

Quantum valley pseudospin controlled by strain

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Valleytronics, as an alternative to traditional electronics or spintronics, is based on the encoding of quantum information in pseudospin valley quantum numbers, rather than in charge or spin states. A key ingredient is the (optical) manipulation of valley states before loss of coherence, which can be as fast as 100 fs. Previous works have shown the possibility of valley state manipulation using external fields. Here, we propose uniaxial strain as a more flexible and robust scheme to manipulate the valley state through the breaking of the crystal symmetry and the concomitant lifting of the degeneracy of the $1s$ exciton energy. Our theory is corroborated by state-of-the-art numerical simulations in monolayer hBN and shows the possibility to control valley pseudospin at the attosecond timescale.

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I. INTRODUCTION

The breaking of symmetries usually gives rise to interesting phenomena such as spin-polarization effects, nonlinear effects, superconductivity, and valleytronics, to just name a few [1], with a wide variety of technology applications and advances in photonics and optoelectronics. The term valleytronics refers to the possibility of encoding information through the crystal momentum of the electrons, specifically in the so-called valley pseudospin, which refers to the momentum at (optically) relevant time-reversed points in the Brillouin zone. The unique properties of two-dimensional (2D) materials are essential to deploy the potential of valleytronics [2]. In monolayer materials such as hBN and transition metal dichalcogenides (TMDCs), inversion symmetry breaking gives rise to a nontrivial Berry connection around K and K' points in reciprocal space. This, along with spin-orbit coupling in TMDCs, allows for selection rules that permit to selectively excite carriers at the K or K' valleys, by using circularly polarized pulses [2]. This selectivity can be used to encode information, opening a promising framework

for electronics and quantum information. Furthermore, it is based on an all-optical scheme, which enables to manipulate the information at the ultimate speed of electrons, i.e., at the attosecond timescale [3,4].

In 2D materials, due to their low dimensionality and reduced screening, the optical response is dominated by excitons. Excitons can be considered quasiparticles composed by an electron-hole pair bound via Coulomb interaction. In particular, the degenerate $1s$ excitonic state dominates the absorption spectrum. Previous works demonstrated rotations on the pseudospin Bloch sphere of the excitonic quantum states, see Fig. 1(b), by using magnetic or electric external fields [5–8]. There is also extensive research on manipulating the pseudospin degrees of freedom in quantum dots using external electrostatic fields [9–11].

Current technology allows to break and control the symmetry of 2D materials by relying on external fields, layer stacking, or strain [1]. In particular, the potential of strain engineering to tailor the valley-related behavior of carriers in TMDCs has been vastly explored in the literature [13–24]. Despite the relevance of the $1s$ exciton peak in the optical response, certain effects of strain on excitons have scarcely been explored, such as how it modifies the character of the $1s$ exciton states, induces energy splitting, and alters their excitation under circular polarization [18,20,23,24]. In contrast to previous studies, in which an external electromagnetic field [5] or a laser pulse field [6,7] is used to modify the exciton energies and produce a rotation in the Bloch sphere, here we exploit strain. We prove that global static strain, by breaking the spatial symmetry, lifts the $1s$ exciton degeneracy

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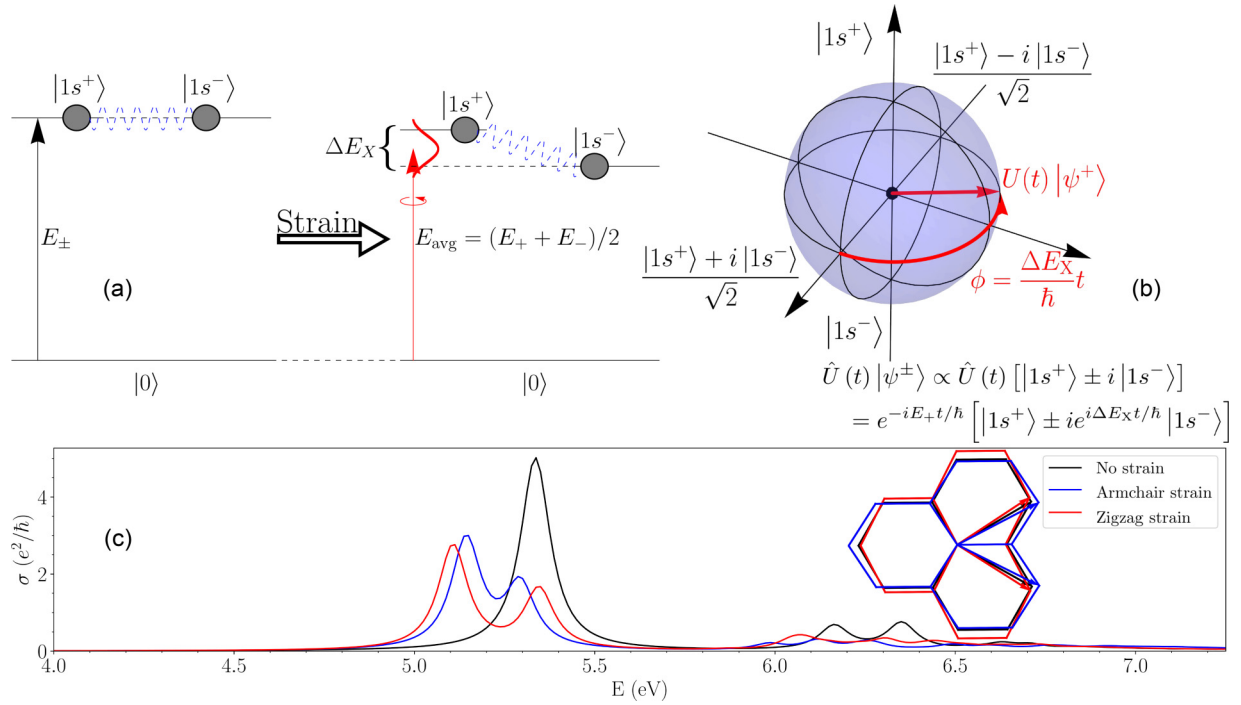


FIG. 1. (a) Scheme of the energy degeneracy lifting of $1s$ exciton states due to strain, together with the pulse designed to excite the two relevant states. (b) View of the rotations of the excitonic quantum states on the pseudospin Bloch sphere induced by strain. (c) Circularly polarized optical conductivity for unstrained system (black line) as well as for the system under armchair (blue line) and zigzag (red line) strains, as obtained through XATU [12]. Inset represents the lattice deformation for each corresponding strain.

and consequently the excitation with a circularly polarized pulse induces a valley rotation. This has two main advantages: (1) the degeneracy can be permanently lifted and (2) the orientation and the strength of the strain offer an additional control knob without the energy cost of an external field, which is more attractive for technology purposes. We show that the speed of the full valley pseudospin rotation could reach the few-femtosecond timescale with realistic strains, being comparable or superior to reported schemes with external fields [5–7,16,25,26].

