma_0 = \frac{e^2}{4\hbar}$, α/β are Cartesian directions, and E_n is the energy of the excitation, in which an imaginary broadening $\Gamma = 20$ meV is introduced via the transformation $E_n \rightarrow E_n - i\Gamma$ to model a realistic spectrum. The generic exciton dipole matrix element reads [8,91,92]

$$X_{0n}^\alpha = i \frac{\hbar}{m_0} \sum_{c,v} \int A_{vc\mathbf{k}}^{(n)} \frac{p_{vc\mathbf{k}}^\alpha}{E_{c\mathbf{k}} - E_{v\mathbf{k}}} d^2\mathbf{k}, \quad (12)$$

with $A_{vc\mathbf{k}}^{(n)}$ the exciton wave function between conduction band c and valence band v , $p_{vc\mathbf{k}}^\alpha$ the interband momentum matrix element between the same band pair, defined as

$$p_{vc\mathbf{k}}^\alpha = \frac{m_0}{\hbar} \langle v, \mathbf{k} | \frac{\partial \mathcal{H}(\mathbf{k})}{\partial k_\alpha} | c, \mathbf{k} \rangle,$$

and $E_{c/v\mathbf{k}}$ the dispersion of the bands in question.

The IPA contribution to the linear optical response will be obtained by directly applying the Kubo formalism as defined in Refs. [80,91] and computed with the OPTICX code [78,93].

As the dominant contribution to the subgap response will stem from the bands closest to the Fermi level, we perform the excitonic computations while taking into account the two valence and two conduction bands highlighted in red in Fig. 2. This decreases the computational cost without compromising the accuracy of the calculations and it makes possible to consider a greater number of neighboring unit cells in

the calculation. Considering $N = 90$ neighboring cells and an imaginary broadening of $\Gamma = 0.025$ eV, we compute the linear optical conductivity under both A and B strain (see Fig. 5).

Figure 5 portrays the xx (top panels) and yy (bottom panels) tensor components of the linear conductivity tensor for five distinct strain configurations: an unstrained system, 95% strain along both A and B directions, and 105% strain along the same directions. In this figure, the panels in the diagonal (top left and bottom right) correspond to strains parallel to the tensor component of the linear conductivity, while the off-diagonal panels (top right and bottom left) correspond to strains perpendicular to the tensor component of the linear conductivity.

First, we note that the excitonic optical conductivity presents strong exciton peaks within the band gap for y polarization (B axis), while excitonic peaks for x polarization are very small. This is in agreement with what is observed in experiments (see, for example, Ref. [69]). This results in significant birefringence or linear dichroism for photon energies within the energy gap.

By first examining the IPA calculations, Fig. 5 reveals that strain effects are significantly more pronounced when the strain direction is collinear with the diagonal component of the linear optical response under consideration. This is because strain alters the orbitals involved in bonding along that direction, thereby modifying the band energy structure. The primary manifestation of these changes is a redshift or blueshift in energy, corresponding to tensile or compressive strain, respectively, which are consistent with variations in the band gap. The excitonic optical conductivity also inherits the same behavior, with its dominant feature being a redshift or blueshift depending on the sign of the applied strain.

When examining the effects of strain applied perpendicular to the diagonal component of the linear optical response, we find that the IPA optical conductivity remains largely unchanged. However, significant modifications appear in the

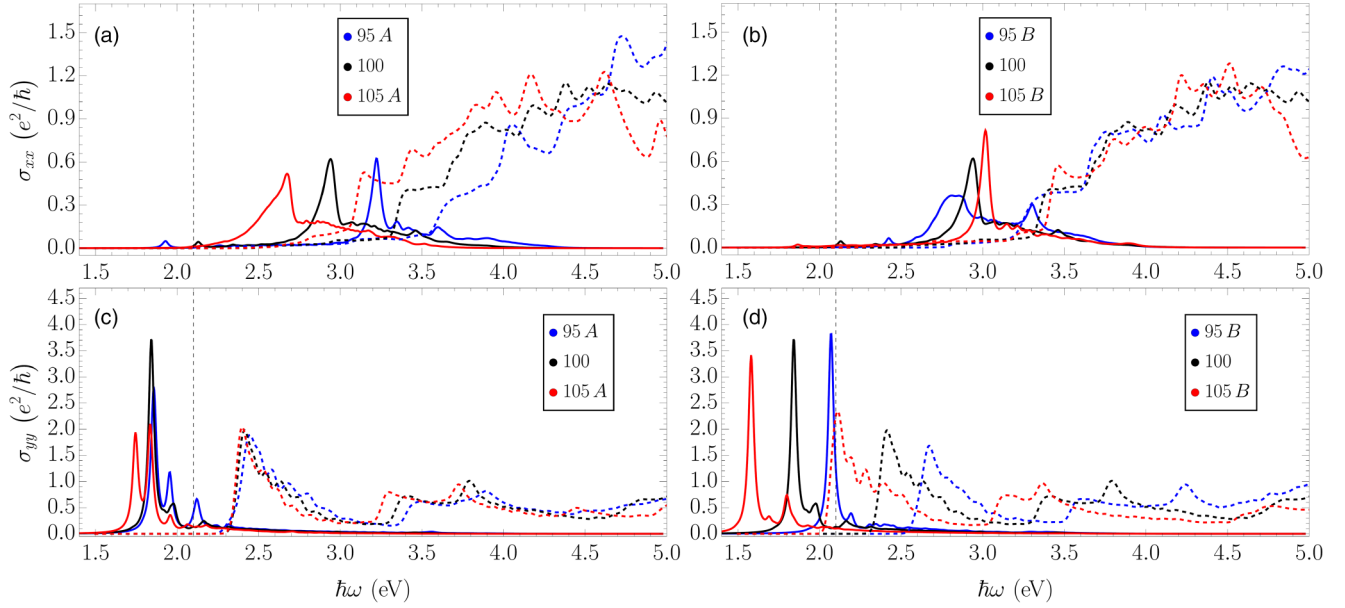


FIG. 5. Excitonic (solid lines) and IPA (dashed lines) contribution to the diagonal tensor elements of the linear optical conductivity (top: σ_{xx} , bottom: σ_{yy}). Left panels (a) and (c) correspond to strain in the A direction (x axis), while right panels (b) and (d) correspond to strain in the B direction (y axis). Blue, black, and red lines correspond to 95% strain, unstrained, and 105% strain in the corresponding column's direction, respectively. In all panels, vertical dashed line at $\hbar\omega = 2.1$ eV corresponds to the band gap at the Γ point for the unstrained system.

excitonic states, particularly those within the band gap along the y direction. This behavior can be understood by analyzing the exciton wave functions shown in Fig. 4, especially bright excitons that contribute to the optical response of the system. These wave functions are localized in regions of k space where the band energies are sensitive to strain, as illustrated in the conduction and valence energy bands in Fig. 3. This is particularly visible under tensile strain, in which we observe a strong redshift energy. Although bound excitons in CrSBr exhibit quasi-1D behavior along the y (B) direction, they are clearly influenced by strain applied along the x (A) direction.

Moreover, the lineshape of the excitonic optical conductivity evolves under strain, an effect attributed to the high sensitivity of exciton wave functions to lattice distortions. For instance, the wave functions of excitons 7 and 26 in the unstrained system differ notably; exciton 7 is primarily extended along the k_y direction, while exciton 26 has a stronger contribution along the k_x direction. This wave function distribution implies a distinct response to strain, with direct consequences for the energy positions of the excitonic series (see more details in Appendix B) and the corresponding oscillator strengths.