Detecting the valley state is a challenging task due to its short coherence lifetime, which is reported in TMDCs to lie between 98 and 520 fs [5,27]. It is then desired to have a fast valley-pseudospin manipulation and therefore also a detection scheme to track the state changes. Previous detection schemes are based on photoluminescence [6], two-dimensional coherent spectroscopy [28], second-harmonic generation [29], and Faraday rotation [26]. Here, due to our fast few-femtosecond timescales to manipulate the valley pseudospin rotation, we explore the possibility to follow the state changes via attosecond transient absorption spectroscopy (ATAS). The recent generation of attosecond (10^{-18} s) pulses [30] allowed us to perform ultrafast (pump-probe) experiments to track dynamics at the ultimate speed of electron motion. ATAS has been successfully applied to track exciton dynamics [31,32], and it is sensitive to the coherent laser-induced dynamics [33,34] and to the topological phase [35]. In this context, we provide the interpretation of the spectral features of a possible ATAS study that would enable us to retrieve the valley state changes.

In this manuscript, we focus on monolayer hBN, which enables us to simplify the system and introduce the main

concept in the context of a two-band tight-binding model, but the theory can be easily extended to TMDCs. Our theoretical results are supported by state-of-the-art real-time simulations performed with the EDUS code [36], which accounts for both light-matter and electron-electron interactions.

II. COHERENT VALLEY OSCILLATIONS

A circularly polarized laser pulse can selectively excite a valley. This is dictated by the valley-pseudospin selection rule, which is the essence for valleytronics in hBN and TMDCs [37]. For $1s$ exciton states, this selection rule is also inherited [38]. For an unstrained system, see Fig. 1(a), circularly polarized light excites a linear combination of the two degenerate $1s$ states as

$$|\psi^\pm\rangle = \frac{|1s^+\rangle \pm i|1s^-\rangle}{\sqrt{2}}, \quad (1)$$

which leads to a valley localization [39]. The $\pm$ superscript corresponds to positive/negative circular polarization. In monolayer hBN, this degeneracy is fundamental and stems from the intrinsic symmetry of the lattice itself (i.e., the D_{3h} point group). The presence of uniaxial strain breaks this symmetry, leading to the $1s$ exciton states being split and the degeneracy lifted [40,41]. When the strain is introduced, the anisotropic optical response would change the excitation from circularly polarized light, which can be expressed as a sum of the linear conductivity for linear polarization in the x and y directions (see Appendix C). We calculate the optical conductivity for unstrained and strained monolayer hBN, see Fig. 1(c), using the standard Bethe-Salpeter equation (BSE).

In the BSE, a superposition of electron-hole pairs in the reciprocal space is used as an ansatz to solve the Hamiltonian with electron-hole interactions [42–44]. We consider a two-band tight-binding model to describe the electronic structure of hBN (see more details in Appendix B), and we employ the XATU code to solve the BSE [12]. For this, we consider $N = 60$ neighboring unit cells, the hBN layer to be freely suspended, and a screening length $r_0 = 10 \text{ \AA}$. In the unstrained system, the first dominant peak in the optical conductivity around 5.4 eV corresponds to the two degenerate $1s$ excitons, which are located below the bandgap (in our case at 7.25 eV). In the strained system, the energy degeneracy of the $1s$ excitons is broken and the absorption peaks split into two. We consider strain strengths (ϵ) of 10%. The optical and electronic properties of 2D materials can be tailored to a large extent via external mechanical deformation. While bulk crystalline materials can rarely sustain mechanical strains beyond 1% without breaking, 2D crystals can withstand extreme deformations, reaching strain limits of up to 25% for graphene, 20% for hBN, and 11% for MoS₂, to name a few [45]. Furthermore, the orientation of the uniaxial strain (θ_s) also offers an additional knob to split the $1s$ exciton peaks [13,14]. We observe in Fig. 1(c) how the zigzag ($\theta_s = \pi/2$) strain provides a larger energy splitting than the one induced by the armchair ($\theta_s = 0$) strain. It is worth noting that both armchair and zigzag strain directions lift the energy degeneracy (see Fig. 7), thereby enabling valley rotation, unlike other schemes based on external electrostatic potentials [46].

It seems reasonable to use an ultrashort (broad bandwidth) pulse to excite both $1s$ states and produce a superposition as in Eq. (1). However, due to the lifted degeneracy, we expect the time evolution of the superposition to be

$$\hat{U}(t)|\psi^\pm\rangle \propto \hat{U}(t)[|1s^+\rangle \pm i|1s^-\rangle] = e^{-iE_+t/\hbar}[|1s^+\rangle \pm ie^{i\Delta E_X t/\hbar}|1s^-\rangle], \quad (2)$$

where $\Delta E_X = E_+ - E_-$ is the energy splitting between the eigenvalues of the states $|1s^{+/-}\rangle$ [see Fig. 7(c)]. While the global $e^{-iE_+t/\hbar}$ factor simply introduces a global phase to the state as it evolves in time, the $e^{i\Delta E_X t/\hbar}$ factor multiplying $|1s^-\rangle$ gives rise to the rotation of the valley state, which is represented by a rotation around the z axis in the Bloch sphere of Fig. 1(b). The presence of this complex exponential means that the phase of the $|1s^-\rangle$ state changes in time and, more specifically, after a time

$$\tau = \frac{\pi \hbar}{\Delta E_X}, \quad (3)$$

the state $|\psi^\pm\rangle$ evolves to

$$\hat{U}(\tau)|\psi^\pm\rangle = e^{-i\frac{E_+}{\Delta E_X}\pi}|\psi^\mp\rangle. \quad (4)$$

Hence, the time τ defines a “valley migration time” between two states $|\psi^{+/-}\rangle$, mostly localized in the K/K' valleys, respectively. The dependence of this valley migration time between the two states $|\psi^{+/-}\rangle$ on the strain configuration is showcased in Fig. 7(d). In order to prove the strain-tunable valley rotation, we perform real-time simulations in strained hBN with the EDUS code [33–36], which consists in evolving the one-electron reduced density matrix $\rho_{ij}(\mathbf{k})$ in the reciprocal space. We consider a circularly polarized pulse with

photon frequency centered at $E_{\text{avg}} = (E_+ + E_-)/2$ between the two $1s$ exciton peaks in order to produce the $|\psi^\pm\rangle$ state given by Eq. (1). The pulse must be short enough to excite both $1s$ exciton peaks. For a strain strength $\epsilon = 0.1$, the pulse has a total time duration of approximately 12 fs (more details about the pump pulse parameters are presented in Appendix D). The evolution of the exciton wave function given by the $\rho_{cv}(\mathbf{k})$ term, where the index c (v) stands for the conduction (valence) band, is represented in Fig. 2. We observe the valley rotation for the zigzag and armchair strain directions. The panels in each row are plotted at specific time steps $\delta t = n\frac{\tau}{4}$, with the peak localized in the K valley moving from left to right, transitioning into a K' peak at $t = \tau$. Furthermore, these plots also clearly showcase the effects of the deformation of the Brillouin zone on the valley migration. The valley migration time τ is approximately 12.5 fs for $\epsilon = 0.1$. This demonstrates the control of quantum rotations at the attosecond timescale by using uniaxial strain.