Now, we consider the optical response to circularly polarized light, which is related to the magnetic circular dichroism (MCD) (see Fig. 6). The circular optical conductivity can be related to the off-diagonal components of the linear optical conductivity. Simplifying Eq. (12) for circularly polarized light, we have

$$\begin{aligned} X_{0n}^{\pm} &= \frac{i}{\sqrt{2}} \sum_{c,v} \int A_{v\mathbf{k}}^{(n)} \frac{\langle v, \mathbf{k} | [\frac{\partial \mathcal{H}(\mathbf{k})}{\partial k_x} \pm i \frac{\partial \mathcal{H}(\mathbf{k})}{\partial k_y}] | c, \mathbf{k} \rangle}{E_{c\mathbf{k}} - E_{v\mathbf{k}}} d^2\mathbf{k} \\ &= \frac{i}{\sqrt{2}} [X_{0n}^x \pm i X_{0n}^y], \end{aligned} \quad (13)$$

meaning that circular polarization will, in general, mix the four in-plane tensor components as

$$\sigma_{\pm}(\omega) = \frac{\sigma_{xx}(\omega)}{2} + \frac{\sigma_{yy}(\omega)}{2} \pm \frac{i}{2} [\sigma_{yx}(\omega) - \sigma_{xy}(\omega)]. \quad (14)$$

When all four tensor components are mixed, the effects of strain become considerably more complex. However, in monolayer CrSBr, the yy tensor component is the dominant one until $\hbar\omega \approx 3$ – 3.5 eV and, examining Eq. (14), one expects the circular optical conductivity under strain to closely resemble the features observed in the yy component of the linear optical conductivity within this frequency range. The MCD signal, which is computed by taking the difference of the left- and right-handed circular optical conductivity, is found to be very small within the band gap region (see bottom panels of Fig. 6). The MCD is directly connected to the xy and yx tensor components, which are antisymmetrical between themselves. The small MCD signal is understood because the xy and yx tensor components are 3 orders of magnitude smaller than the xx and yy tensor components. Additionally, while a subtle difference is observable below the band gap (more clearly visible when considering strain in the B direction), the effect is much smaller than what is observed in the single-particle regime and, therefore, is barely observable even when magnified by a factor of 10^3 . As a final comment, the xy and yx tensor components are also responsible for magneto-optical phenomena such as the Faraday and Kerr effects. Due to their small magnitude, these effects are likewise weak, consistent with experimental observations.

In the ground state, the magnetization orientation in CrSBr lies along the y (B) direction. This orientation, which can be modified by an external magnetic field, influences the optical and the magneto-optical response of the material. In Appendix A, we compare the effects of the three distinct

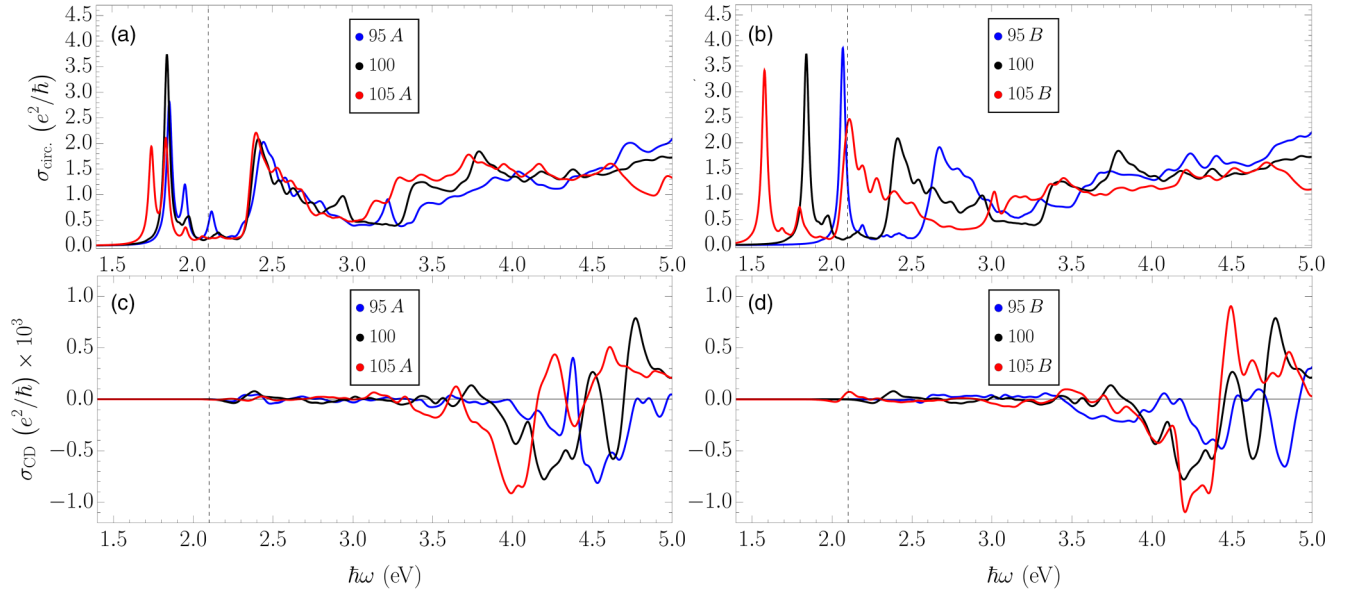


FIG. 6. Linear optical conductivity with both excitonic and IPA contributions for circularly polarized light. Left panels (a) and (c) correspond to strain in the A direction (x axis), while right panels (b) and (d) correspond to strain in the B direction (y axis). Top panels correspond to left-handed circular polarization, while bottom panels correspond to difference between left- and right-handed polarization. Blue, black, and red lines correspond to 95% strain, unstrained, and 105% strain in the corresponding column's direction, respectively. In both panels, vertical dashed line at $\hbar\omega = 2.1$ eV corresponds to the band gap at the Γ point for the unstrained system.

magnetization orientations on the diagonal tensor components of the conductivity and the circular dichroism. Notably, we observe that the MCD signal becomes two orders of magnitude stronger above the band gap when the magnetization is aligned along the z direction. This enhancement is consistent with observations in other materials, such as CrI_3 , where out-of-plane magnetization leads to strong MCD signals [94].

V. SUMMARY

In this work, we investigate the influence of strain on the linear optical response of monolayer CrSBr . By solving the Bethe-Salpeter equation, we compute the linear optical conductivity with explicit consideration of excitonic effects. We find that bound excitons predominantly form along the B direction and exhibit pronounced sensitivity to the strain configuration.

Despite the quasi-one-dimensional nature of the exciton wave functions, strain applied along both the A and B directions significantly alters their energies and directly impacts the subband gap optical conductivity. When strain is applied collinearly to the polarization direction of the optical conductivity, we observe an energy redshift and blueshift for tensile and compressive strain, respectively. In contrast, strain applied perpendicular to the polarization direction leads to substantial modifications in the spectral lineshape, which we attribute to changes in the energetic ordering of the excitonic series.

Furthermore, magnetic circular dichroism is found to be negligible for bound excitons, with the signal primarily emerging at energies above the band gap. The MCD signal above the gap is notably sensitive to the orientation

of the magnetization. This work opens the door to investigate coherent exciton migration controlled by strain [63,95] in monolayer CrSBr and the manipulation of the magnetization at the attosecond time scale by using strong laser pulses [96]. For that, we could extend the methodology used here to real-time approaches that also consider excitonic effects [97–99].

ACKNOWLEDGMENTS

The authors acknowledge financial support to the Spanish Ministry of Science, Innovation and Universities and the State Research Agency through a Grants No. PID2024-157663NB-I00, No. PID2021-126560NB-I00, No. CNS2022-135803, No. TED2021-131323B-I00, No. PID2022-141712NB-C21, and No. PID2024-162182NAI00 (MCIU/AEI/FEDER, UE), and the “María de Maeztu” and “Severo Ochoa” Programme for Units of Excellence in R&D (CEX2023-001316-M and CEX2024-001445-S), “Disruptive 2D materials” (MAD2D-CM-UAM7), funded by Comunidad de Madrid within the Recovery, Transformation and Resilience Plan, and by NextGenerationEU programme from the European Union, the Generalitat Valenciana through the Program Prometeo (2021/017). We also acknowledge computer resources and assistance provided by Centro de Computación Científica de la Universidad Autónoma de Madrid and RES resources (FI-2024-3-0010, FI-2024-3-0011, FI-2024-2-0034, FI-2023-2-0012, FI-2022-3-0022, FI-2022-1-0031). J.J.B. acknowledges the European Union (ERC-2021-StG101042680 2D-SMARTIES) and the Generalitat Valenciana (Grant No. CIDEXG/2023/1), CEX2024-001467-M (ICMol). A.M.R. thanks the Spanish MIU (Grant No. FPU21/04195).

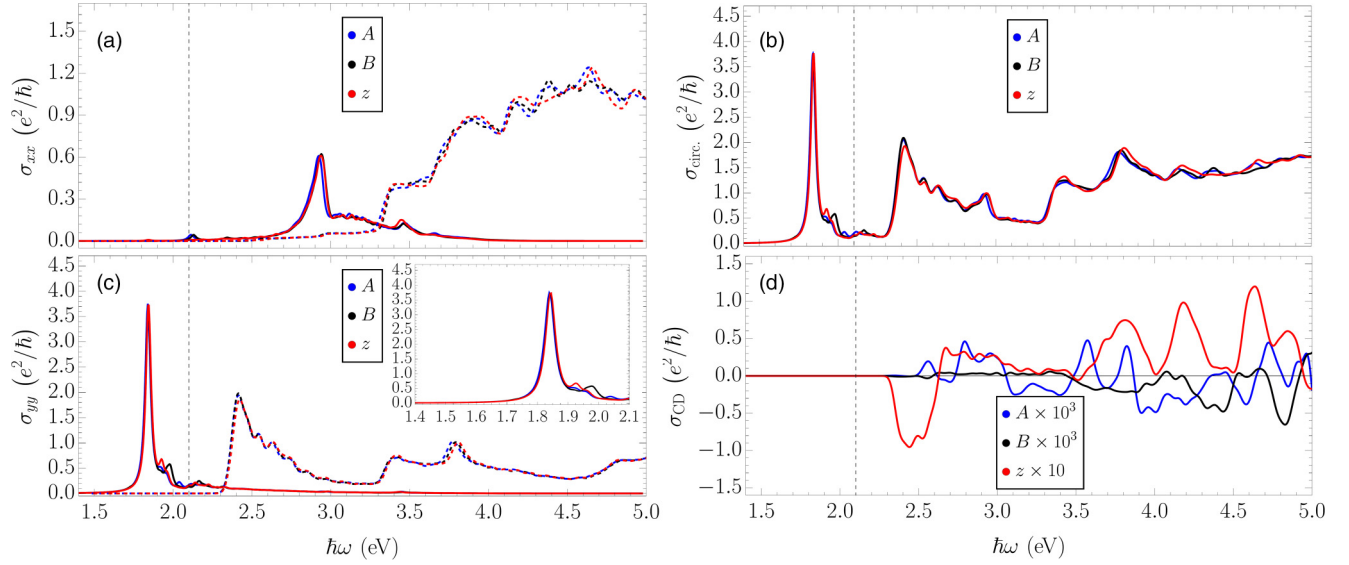


FIG. 7. Influence of magnetization direction on linear optical conductivity with both excitonic and IPA contributions for (left panels) linearly polarized light and (right panels) circularly polarized light. Blue, black, and red lines correspond to magnetization chosen to be along the A , B , and z axis for the Wannierization process, respectively. In all panels, vertical dashed line at $\hbar\omega = 2.1$ eV corresponds to the band gap at the Γ point for the unstrained system. For linearly polarized light, excitonic (solid lines) and IPA (dashed lines) contributions to the diagonal tensor elements of the linear optical conductivity (top: σ_{xx} , bottom: σ_{yy}) are considered separately to better showcase the different effects of the magnetization direction on either component. Inset in the bottom-left panel presents the subgap region of the conductivity to more clearly observe the changes in the excitonic peaks.

DATA AVAILABILITY

The data that support the findings of this article are not publicly available upon publication because it is not technically feasible and/or the cost of preparing, depositing, and hosting the data would be prohibitive within the terms of this research project. The data are available from the authors upon reasonable request.

APPENDIX A: EFFECTS OF MAGNETIC MOMENTUM DIRECTION

In this Appendix, we provide a comparison for the xx and yy components of the linear optical conductivity for the three distinct directions of the magnetization chosen during the Wannierization process (specifically, along either A or B axis, or perpendicular to the plane of the monolayer). As can be seen in Fig. 7, the xx component of the linear optical conductivity barely changes depending on the magnetization choice. On the other hand, the yy component presents quite clear changes in the subgap response of the material (see inset in the bottom panel), with the two most pronounced excitonic peaks having quite distinct intensities and locations depending on the axis chosen for the magnetization. However, as can be seen in both the top and bottom panels, the conductivity above the band gap remains essentially unchanged between the three distinct magnetization directions.

APPENDIX B: STRAIN EFFECTS ON EXCITONIC WAVE FUNCTIONS

In this Appendix, we provide a comparison between the excitonic states for strains along the A and B directions. These

are presented in Fig. 8 for systems under (top to bottom, in pairs) 95% A , 105% A , 95% B , and 105% B strain. In the conductivity panels, the lines follow the same notation as those in Fig. 4, with blue dot-dashed line corresponding to the lowest-energy excitonic state, dot-dashed lines representing first few dark states, solid lines representing the plotted bright states, and dashed line representing the gap at the Γ point. As it can be clearly seen, the overall shape of the state corresponding to the dominant peak changes slightly with strain (see third wave function for strain 95% A and second wave function for the remaining strains in Fig. 8), although its position in the excitonic series differs depending on the strain configuration. For easier comparison, we list the energies of each of these five states in Table I.

We emphasize that the excitonic evolution presented here arises from strain-induced modifications of the electronic structure while maintaining a fixed in-plane ferromagnetic configuration of the monolayer. This assumption is supported by recent first-principles studies showing that monolayer

TABLE I. First energy eigenvalue, corresponding to the dark exciton state, along with the energy eigenvalues of the four lowest bright exciton states, as a function of strain configuration, as illustrated in Fig. 8.