III. ATTOSECOND SPECTROSCOPY

The exciton quantum state oscillation between valleys relies on coherence, and therefore, it should be observed before the dynamics couples to other degrees of freedom. Current technology permits the tracking of exciton dynamics on the attosecond scale via transient absorption or reflectivity spectroscopy [31,32]. To simulate an attosecond experiment with the EDUS code, we need to model a pump-probe scheme [47,48]. The first pump pulse excites the material and induces the above-mentioned exciton oscillation, while a second probe pulse is absorbed in a later stage, with a certain time delay that is controlled. The probe pulse has photon energies around 410 eV in order to excite core transitions from the N $1s$ orbital band to the valence or conduction band. We note that ultrafast experiments can be currently performed using those photon energies in thin materials [48]. The probe pulse is short enough to have a bandwidth to cover the whole valence and conduction bands in our hBN model. We include therefore the N $1s$ orbital band in our tight-binding model, as in Ref. [34]. For the simulations, we consider a range of time delays $\Delta\tau_d \in [0, 28 \text{ fs}]$ after the pump pulse.

The pump-probe signal is strong when the probe excites core electrons into the valence holes produced by the pump pulse; see scheme in Fig. 3(a). For that particular energy window, we observe strong oscillations in the absorption with respect to the time delay; see Fig. 3(b). The energy scale refers to the energy from the N $1s$ band to the Fermi level, i.e., $E_{\text{ch}} = 409.9 \text{ eV}$, and the intensity is normalized with respect to the maximum peak, which corresponds to the core-to-conduction excitation. From the way the exciton superposition is created following Eq. (2), at least two distinct periodicities are found in the pump-probe absorption signal; see further details in Appendix D. One slow oscillation associated with the valley migration, $T_\tau = \frac{2\pi\hbar}{\Delta E_X} \approx 12.5 \text{ fs}$, and one fast oscillation associated with the global phase of the wave function at the instant of the probe arrival, $T_{\tau+} = \frac{2\pi\hbar}{E_+} \approx 0.8 \text{ fs}$. The fast oscillations are clearly observed in Fig. 3(b) by taking snapshots with small steps of time delays. By filtering out the fast oscillations, the remaining signal shows the period of the exciton valley oscillations; see Fig. 3(c) in which the intensity of the peak

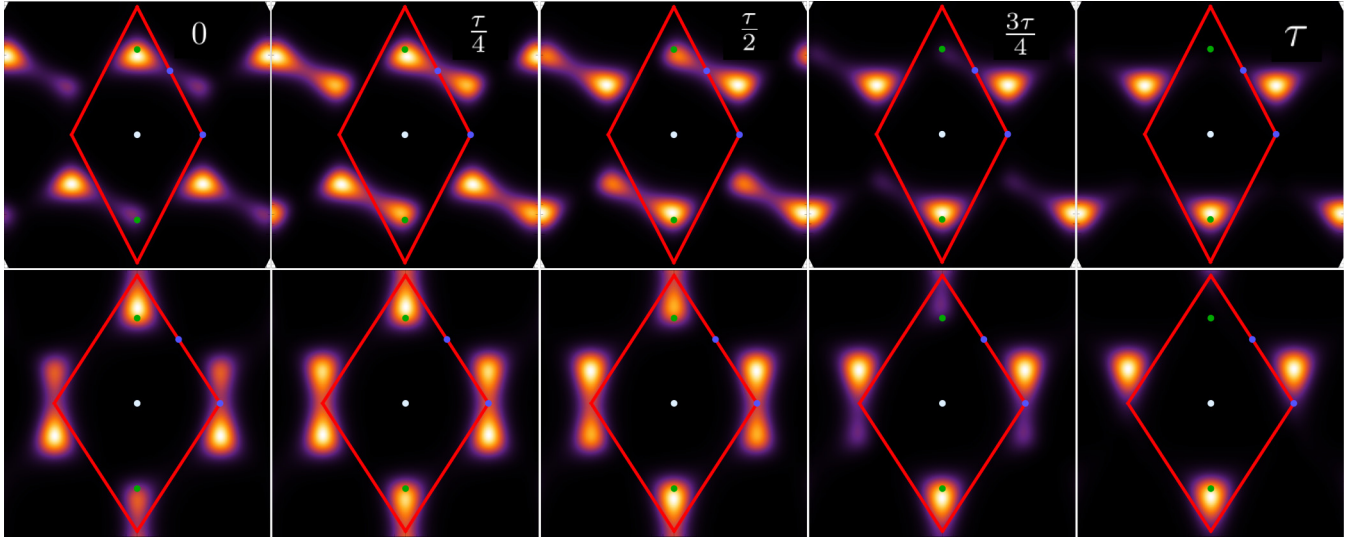


FIG. 2. Time evolution (left to right) of the exciton wave function $\rho_{cv}(\mathbf{k})$, from $t \approx t_f$ to $t \approx t_f + \tau$, right after excitation under $\epsilon = 0.1$ strain, computed via EDUS [36]. Top row: armchair ($\theta_s = 0$) strain. Bottom row: zigzag ($\theta_s = \pi/2$) strain. The fifth panel in each row corresponds to $t \approx t_f + \tau$, where the $|\psi^+\rangle$ state has fully transitioned into the $|\psi^-\rangle$ state. Red outline denotes the first Brillouin zone, with points green, white, and blue representing the $\mathbf{K}/\mathbf{K}'$, Γ , and $\mathbf{M}/\mathbf{M}'$ points, respectively.