	100%	95% A	105% A	95% B	105% B
$n = 1$	1.60 eV	1.67 eV	1.56 eV	1.80 eV	1.38 eV
First bright	1.84 eV	1.79 eV	1.74 eV	2.07 eV	1.58 eV
Second bright	1.92 eV	1.86 eV	1.75 eV	2.11 eV	1.69 eV
Third bright	1.96 eV	1.88 eV	1.84 eV	2.19 eV	1.72 eV
Fourth bright	1.98 eV	1.96 eV	1.96 eV	2.20 eV	1.77 eV

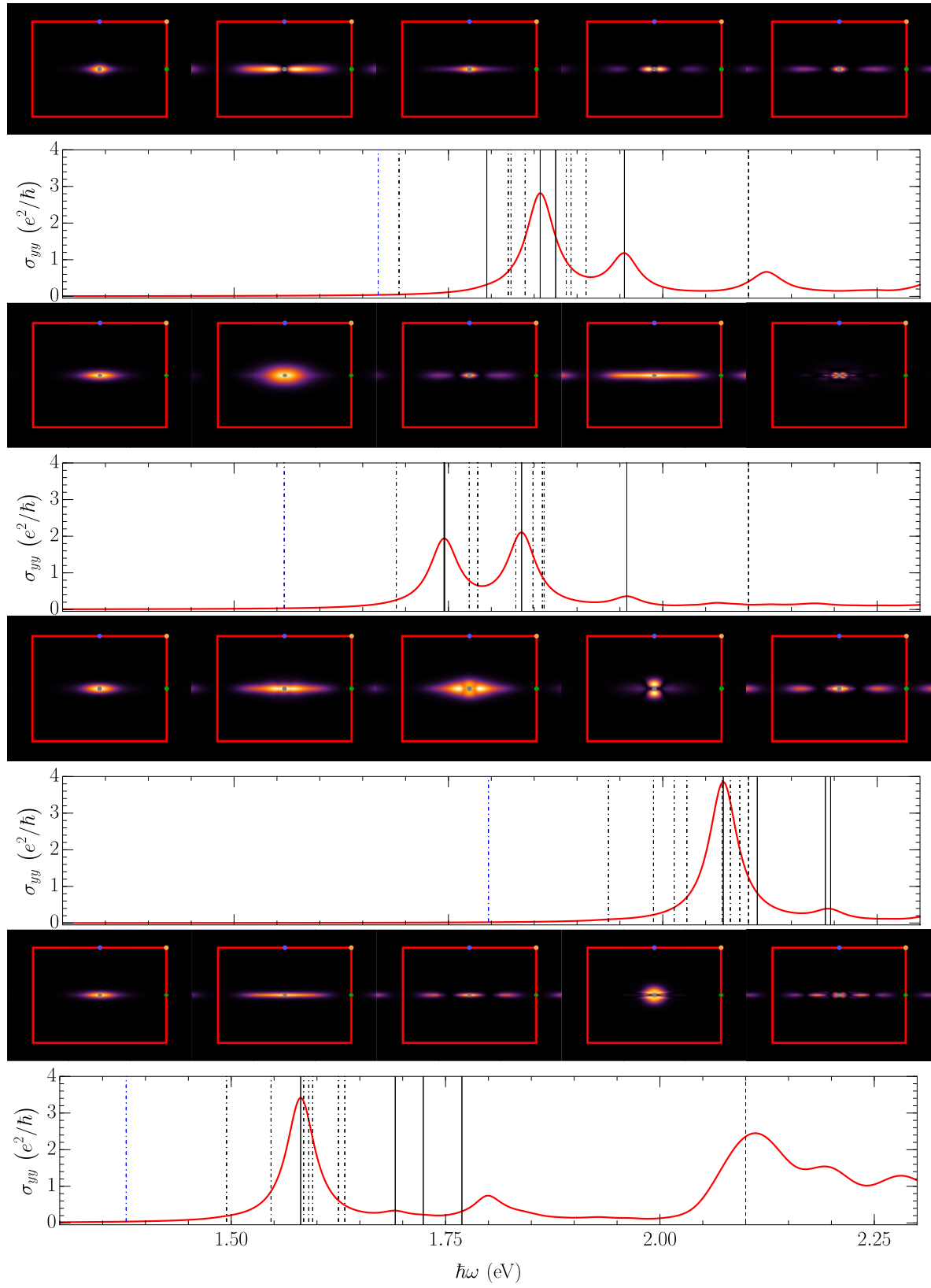


FIG. 8. Excitonic wave functions of first (dark) state, together with first four bright states and the corresponding subgap response for clearer identification for systems under (top to bottom, in pairs) 95% A, 105% A, 95% B, and 105% B strain.

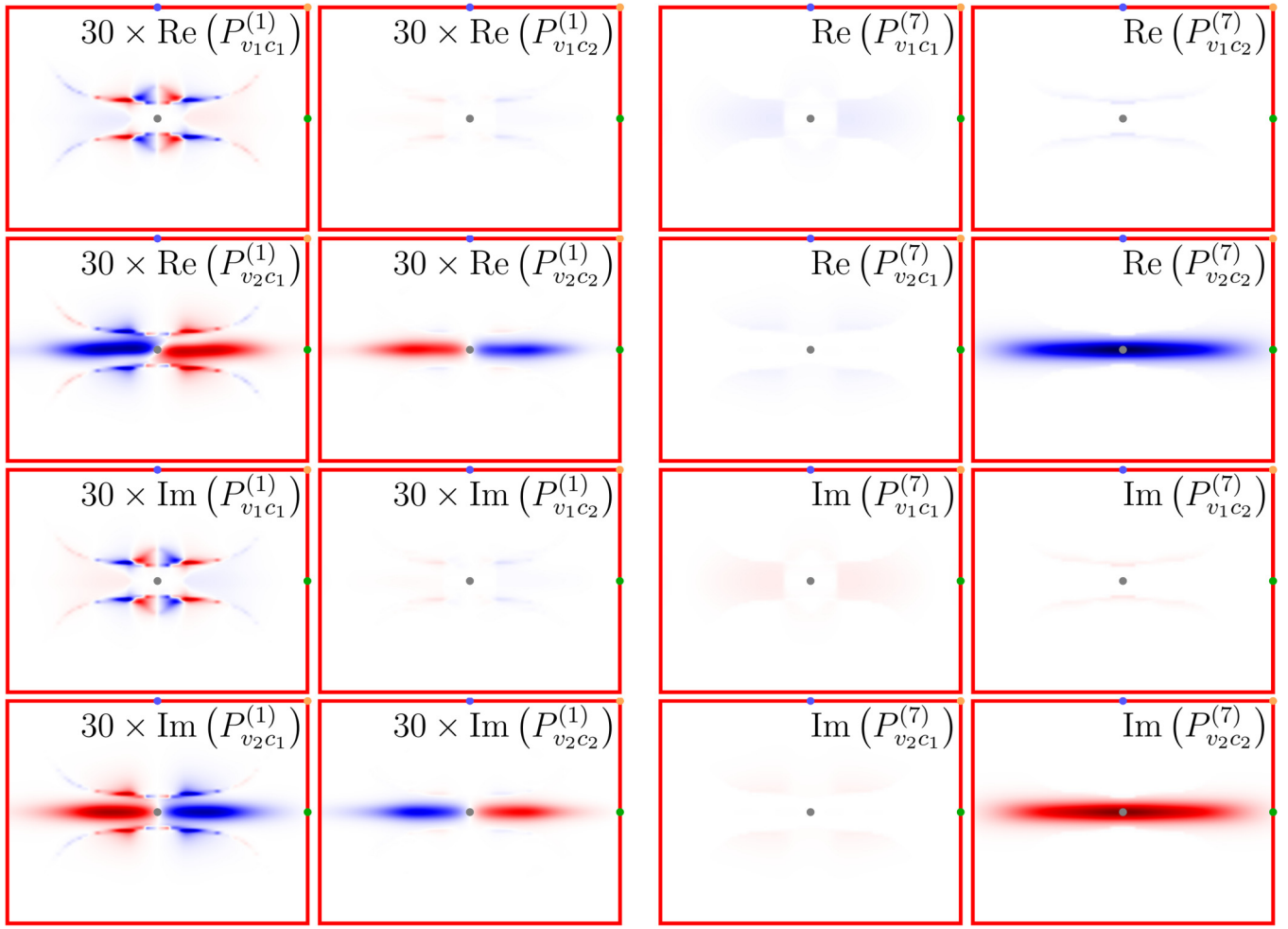


FIG. 9. Real and imaginary parts of the $\mathbf{k}$ -resolved exciton momentum matrix elements of the $n = 1$ and $n = 7$ exciton states for band pairs $v_{1(2)}c_{1(2)}$. Color scales have been normalized by the extreme of $\text{Re}(P_{v_2c_2}^{(7)})$ and $\text{Im}(P_{v_2c_2}^{(7)})$ for the real and imaginary components, respectively. For clarity, the matrix elements corresponding to the $n = 1$ state have been magnified by a factor of 30.

CrSBr preserves its ferromagnetic order under substantial lattice distortions, with the primary effect being a renormalization of the band structure [100].

APPENDIX C: EXCITONIC DIPOLE MATRIX ELEMENTS

In this Appendix, we provide a comparison between the $\mathbf{k}$ -resolved exciton momentum matrix elements along the y direction in unstrained CrSBr, defined from Eq. (12) as

$$P_{v\mathbf{ck}}^{(n)} = A_{v\mathbf{ck}}^{(n)} p_{v\mathbf{ck}}^y, \quad (\text{C1})$$

where the y index has been dropped from the $P_{v\mathbf{ck}}^{(n)}$ notation for compactness. Upon integration in $\mathbf{k}$ and sum over bands [see Eq. (12)], these $\mathbf{k}$ -resolved momentum matrix elements

give rise to the excitonic optical selection rules governing whether a state is optically dark ($n = 1$ exciton in this system) or optically bright ($n = 7$ exciton).

In Fig. 9, we plot both real and imaginary components of the $\mathbf{k}$ -resolved exciton momentum matrix elements for each of the band pairings considered in the BSE calculation (see Fig. 2), where valence and conduction bands are labeled $v_{1/2}c_{1/2}$ in ascending order. The optically dark character of the $n = 1$ state arises from both its significantly smaller amplitude and its antisymmetric distribution around the Γ point. Notably, for this dark state, $P_{v_2c_2}^{(1)}$ and $P_{v_2c_1}^{(1)}$ exhibit comparable amplitudes, whereas the bright $n = 7$ state is dominated by a single transition, $P_{v_2c_2}^{(7)}$, which is symmetric with respect to Γ .

- [1] K. S. Novoselov, A. K. Geim, S. V. Morozov, D. Jiang, Y. Zhang, S. V. Dubonos, I. V. Grigorieva, and A. A. Firsov, Electric field effect in atomically thin carbon films, *Science* **306**, 666 (2004).
- [2] K. F. Mak, C. Lee, J. Hone, J. Shan, and T. F. Heinz, Atomically thin MoS_2 : A new direct-gap semiconductor, *Phys. Rev. Lett.* **105**, 136805 (2010).

- [3] Y. Li, A. Chernikov, X. Zhang, A. Rigosi, H. M. Hill, A. M. van der Zande, D. A. Chenet, E.-M. Shih, J. Hone, and T. F. Heinz, Measurement of the optical dielectric function of monolayer transition-metal dichalcogenides: MoS_2 , MoSe_2 , WS_2 , and WSe_2 , *Phys. Rev. B* **90**, 205422 (2014).
- [4] H. Sahin, S. Cahangirov, M. Topsakal, E. Bekaroglu, E. Akturk, R. T. Senger, and S. Ciraci, Monolayer honeycomb