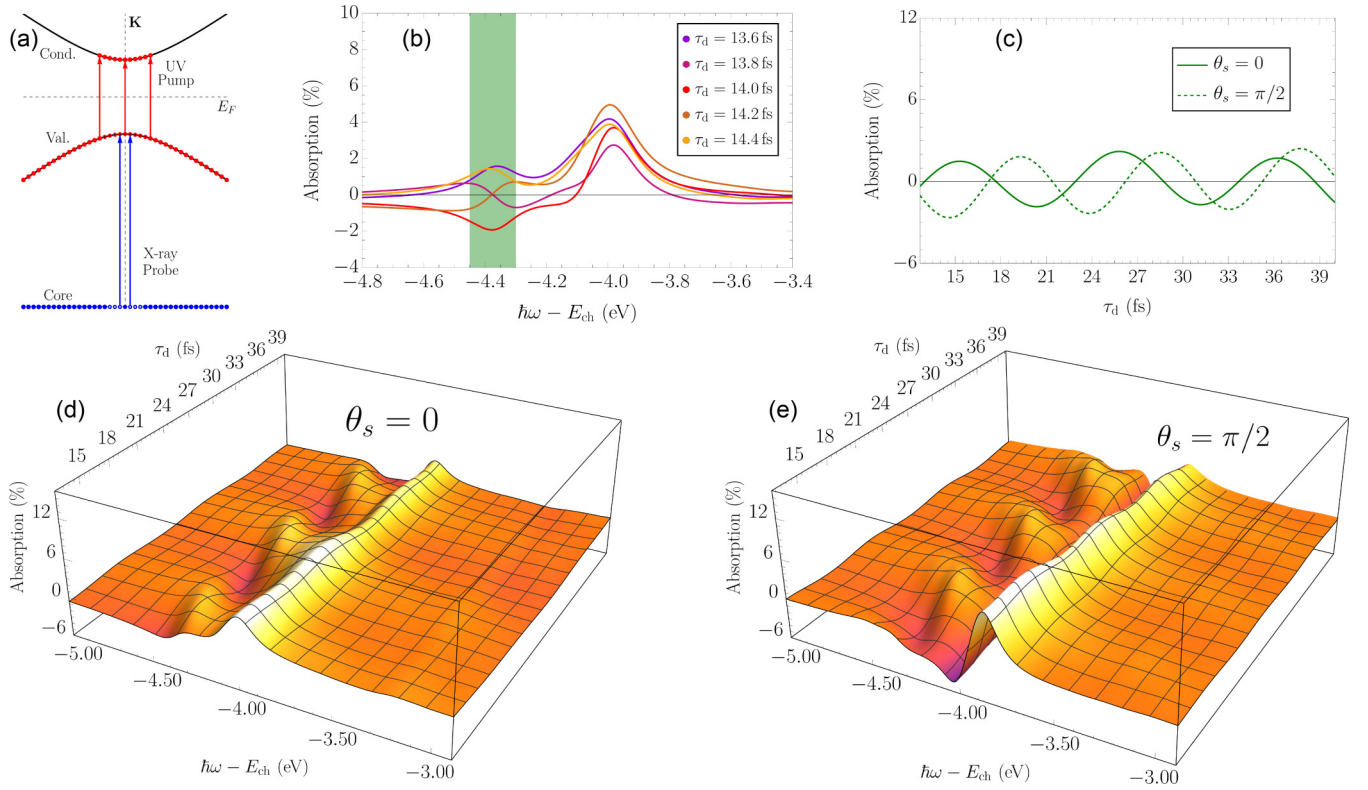


FIG. 3. (a) Illustration of the relevant transitions involved in the pump-probe signal. (b) Transient absorption spectrum in the energy range corresponding to transitions from core to valence states. Fast oscillations are observed with a period $T_{\tau_+} \approx 0.8$ fs, consistent with the probe pulse capturing the global phase of an exciton coherent state. Data for hBN strained along the armchair direction ($\epsilon = 0.1$, $\theta_s = 0$). (c) Oscillations in time delay τ_d for the peaks in the absorption spectra (highlighted in green) in panels (b), (d), and (e) for both armchair (solid lines) and zigzag (dashed lines) strain directions. (d), (e) Transient absorption spectrum in hBN strained along the armchair ($\epsilon = 0.1$, $\theta_s = 0$) and zigzag ($\epsilon = 0.1$, $\theta_s = \pi/2$) directions, respectively.

around -4.4 eV is represented as a function of the time delay. We show the whole transient absorption spectrum in Figs. 3(d) and 3(e) for armchair and zigzag strains, respectively. The numerical simulations show the sensitivity of ATAS to follow the valence holes at the N site during the valley state rotation.

IV. CONCLUSIONS

In conclusion, we propose a scheme to manipulate the valley pseudospin via uniaxial strain. This is supported by numerical real-time simulations in hBN, which show a perfect valley rotation whose speed is determined by the energy split of the $1s$ excitons, which depends on both the strength and the orientation of the strain. Furthermore, we also demonstrate the feasibility to characterize the valley rotation by using attosecond absorption spectroscopy. It is worth noting that, while here we focused our discussion on hBN, our approach can be easily extended to a wide variety of 2D materials such as mono- and bilayer TMDCs, as well as other materials where a fundamental degeneracy can be broken via the discussed uniaxial strain. This work opens strategies to harness energy-efficient schemes for valleytronics based on mechanical distortions of the crystal, which can be combined with stacking schemes to increase the valley coherence time [27]. Additionally, further investigations in dynamic strain or in magnetic materials may enrich our implementation of manipulating valley degrees of freedom [18,49].

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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: LATTICE STRUCTURE OF hBN

To study the effect of deformation on excitons in hBN, we first study the effects on the unit cell, the vectors joining nearest neighbors, and the Bravais vectors. The vectors δ_i are defined as

$$\delta_1 = a_0 \begin{bmatrix} 1 \\ 0 \end{bmatrix}, \quad \delta_2 = a_0 \begin{bmatrix} -\frac{1}{2} \\ \frac{\sqrt{3}}{2} \end{bmatrix}, \quad \delta_3 = a_0 \begin{bmatrix} -\frac{1}{2} \\ -\frac{\sqrt{3}}{2} \end{bmatrix},$$

with the unit cell being aligned with δ_1 , and the Bravais vectors read

$$\mathbf{a}_1 = \delta_1 - \delta_3 = a_0 \begin{bmatrix} \frac{3}{2} \\ \frac{\sqrt{3}}{2} \end{bmatrix}, \quad \mathbf{a}_2 = \delta_1 - \delta_2 = a_0 \begin{bmatrix} \frac{3}{2} \\ -\frac{\sqrt{3}}{2} \end{bmatrix}.$$

This lattice structure is then portrayed in Fig. 1(a). As zigzag strain is not parallel to any of the three δ_i vectors defined above, its effects will be qualitatively distinct from armchair strain. This thus leads to a qualitatively distinct evolution of the hopping parameters when compared to armchair strain.

Knowing the Bravais vectors, the primitive vectors in reciprocal space read

$$\mathbf{b}_1 = \frac{2\pi}{\sqrt{3}a_0} \begin{bmatrix} \frac{1}{\sqrt{3}} \\ 1 \end{bmatrix}, \quad \mathbf{b}_2 = \frac{2\pi}{\sqrt{3}a_0} \begin{bmatrix} \frac{1}{\sqrt{3}} \\ -1 \end{bmatrix},$$

which means that the high-symmetry Dirac points are given by

$$\mathbf{K} = \frac{\mathbf{b}_1 - \mathbf{b}_2}{3} = \frac{4\pi}{3\sqrt{3}a_0} \begin{bmatrix} 0 \\ 1 \end{bmatrix},$$

$$\mathbf{K}' = \frac{\mathbf{b}_2 - \mathbf{b}_1}{3} = \frac{4\pi}{3\sqrt{3}a_0} \begin{bmatrix} 0 \\ -1 \end{bmatrix}.$$

APPENDIX B: STRAINED DIRAC POINTS

To introduce strain in the hBN lattice, we must first define how uniaxial deformation transforms generic two-dimensional vectors. From the generalized Hooke's law [50], the strain tensor for uniaxial deformation in the lattice coordinate system reads [12,51]

$$\epsilon = \epsilon \begin{bmatrix} \cos^2 \theta_s - \sigma \sin^2 \theta_s & (1 + \sigma) \cos \theta_s \sin \theta_s \\ (1 + \sigma) \cos \theta_s \sin \theta_s & \sin^2 \theta_s - \sigma \cos^2 \theta_s \end{bmatrix}, \quad (\text{B1})$$

where θ_s is the direction of the strain, measured (without loss of generality) from the x axis, ϵ is the strain strength, and $\sigma = 0.211$ is the Poisson ratio in hBN [52–54], meaning a generic

vector $\begin{bmatrix} x \\ y \end{bmatrix}$ will transform as

$$\begin{bmatrix} x \\ y \end{bmatrix} \rightarrow (\mathbb{1} + \epsilon) \cdot \begin{bmatrix} x \\ y \end{bmatrix} \rightarrow \begin{bmatrix} x(1 + \epsilon)(\cos^2 \theta_s - \sigma \sin^2 \theta_s) + y\epsilon(1 + \sigma) \cos \theta_s \sin \theta_s \\ x\epsilon(1 + \sigma) \cos \theta_s \sin \theta_s + y(1 + \epsilon)(\sin^2 \theta_s - \sigma \cos^2 \theta_s) \end{bmatrix}, \quad (\text{B2})$$

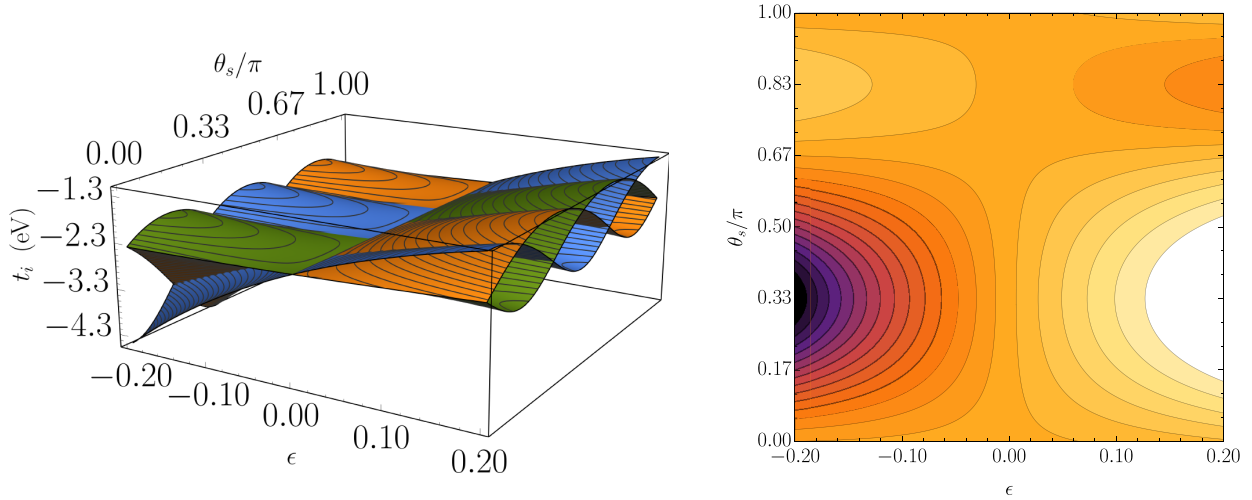


FIG. 4. (Left) Hopping parameter along δ_1 (orange curve), δ_2 (blue curve), and δ_3 (green curve) as a function of strain strength ϵ and strain direction θ_s . (Right) Detailed view of hopping parameter along δ_1 presented as a contour plot, corresponding to a top-down view of the left panel.

where $\mathbb{1}$ is the 2×2 identity matrix. While the strain effects on the lattice vectors lead to rather unwieldy expressions due to the many cross terms present in Eq. (B1), the strained Dirac points $\mathbf{K}/\mathbf{K}'$ can be simply written as

$$\tilde{\mathbf{K}} = \frac{2\pi}{3\sqrt{3}a_0} \begin{bmatrix} -\frac{\epsilon(1+\sigma)\sin 2\theta_s}{(1+\epsilon)(1-\epsilon\sigma)} \\ \frac{2+\epsilon(1-\sigma)+\epsilon(1+\sigma)\cos 2\theta_s}{(1+\epsilon)(1-\epsilon\sigma)} \end{bmatrix},$$

$$\tilde{\mathbf{K}}' = \frac{2\pi}{3\sqrt{3}a_0} \begin{bmatrix} \frac{\epsilon(1+\sigma)\sin 2\theta_s}{(1+\epsilon)(1-\epsilon\sigma)} \\ -\frac{2+\epsilon(1-\sigma)+\epsilon(1+\sigma)\cos 2\theta_s}{(1+\epsilon)(1-\epsilon\sigma)} \end{bmatrix}.$$

Under strain, and identifying hoppings along the vectors δ_i as γ_i , the hopping parameters change as

$$\gamma_{mn} = \gamma_0 e^{-3.37(\frac{a}{a_0}-1)}, \quad (\text{B3})$$

where $\gamma_0 = 2.3$ eV is the hopping integral for the undeformed lattice, a_0 is the lattice parameter for the undeformed lattice, and a is the interatomic distance after deformation, as discussed previously. The decay rate 3.37 is extracted from experimental results and is chosen so that the nearest-neighbor hopping would have the value

$$\gamma'_{mn} = \gamma_0 e^{-3.37(\frac{\sqrt{3}a_0}{a}-1)} = 0.23 \text{ eV}, \quad (\text{B4})$$

matching existing estimates of this hopping in graphene and similar materials [51,55,56]. Careful inspection also reveals that the hopping parameters for bonds along two of the three different δ_i directions match when $\theta_s = n'\frac{\pi}{6}$, in accordance with what would be expected from the lattice symmetry. More concretely, strain at $\theta_s = n'\frac{\pi}{6}$ is either:

(1) parallel to a bond δ_i (armchair strain), and will occur for even $n = 2n'$ (i.e., $\theta_s = 2n'\frac{\pi}{6}$), or

(2) perpendicular to a bond δ_i (zigzag strain), and will occur for odd $n = 2n' + 1$ (i.e., $\theta_s = (2n' + 1)\frac{\pi}{6}$).