- structures of group-IV elements and III-V binary compounds: First-principles calculations, *Phys. Rev. B* **80**, 155453 (2009).
- [5] H. K. Avetissian and G. F. Mkrtchian, Higher harmonic generation by massive carriers in buckled two-dimensional hexagonal nanostructures, *Phys. Rev. B* **99**, 085432 (2019).
 - [6] M.-Q. Le, H.-T. Nguyen, and T.-L. Bui, Fracture of 28 buckled two-dimensional hexagonal sheets, *Mech. Adv. Mater. Struct.* **29**, 4993 (2022).
 - [7] R. Y. Kezerashvili and A. Spiridonova, Effects of parallel electric and magnetic fields on Rydberg excitons in buckled two-dimensional materials, *Phys. Rev. B* **103**, 165410 (2021).
 - [8] M. F. C. M. Quintela and T. G. Pedersen, Anisotropic linear and nonlinear excitonic optical properties of buckled monolayer semiconductors, *Phys. Rev. B* **107**, 235416 (2023).
 - [9] A.-Y. Lu, H. Zhu, J. Xiao, C.-P. Chuu, Y. Han, M.-H. Chiu, C.-C. Cheng, C.-W. Yang, K.-H. Wei, Y. Yang, Y. Wang, D. Sokaras, D. Nordlund, P. Yang, D. A. Muller, M.-Y. Chou, X. Zhang, and L.-J. Li, Janus monolayers of transition metal dichalcogenides, *Nat. Nanotechnol.* **12**, 744 (2017).
 - [10] J. Zhang, S. Jia, I. Kholmanov, L. Dong, D. Er, W. Chen, H. Guo, Z. Jin, V. B. Shenoy, L. Shi, and J. Lou, Janus monolayer transition-metal dichalcogenides, *ACS Nano* **11**, 8192 (2017).
 - [11] T. Zheng, Y.-C. Lin, Y. Yu, P. Valencia-Acuna, A. A. Puzosky, R. Torsi, C. Liu, I. N. Ivanov, G. Duscher, D. B. Geohegan, Z. Ni, K. Xiao, and H. Zhao, Excitonic dynamics in Janus MoSSe and WSSe monolayers, *Nano Lett.* **21**, 931 (2021).
 - [12] O. Dogadov, C. Trovatiello, B. Yao, G. Soavi, and G. Cerullo, Parametric nonlinear optics with layered materials and related heterostructures, *Laser Photon. Rev.* **16**, 2100726 (2022).
 - [13] J. Shi, H. Xu, C. Heide, C. HuangFu, C. Xia, F. de Quesada, H. Shen, T. Zhang, L. Yu, A. Johnson, F. Liu, E. Shi, L. Jiao, T. Heinz, S. Ghimire, J. Li, J. Kong, Y. Guo, and A. M. Lindenberg, Giant room-temperature nonlinearities in a monolayer Janus topological semiconductor, *Nat. Commun.* **14**, 4953 (2023).
 - [14] H. Yu, D. Talukdar, W. Xu, J. B. Khurgin, and Q. Xiong, Charge-induced second-harmonic generation in bilayer WSe₂, *Nano Lett.* **15**, 5653 (2015).
 - [15] S. J. Brun and T. G. Pedersen, Intense and tunable second-harmonic generation in biased bilayer graphene, *Phys. Rev. B* **91**, 205405 (2015).
 - [16] J. Klein, J. Wierzbowski, A. Steinhoff, M. Florian, M. Rösner, F. Heimbach, K. Müller, F. Jahnke, T. O. Wehling, J. J. Finley, and M. Kaniber, Electric-field switchable second-harmonic generation in bilayer MoS₂ by inversion symmetry breaking, *Nano Lett.* **17**, 392 (2017).
 - [17] Z. Zheng, K. Chang, and J. L. Cheng, Gate voltage induced injection and shift currents in AA- and AB-stacked bilayer graphene, *Phys. Rev. B* **108**, 235401 (2023).
 - [18] M. F. C. M. Quintela, N. M. R. Peres, and T. G. Pedersen, Tunable nonlinear excitonic optical response in biased bilayer graphene, *Phys. Rev. B* **110**, 085433 (2024).
 - [19] Y. Gong, J. Lin, X. Wang, G. Shi, S. Lei, Z. Lin, X. Zou, G. Ye, R. Vajtai, B. I. Yakobson, H. Terrones, M. Terrones, B. Tay, J. Lou, S. T. Pantelides, Z. Liu, W. Zhou, and P. M. Ajayan, Vertical and in-plane heterostructures from WS₂/MoS₂ monolayers, *Nat. Mater.* **13**, 1135 (2014).
 - [20] P. Rivera, K. L. Seyler, H. Yu, J. R. Schaibley, J. Yan, D. G. Mandrus, W. Yao, and X. Xu, Valley-polarized exciton dynamics in a 2D semiconductor heterostructure, *Science* **351**, 688 (2016).
 - [21] Z. Peng, X. Chen, Y. Fan, D. J. Srolovitz, and D. Lei, Strain engineering of 2D semiconductors and graphene: From strain fields to band-structure tuning and photonic applications, *Light: Sci. Appl.* **9**, 190 (2020).
 - [22] L. Du, T. Hasan, A. Castellanos-Gomez, G.-B. Liu, Y. Yao, C. N. Lau, and Z. Sun, Engineering symmetry breaking in 2D layered materials, *Nat. Rev. Phys.* **3**, 193 (2021).
 - [23] M. M. Glazov, F. Dirnberger, V. M. Menon, T. Taniguchi, K. Watanabe, D. Bougeard, J. D. Ziegler, and A. Chernikov, Exciton fine structure splitting and linearly polarized emission in strained transition-metal dichalcogenide monolayers, *Phys. Rev. B* **106**, 125303 (2022).
 - [24] A. Castellanos-Gomez, L. Vicarelli, E. Prada, J. O. Island, K. L. Narasimha-Acharya, S. I. Blanter, D. J. Groenendijk, M. Buscema, G. A. Steele, J. V. Alvarez, H. W. Zandbergen, J. J. Palacios, and H. S. J. van der Zant, Isolation and characterization of few-layer black phosphorus, *2D Mater.* **1**, 025001 (2014).
 - [25] V. Tran and L. Yang, Scaling laws for the band gap and optical response of phosphorene nanoribbons, *Phys. Rev. B* **89**, 245407 (2014).
 - [26] K. Cho, J. Yang, and Y. Lu, Phosphorene: An emerging 2D material, *J. Mater. Res.* **32**, 2839 (2017).
 - [27] H. C. Kamban, T. G. Pedersen, and N. M. R. Peres, Anisotropic Stark shift, field-induced dissociation, and electroabsorption of excitons in phosphorene, *Phys. Rev. B* **102**, 115305 (2020).
 - [28] B. Huang, G. Clark, E. Navarro-Moratalla, D. R. Klein, R. Cheng, K. L. Seyler, D. Zhong, E. Schmidgall, M. A. McGuire, D. H. Cobden, W. Yao, D. Xiao, P. Jarillo-Herrero, and X. Xu, Layer-dependent ferromagnetism in a van der Waals crystal down to the monolayer limit, *Nature (London)* **546**, 270 (2017).
 - [29] C. Gong, L. Li, Z. Li, H. Ji, A. Stern, Y. Xia, T. Cao, W. Bao, C. Wang, Y. Wang, Z. Q. Qiu, R. J. Cava, S. G. Louie, J. Xia, and X. Zhang, Discovery of intrinsic ferromagnetism in two-dimensional van der Waals crystals, *Nature (London)* **546**, 265 (2017).
 - [30] G. Shi, N. Huang, J. Qiao, X. Zhang, F. Hu, H. Hu, X. Zhang, and J. Shang, Recent progress in two-dimensional magnetic materials, *Nanomaterials* **14**, 1759 (2024).
 - [31] M. Gibertini, M. Koperski, A. F. Morpurgo, and K. S. Novoselov, Magnetic 2D materials and heterostructures, *Nat. Nanotechnol.* **14**, 408 (2019).
 - [32] Z. Zhang, J. Shang, C. Jiang, A. Rasmita, W. Gao, and T. Yu, Direct photoluminescence probing of ferromagnetism in monolayer two-dimensional CrBr₃, *Nano Lett.* **19**, 3138 (2019).
 - [33] A. Bedoya-Pinto, J.-R. Ji, A. K. Pandeya, P. Gargiani, M. Valvidares, P. Sessi, J. M. Taylor, F. Radu, K. Chang, and S. S. P. Parkin, Intrinsic 2D-XY ferromagnetism in a van der Waals monolayer, *Science* **374**, 616 (2021).
 - [34] N. P. Wilson, K. Lee, J. Cenker, K. Xie, A. H. Dismukes, E. J. Telford, J. Fonseca, S. Sivakumar, C. Dean, T. Cao, *et al.*, Interlayer electronic coupling on demand in a 2D magnetic semiconductor, *Nat. Mater.* **20**, 1657 (2021).
 - [35] K. Lee, A. H. Dismukes, E. J. Telford, R. A. Wiscons, J. Wang, X. Xu, C. Nuckolls, C. R. Dean, X. Roy, and X. Zhu, Magnetic