In both cases, one bond δ_i will be subjected to a specific transformation while the other two bonds $\delta_{j/k}$ will undergo a different transformation (but identical among themselves). These two distinct strains are portrayed via the blue (armchair

strain) and red (zigzag strain) lines in Fig. 1(b). This is clearly visible in the left panel of Fig. 4, where the three distinct hoppings are plotted as a function of both strain intensity and strain direction. Taking both these periodicities together, one can also see that the deformation effects will be periodic at intervals $\theta_s = n'\frac{\pi}{3}$, as expected from the rotational symmetry of the honeycomb lattice.

Finally, the band structure and Brillouin zone themselves will also change, both from the changing Bravais vectors and from the changing hoppings in each direction. The band structure of hBN reads [51,57,58]

$$E(\mathbf{k}) = \pm \sqrt{\frac{E_g^2}{4} + |\gamma_1 + \gamma_3 e^{-i\mathbf{k}\cdot\mathbf{a}_1} + \gamma_2 e^{-i\mathbf{k}\cdot\mathbf{a}_2}|^2}.$$

Introducing strain, and as discussed previously, we now obtain

$$E'(\mathbf{k}) = \pm \sqrt{\frac{E_g^2}{4} + |\tilde{\gamma}_1 + \tilde{\gamma}_3 e^{-i\mathbf{k}\cdot\tilde{\mathbf{a}}_1} + \tilde{\gamma}_2 e^{-i\mathbf{k}\cdot\tilde{\mathbf{a}}_2}|^2},$$

where $\tilde{Z}$ indicates that the object Z will change under strain following the relations outlined in Eqs. (B2) and (B3). As both the hopping integrals and the Bravais vectors will change under strain, the band structure will evolve in a nontrivial way, as portrayed in Fig. 5 for distinct strain strengths and directions. The absence of collinearity between the strain axis of zigzag and any of the three δ_i vectors leads to a qualitatively distinct evolution of the hopping parameters when compared to armchair strain. This is especially clear when one analyzes the band structure at the $\mathbf{M}$ saddle points connecting the two Dirac points $\mathbf{K}/\mathbf{K}'$, where the bands become much flatter for zigzag strain when compared to the unstrained system, to the armchair strained system, or even to hybrid strain (not zigzag nor armchair). This important distinction implies distinct physics depending on the strain direction, leading to different evolution of the exciton binding energies for the distinct strain configurations, as will be discussed in the following Appendix. Additionally, the obtained band structure

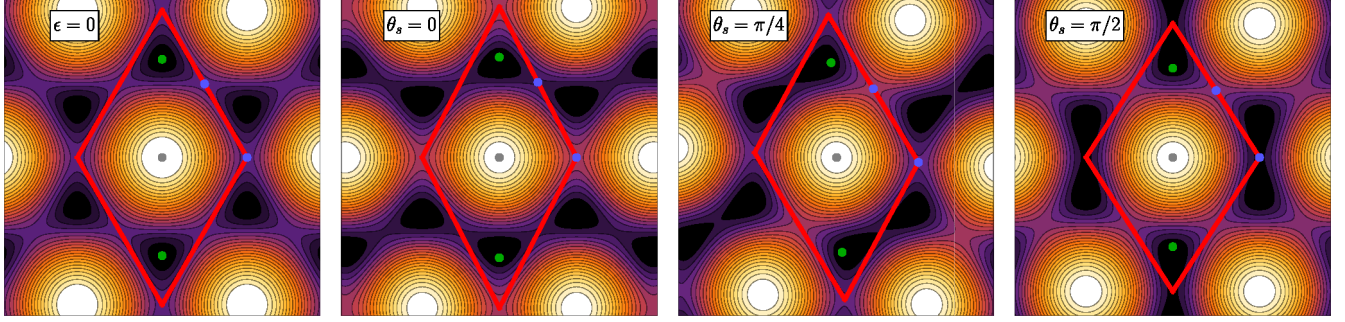


FIG. 5. Contour plot of conduction band of hBN for strain configurations (left to right) $[\epsilon, \theta_s] = [0, 0]$, $[\epsilon, \theta_s] = [0.1, 0]$, $[\epsilon, \theta_s] = [0.1, \pi/4]$, and $[\epsilon, \theta_s] = [0.1, \pi/2]$. Important points in the first Brillouin zone (edges marked by red lines) are highlighted: $\mathbf{K}/\mathbf{K}'$ (green top/bottom, respectively), $\mathbf{M}$ (blue), and $\mathbf{\Gamma}$ (gray).

qualitatively matches against previous results in the literature for strained graphene, where a similar flattening of the bands was also observed [51].

APPENDIX C: EXCITONIC CONDUCTIVITY

The generic component of the linear conductivity is given by [59–61]

$$\frac{\sigma_{\alpha\beta}(\omega)}{\sigma_0} = \frac{-i}{2\pi^3} \sum_n \left[\frac{E_n X_{0n}^\alpha X_{n0}^\beta}{E_n - \hbar\omega} - (\omega \rightarrow -\omega)^* \right], \quad (\text{C1})$$

where $\sigma_0 = \frac{e^2}{4\hbar}$, an imaginary broadening is introduced via the transformation $\hbar\omega \rightarrow \hbar\omega + i\Gamma$, and the generic exciton dipole matrix element reads [59–61]

$$X_{0n}^\alpha = i \frac{\hbar}{m_0} \int \psi_{cv\mathbf{k}}^{(n)} \frac{p_{v\mathbf{k}}^\alpha}{E_{c\mathbf{k}} - E_{v\mathbf{k}}} d^2\mathbf{k}, \quad (\text{C2})$$

where α/β represent Cartesian directions, ω is the frequency of the incident field, E_n is the energy of the excitonic state n , $p_{v\mathbf{k}}^\alpha$ is the interband momentum matrix element in the α direction, m_0 is the bare electron mass, and $\psi_{cv\mathbf{k}}^{(n)}$ is the $\mathbf{k}$ -space exciton wave function for the state n , obtained by solving Bethe-Salpeter equation for the considered system.

The interband momentum matrix elements for circularly polarized light can be written as a superposition of the matrix elements for linearly polarized light [60–62],

$$\begin{aligned} p_{v\mathbf{k}}^\pm &= \frac{p_{v\mathbf{k}}^x \pm ip_{v\mathbf{k}}^y}{\sqrt{2}} \\ &= \frac{1}{\sqrt{2}} \langle v, \mathbf{k} | \frac{m_0}{\hbar} \left[\frac{\partial \mathcal{H}(\mathbf{k})}{\partial k_x} \pm i \frac{\partial \mathcal{H}(\mathbf{k})}{\partial k_y} \right] | c, \mathbf{k} \rangle, \end{aligned} \quad (\text{C3})$$

where $\mathcal{H}$ is the tight-binding Hamiltonian and m_0 is the free-electron mass. This interband momentum matrix element includes both $p_{v\mathbf{k}}^x$ and $p_{v\mathbf{k}}^y$ components, where the $\pm$ sign defines left-handed (positive) and right-handed (negative) circularly polarized light [63].

Reidentifying the left- and right-handed polarization directions with the $\pm$ sign, we can write the linear conductivity for circularly polarized light as

$$\frac{\sigma_\pm(\omega)}{\sigma_0} = \frac{-i\hbar^2}{2\pi^3 m_0^2} \sum_n \frac{E_n |X_{0n}^\pm|^2}{E_n - \hbar\omega}.$$

Directly substituting $p_{v\mathbf{k}}^\pm$ from Eq. (C3) and separating the two terms, we have

$$X_{0n}^\pm = i \int \psi_{cv\mathbf{k}}^{(n)} \frac{p_{v\mathbf{k}}^\pm}{E_{c\mathbf{k}} - E_{v\mathbf{k}}} d^2\mathbf{k} = \frac{1}{\sqrt{2}} [X_{0n}^x \pm iX_{0n}^y], \quad (\text{C4})$$

and then the linear conductivity for circular polarization is related to the linear polarization one by

$$\sigma_\pm(\omega) = \frac{\sigma_{xx}(\omega)}{2} + \frac{\sigma_{yy}(\omega)}{2} \pm \frac{i}{2} [\sigma_{yx}(\omega) - \sigma_{xy}(\omega)]. \quad (\text{C5})$$

Hence, we can compute the linear conductivity for circularly polarized light knowing only the various components from the optical response to linearly polarized light, having only to apply the Kramers-Kronig relations [64–68] to obtain the imaginary part of the off-diagonal components from their real part. Furthermore, the lattice symmetry of hBN in the nearest-neighbor tight-binding approach results in $\sigma_{yx}(\omega) = \sigma_{xy}(\omega)$, meaning that the linear conductivity for both circular polarization directions is equivalent. The strain effects on the linear conductivity are showcased in Fig. 6, where the different preferential polarization directions for each exciton are clearly visible [13,14].

APPENDIX D: REAL-TIME SIMULATIONS

We use the EDUS code [36] to compute the laser-driven dynamics in hBN. The numerical approach considers the light-matter and exciton interactions on the time domain. The approach evolves the one-electron reduced density matrix in reciprocal space. We use a grid of 200×200 points and periodic boundary conditions, modeling the electron-hole interaction via the Rytova-Kelysh potential with a screening length $r_0 = 10 \text{ \AA}$ and average medium dielectric constant $\epsilon_r = 1$. The laser pump pulse that induces the exciton migration is modeled in time with a $\sin^2$ envelope as

$$\begin{aligned} E(t) &= E_0 \sin(\omega(t - t_0)) \sin^2 \left(\pi \frac{t - t_0}{t_f - t_0} \right) \\ &= E_0 \sin(\omega t) \sin^2 \left(\pi \frac{t}{t_f} \right), \end{aligned} \quad (\text{D1})$$

where t_0 is the beginning of the pulse, set at $t_0 = 0$, $t_f = n_{\text{cycles}} \frac{2\pi\hbar}{E_{\text{avg}}}$ is the duration of the pulse, ω is the photon

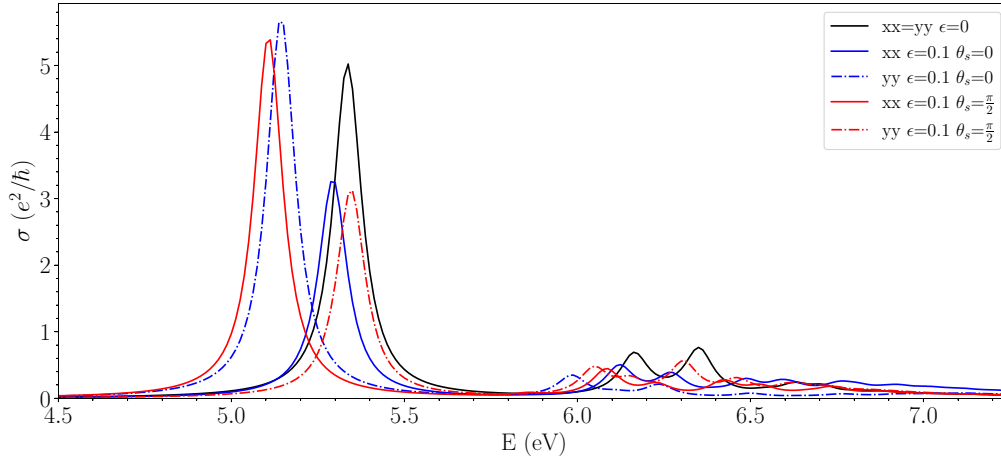


FIG. 6. Diagonal components of excitonic linear conductivity for an unstrained system (solid lines), and $\epsilon = 0.1$ strain along $\theta_s = 0$ (armchair, dashed lines) and along $\theta_s = \pi/2$ (zigzag, dot-dashed lines).

frequency, and considering time steps of $dt = 0.00024$ fs in the time simulation up to a final time of $T_f = 150$ fs. The photon frequency is centered between the two $1s$ excitons peaks at the energy $\omega = E_{\text{avg}}/\hbar$ in order to excite both of them. The specific duration will depend on the average energy of the two $1s$ states as $T = n_{\text{cycles}} \frac{2\pi\hbar}{E_{\text{avg}}}$, where $n_{\text{cycles}} = 16$ is the number of cycles of the pulse, meaning the full duration of the pulse will be approximately $T \approx 12.5$ fs for the considered exciton states. The pulse intensity is set at $E_0 = 10^8$ W cm $^{-2}$. In order to induce a superposition between the two nondegenerate $1s$ excitonic states, the pulse is left-handed circularly polarized.