- order and symmetry in the 2D semiconductor CrSBr, *Nano Lett.* **21**, 3511 (2021).
- [36] J. Klein, B. Pingault, M. Florian, M.-C. Heissenbüttel, A. Steinhoff, Z. Song, K. Torres, F. Dirnberger, J. B. Curtis, M. Weile, *et al.*, The bulk van der Waals layered magnet CrSBr is a quasi-1D material, *ACS Nano* **17**, 5316 (2023).
- [37] K. S. Burch, D. Mandrus, and J.-G. Park, Magnetism in two-dimensional van der Waals materials, *Nature (London)* **563**, 47 (2018).
- [38] S. Neusser and D. Grundler, Magnonics: Spin waves on the nanoscale, *Adv. Mater.* **21**, 2927 (2009).
- [39] S. A. Nikitov, D. V. Kalyabin, I. V. Lisenkov, A. N. Slavin, Y. N. Barabanenkov, S. A. Osokin, A. V. Sadovnikov, E. N. Beginin, M. A. Morozova, Y. P. Sharaevsky, Y. A. Filimonov, Y. V. Khivintsev, S. L. Vysotsky, V. K. Sakharov, and E. S. Pavlov, Magnonics: A new research area in spintronics and spin wave electronics, *Phys. Usp.* **58**, 1002 (2015).
- [40] A. V. Chumak, V. I. Vasyuchka, A. A. Serga, and B. Hillebrands, Magnon spintronics, *Nat. Phys.* **11**, 453 (2015).
- [41] J.-U. Lee, S. Lee, J. H. Ryoo, S. Kang, T. Y. Kim, P. Kim, C.-H. Park, J.-G. Park, and H. Cheong, Ising-type magnetic ordering in atomically thin FePS₃, *Nano Lett.* **16**, 7433 (2016).
- [42] S. N. Kajale, J. Hanna, K. Jang, and D. Sarkar, Two-dimensional magnetic materials for spintronic applications, *Nano Res.* **17**, 743 (2024).
- [43] L. Šmejkal, Y. Mokrousov, B. Yan, and A. H. MacDonald, Topological antiferromagnetic spintronics, *Nat. Phys.* **14**, 242 (2018).
- [44] A. Rodin, M. Trushin, A. Carvalho, and A. H. Castro Neto, Collective excitations in 2D materials, *Nat. Rev. Phys.* **2**, 524 (2020).
- [45] H. Katscher and H. Hahn, Über chalkogenidhalogenide des dreiwertigen chroms, *Naturwissenschaften* **53**, 361 (1966).
- [46] O. Göser, W. Paul, and H. Kahle, Magnetic properties of CrSBr, *J. Magn. Magn. Mater.* **92**, 129 (1990).
- [47] C. Wang, X. Zhou, L. Zhou, N.-H. Tong, Z.-Y. Lu, and W. Ji, A family of high-temperature ferromagnetic monolayers with locked spin-dichroism-mobility anisotropy: MnNX and CrCX (X = Cl, Br, I; C = S, Se, Te), *Sci. Bull.* **64**, 293 (2019).
- [48] H. Wang, J. Qi, and X. Qian, Electrically tunable high Curie temperature two-dimensional ferromagnetism in van der Waals layered crystals, *Appl. Phys. Lett.* **117**, 083102, (2020).
- [49] E. J. Telford, A. H. Dismukes, K. Lee, M. Cheng, A. Wieteska, A. K. Bartholomew, Y.-S. Chen, X. Xu, A. N. Pasupathy, X. Zhu, *et al.*, Layered antiferromagnetism induces large negative magnetoresistance in the van der Waals semiconductor CrSBr, *Adv. Mater.* **32**, 2003240 (2020).
- [50] K. Yang, G. Wang, L. Liu, D. Lu, and H. Wu, Triaxial magnetic anisotropy in the two-dimensional ferromagnetic semiconductor CrSBr, *Phys. Rev. B* **104**, 144416 (2021).
- [51] J. Klein, T. Pham, J. Thomsen, J. Curtis, T. Denneulin, M. Lorke, M. Florian, A. Steinhoff, R. Wiscons, J. Luxa, *et al.*, Control of structure and spin texture in the van der Waals layered magnet CrSBr, *Nat. Commun.* **13**, 5420 (2022).
- [52] J. Klein, Z. Song, B. Pingault, F. Dirnberger, H. Chi, J. B. Curtis, R. Dana, R. Bushati, J. Quan, L. Dekanovsky, *et al.*, Sensing the local magnetic environment through optically active defects in a layered magnetic semiconductor, *ACS Nano* **17**, 288 (2023).
- [53] E. J. Telford, A. H. Dismukes, R. L. Dudley, R. A. Wiscons, K. Lee, D. G. Chica, M. E. Ziebel, M.-G. Han, J. Yu, S. Shabani, *et al.*, Coupling between magnetic order and charge transport in a two-dimensional magnetic semiconductor, *Nat. Mater.* **21**, 754 (2022).
- [54] F. Wu, I. Gutiérrez-Lezama, S. A. López-Paz, M. Gibertini, K. Watanabe, T. Taniguchi, F. O. von Rohr, N. Ubrig, and A. F. Morpurgo, Quasi-1D electronic transport in a 2D magnetic semiconductor, *Adv. Mater.* **34**, 2109759 (2022).
- [55] S. A. López-Paz, Z. Guguchia, V. Y. Pomjakushin, C. Witteveen, A. Cervellino, H. Luetkens, N. Casati, A. F. Morpurgo, and F. O. von Rohr, Dynamic magnetic crossover at the origin of the hidden-order in van der Waals antiferromagnet CrSBr, *Nat. Commun.* **13**, 4745 (2022).
- [56] K. Torres, A. Kuc, L. Maschio, T. Pham, K. Reidy, L. Dekanovsky, Z. Sofer, F. M. Ross, and J. Klein, Probing defects and spin-phonon coupling in CrSBr via resonant Raman scattering, *Adv. Funct. Mater.* **33**, 2211366 (2023).
- [57] T.-X. Qian, J. Zhou, T.-Y. Cai, and S. Ju, Anisotropic electron-hole excitation and large linear dichroism in the two-dimensional ferromagnet CrSBr with in-plane magnetization, *Phys. Rev. Res.* **5**, 033143 (2023).
- [58] Y. Wang, S.-S. Wang, Y. Lu, J. Jiang, and S. A. Yang, Strain-induced isostructural and magnetic phase transitions in monolayer MoN₂, *Nano Lett.* **16**, 4576 (2016).
- [59] A. V. Sadovnikov, A. A. Grachev, S. E. Sheshukova, Y. P. Sharaevskii, A. A. Serdobintsev, D. M. Mitin, and S. A. Nikitov, Magnon straintronics: Reconfigurable spin-wave routing in strain-controlled bilateral magnetic stripes, *Phys. Rev. Lett.* **120**, 257203 (2018).
- [60] D. L. Esteras, A. Rybakov, A. M. Ruiz, and J. J. Baldoví, Magnon straintronics in the 2D van der Waals ferromagnet CrSBr from first-principles, *Nano Lett.* **22**, 8771 (2022).
- [61] J. Cenker, S. Sivakumar, K. Xie, A. Miller, P. Thijssen, Z. Liu, A. Dismukes, J. Fonseca, E. Anderson, X. Zhu, X. Roy, D. Xiao, J.-H. Chu, T. Cao, and X. Xu, Reversible strain-induced magnetic phase transition in a van der Waals magnet, *Nat. Nanotechnol.* **17**, 256 (2022).
- [62] H. Ren and G. Xiang, Strain engineering of intrinsic ferromagnetism in 2D van der Waals materials, *Nanomaterials* **13**, 2378 (2023).
- [63] M. F. C. M. Quintela, M. Sá, A. J. Uría-Álvarez, M. Malakhov, G. Cistaro, J. Quereda, J. J. Palacios, and A. Picón, Quantum valley pseudospin controlled by strain, *Phys. Rev. Res.* **7**, 043265 (2025).
- [64] M. Onga, Y. Sugita, T. Ideue, Y. Nakagawa, R. Suzuki, Y. Motome, and Y. Iwasa, Antiferromagnet-semiconductor van der Waals heterostructures: Interlayer interplay of exciton with magnetic ordering, *Nano Lett.* **20**, 4625 (2020).
- [65] Y. J. Bae, J. Wang, A. Scheie, J. Xu, D. G. Chica, G. M. Diederich, J. Cenker, M. E. Ziebel, Y. Bai, H. Ren, *et al.*, Exciton-coupled coherent magnons in a 2D semiconductor, *Nature (London)* **609**, 282 (2022).
- [66] G. M. Diederich, J. Cenker, Y. Ren, J. Fonseca, D. G. Chica, Y. J. Bae, X. Zhu, X. Roy, T. Cao, D. Xiao, and X. Xu, Tunable interaction between excitons and hybridized

- magnons in a layered semiconductor, *Nat. Nanotechnol.* **18**, 23 (2023).
- [67] Y. Sun, F. Meng, C. Lee, A. Soll, H. Zhang, R. Ramesh, J. Yao, Z. Sofer, and J. Orenstein, Dipolar spin wave packet transport in a van der Waals antiferromagnet, *Nat. Phys.* **20**, 794 (2024).
- [68] G. M. Diederich, M. Nguyen, J. Cenker, J. Fonseca, S. Pumulo, Y. J. Bae, D. G. Chica, X. Roy, X. Zhu, D. Xiao, Y. Ren, and X. Xu, Exciton dressing by extreme nonlinear magnons in a layered semiconductor, *Nat. Nanotechnol.* **20**, 617 (2025).
- [69] B. Datta, P. C. Adak, S. Yu, A. V. Dharmapalan, S. J. Hall, A. Vakulenko, F. Komissarenko, E. Kurganov, J. Quan, W. Wang, K. Mosina, Z. Sofer, D. Pashov, M. van Schilfgaarde, S. Acharya, A. Kamra, M. Y. Sfeir, A. Alù, A. B. Khanikaev, and V. M. Menon, Magnon-mediated exciton–exciton interaction in a van der Waals antiferromagnet, *Nat. Mater.* **24**, 1027 (2025).
- [70] C. A. Belvin, E. Baldini, I. O. Ozel, D. Mao, H. C. Po, C. J. Allington, S. Son, B. H. Kim, J. Kim, I. Hwang, J. H. Kim, J.-G. Park, T. Senthil, and N. Gedik, Exciton-driven antiferromagnetic metal in a correlated van der Waals insulator, *Nat. Commun.* **12**, 4837 (2021).
- [71] Z. Wang, X.-X. Zhang, Y. Shiomi, T. -h. Arima, N. Nagaosa, Y. Tokura, N. Ogawa, Exciton-magnon splitting in the van der Waals antiferromagnet MnPS₃ unveiled by second-harmonic generation, *Phys. Rev. Res.* **5**, L042032 (2023).
- [72] J. Varela-Manjarres, Y. Ren, and B. K. Nikolic, Ultrafast optical excitation of magnons in 2D antiferromagnetic semiconductors via spin torque mediated by unbound electron-hole pairs and excitons: Signatures in magnonic charge pumping, *arXiv:2507.02793*.
- [73] M. Marsili, A. Molina-Sánchez, M. Palummo, D. Sangalli, and A. Marini, Spinorial formulation of the GW-BSE equations and spin properties of excitons in two-dimensional transition metal dichalcogenides, *Phys. Rev. B* **103**, 155152 (2021).
- [74] A. Esquembre-Kučukalić, K. B. Le, A. García-Cristóbal, M. Bernardi, D. Sangalli, and A. Molina-Sánchez, Magnons in chromium trihalides from *ab initio* Bethe-Salpeter equation, *Phys. Rev. B* **112**, 184412 (2025).
- [75] A. A. Mostofi, J. R. Yates, G. Pizzi, Y.-S. Lee, I. Souza, D. Vanderbilt, and N. Marzari, An updated version of Wannier90: A tool for obtaining maximally-localised Wannier functions, *Comput. Phys. Commun.* **185**, 2309 (2014).
- [76] G. Pizzi, V. Vitale, R. Arita, S. Blügel, F. Freimuth, G. Géranton, M. Gibertini, D. Gresch, C. Johnson, T. Koretsune, *et al.*, Wannier90 as a community code: New features and applications, *J. Phys.: Condens. Matter* **32**, 165902 (2020).
- [77] J. Cenker, J. Fonseca, M. Nguyen, C. Hu, D. G. Chica, T. Taniguchi, K. Watanabe, X. Zhu, X. Roy, J.-H. Chu, and X. Xu, Engineering robust strain transmission in van der Waals heterostructure devices, *Nano Lett.* **25**, 4512 (2025).
- [78] J. J. Esteve-Paredes, M. A. García-Blázquez, A. J. Uría-Álvarez, M. Camarasa-Gómez, and J. J. Palacios, Excitons in nonlinear optical responses: Shift current in MoS₂ and GeS monolayers, *npj Comput. Mater.* **11**, 13 (2025).
- [79] M. Rohlfing and S. G. Louie, Electron-hole excitations and optical spectra from first principles, *Phys. Rev. B* **62**, 4927 (2000).
- [80] A. J. Uría-Álvarez, J. J. Esteve-Paredes, M. García-Blázquez, and J. J. Palacios, Efficient computation of optical excitations in two-dimensional materials with the Xatu code, *Comput. Phys. Commun.* **295**, 109001 (2024).
- [81] M. F. C. M. Quintela, J. C. G. Henriques, L. G. M. Tenório, and N. M. R. Peres, Theoretical methods for excitonic physics in 2D materials, *Physica Status Solidi (b)* **259**, 2200097 (2022).
- [82] J. C. G. Henriques, I. Epstein, and N. M. R. Peres, Absorption and optical selection rules of tunable excitons in biased bilayer graphene, *Phys. Rev. B* **105**, 045411 (2022).
- [83] S. N. Rytova, The screened potential of a point charge in a thin film, *Mosc. Un Phys. Bul.* **3**, 30 (1967).
- [84] L. V. Keldysh, Coulomb interaction in thin semiconductor and semimetal films, *Sov. J. Exp. and Theor. Phys. Lett.* **29**, 658 (1979).
- [85] P. Cudazzo, I. V. Tokatly, and A. Rubio, Dielectric screening in two-dimensional insulators: Implications for excitonic and impurity states in graphane, *Phys. Rev. B* **84**, 085406 (2011).
- [86] J. C. G. Henriques, G. B. Ventura, C. D. M. Fernandes, and N. M. R. Peres, Optical absorption of single-layer hexagonal boron nitride in the ultraviolet, *J. Phys.: Condens. Matter* **32**, 025304 (2020).
- [87] D. Y. Qiu, F. H. da Jornada, and S. G. Louie, Screening and many-body effects in two-dimensional crystals: Monolayer MoS₂, *Phys. Rev. B* **93**, 235435 (2016).
- [88] J. Huang, T. B. Hoang, and M. H. Mikkelsen, Probing the origin of excitonic states in monolayer WSe₂, *Sci. Rep.* **6**, 22414 (2016).
- [89] E. V. Castro, K. S. Novoselov, S. V. Morozov, N. M. R. Peres, J. M. B. Lopes dos Santos, J. Nilsson, F. Guinea, A. K. Geim, and A. H. C. Neto, Electronic properties of a biased graphene bilayer, *J. Phys.: Condens. Matter* **22**, 175503 (2010).
- [90] J. C. G. Henriques, B. Amorim, R. M. Ribeiro, and N. M. R. Peres, Excitonic response of AA' and AB stacked hBN bilayers, *Phys. Rev. B* **105**, 115421 (2022).
- [91] T. G. Pedersen, Intraband effects in excitonic second-harmonic generation, *Phys. Rev. B* **92**, 235432 (2015).
- [92] A. Taghizadeh and T. G. Pedersen, Nonlinear optical selection rules of excitons in monolayer transition metal dichalcogenides, *Phys. Rev. B* **99**, 235433 (2019).
- [93] The optcix package can be found within the repository of the Xatu, GitHub, <https://github.com/xatu-code>.
- [94] M. Wu, Z. Li, T. Cao, and S. G. Louie, Physical origin of giant excitonic and magneto-optical responses in two-dimensional ferromagnetic insulators, *Nat. Commun.* **10**, 2371 (2019).
- [95] M. Malakhov, G. Cistaro, F. Martín, and A. Picón, Exciton migration in two-dimensional materials, *Commun. Phys.* **7**, 196 (2024).
- [96] O. Neufeld, N. Tancogne-Dejean, U. De Giovannini, H. Hübener, and A. Rubio, Attosecond magnetization dynamics in non-magnetic materials driven by intense femtosecond lasers, *npj Comput. Mater.* **9**, 39 (2023).
- [97] G. Cistaro, M. Malakhov, J. J. Esteve-Paredes, A. J. Uría-Álvarez, R. E. F. Silva, F. Martín, J. J. Palacios, and A. Picón, Theoretical approach for electron dynamics and ultrafast spectroscopy (EDUS), *J. Chem. Theory Comput.* **19**, 333 (2023).
- [98] E. B. Molinero, B. Amorim, M. Malakhov, G. Cistaro, Á. Jiménez-Galán, A. Picón, P. San-José, M. Ivanov, and R. E. F. Silva, Subcycle dynamics of excitons under strong laser fields, *Sci. Adv.* **10**, eadn6985 (2024).

- [99] J. F. P. Mosquera, G. Cistaro, M. Malakhov, E. Pisanty, A. Dauphin, L. Plaja, A. Chacón, M. Lewenstein, and A. Picón, Topological phase transitions via attosecond x-ray absorption spectroscopy, [Rep. Prog. Phys.](#) **87**, 117901 (2024).
- [100] E. Henríquez-Guerra, A. M. Ruiz, M. Galbiati, Á. Cortés-Flores, D. Brown, E. Zamora-Amo, L. Almonte, A. Shumilin, J. Salvador-Sánchez, A. Pérez-Rodríguez, *et al.*, Strain engineering of magnetoresistance and magnetic anisotropy in CrSBr, [Adv. Mater.](#) 2506695 (2025).