For studying the core excitons, we also require a probe pulse. This laser pulse is modeled in time with a Gaussian envelope as

$$E(t) = E_0 \sin(\omega'(t - \tau_d)) e^{-\frac{(t - \tau_d)^2}{2\sigma^2}}, \quad (\text{D2})$$

where τ_d and σ are the maximum and variance of the Gaussian envelope, respectively, and ω' is the photon frequency necessary to reach the core $1s$ orbital of nitrogen ($\hbar\omega' \approx 409.9$ eV) [34,69,70]. To capture different time steps in the exciton migration, the maximum of the Gaussian envelope is delayed by different intervals $\tau_d = \Delta\tau_d + T$, where T is the duration of the $\sin^2$ pump pulse as defined previously and $\Delta\tau_d$ is the delay between the two pulses.

By the arrival of the probe pulse, the exciton state that is being probed is then given by

$$|\psi(\tau_d)\rangle = e^{-i\frac{E_+ \tau_d}{\hbar}} [|1s^+\rangle + ie^{i\frac{\Delta E_X \tau_d}{\hbar}} |1s^-\rangle]. \quad (\text{D3})$$

The high-energy probe pulse then excites a core electron into a valence-band hole, which is left behind by the pump-pulse interaction. Under the assumption of the sudden excitation, we expect the core exciton state to have the following form after

the probe pulse:

$$\begin{aligned} |\psi_{\text{ce}}(t')\rangle &= \sum_{\mathbf{k}} B_{\mathbf{k}} c_{v\mathbf{k}}^\dagger c_{\text{co},\mathbf{k}} |\psi(\tau_d)\rangle \\ &= e^{-i\frac{E_+ \tau_d}{\hbar}} \sum_{\mathbf{k}} B_{\mathbf{k}} [c_{v\mathbf{k}}^\dagger c_{\text{co},\mathbf{k}} |1s^+\rangle + ie^{i\frac{\Delta E_X \tau_d}{\hbar}} c_{v\mathbf{k}}^\dagger c_{\text{co},\mathbf{k}} |1s^-\rangle], \end{aligned} \quad (\text{D4})$$

where $c_{\text{co},\mathbf{k}}$ is the core annihilation operator. Core excitons are, therefore, defined over an effective ground state, which is the existing exciton, instead of the Fermi sea from which the initial exciton is defined. The coefficients $B_{\mathbf{k}}$ would be determined variationally as with regular excitons, and this would have to be done at each time t' .

Two distinct oscillations as a function of the pulse delay τ_d are then present: First, the exciton migration that evolves as $e^{i\frac{\Delta E_X \tau_d}{\hbar}}$; second, the global phase of the excitonic state created by the pump pulse will go as $e^{-i\frac{E_+ \tau_d}{\hbar}}$. Those oscillations lead to distinct periods as a function of the time delay, namely,

$$T_\tau = \frac{2\pi\hbar}{\Delta E_X}, \quad T_{\tau_+} = \frac{2\pi\hbar}{E_+}. \quad (\text{D5})$$

The global phase gives rise to changes in the absorption line shape [33,47,71] with quite a fast period. While T_τ will be on the order of 10 fs for the considered strains (see Fig. 7), the much larger value of $E_+ \approx 5.5$ eV corresponds to $T_{\tau_+} \approx 0.79$ fs. Such oscillations are presented in Fig. 3(b) by considering small steps in τ_d , and these are filtered from panels (c) through (e) of Fig. 3 by considering steps in τ_d that are multiples of T_{τ_+} .

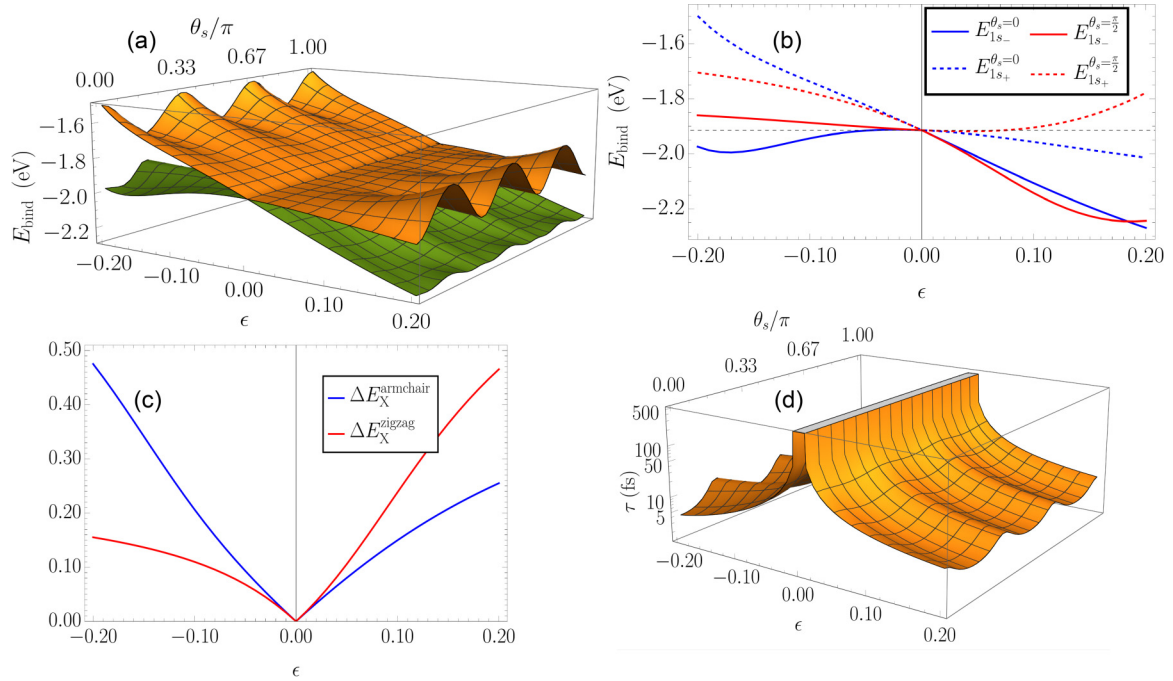


FIG. 7. (a) Binding energy of the 1s exciton states as a function of strain intensity ϵ and strain direction θ_s , as obtained through XATU [12]. (b) Side view of panel (a) along $\theta_s = 0$ and $\theta_s = \pi/2$, corresponding to armchair and zigzag strains, respectively. (c) Splitting of the 1s exciton states as a function of strain intensity ϵ for both armchair and zigzag strains. (d) Valley migration time as a function of strain intensity ϵ and direction θ_s .

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