Topologically localized excitons in single graphene nanoribbons

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Intrinsic optoelectronic properties of atomically precise graphene nanoribbons (GNRs) remain largely unexplored because of luminescence quenching effects that are due to the metallic substrate on which the ribbons are grown. We probed excitonic emission from GNRs synthesized on a metal surface with atomic-scale spatial resolution. A scanning tunneling microscope (STM)–based method to transfer the GNRs to a partially insulating surface was used to prevent luminescence quenching of the ribbons. STM-induced fluorescence spectra reveal emission from localized dark excitons that are associated with the topological end states of the GNRs. A low-frequency vibronic emission comb is observed and attributed to longitudinal acoustic modes that are confined to a finite box. Our study provides a path to investigate the interplay between excitons, vibrons, and topology in graphene nanostructures.

Since their first on-surface synthesis (1), atomically precise graphene nanoribbons (GNRs) have attracted tremendous interest in the nanoscience and technology communities for their topology-related physical properties (2–6). Indeed, their specific edge conformations host peculiar electronic states that in turn lead to unconventional transport or magnetic properties (7–12). In addition, their optical properties hold great promise for realizing robust and controllable atomically thin optoelectronic devices (13). Indeed, GNRs combine many of the outstanding characteristics of graphene with an electronic gap, which is a necessary property for many applications, including light-emitting devices. Whereas theoretical studies discuss in detail how the optical properties of GNRs may be advantageously controlled through atomic-scale variations of their width, length, and edge shapes (14–21), experiments reporting on the excitonic properties of GNRs are scarce (22–27), especially those that focus on fluorescence of on-surface grown GNRs. These experiments either are limited to ensemble averaging measurements where the light emission is dominated by the response of defects (28–30) or focus on individual GNRs in direct contact with metallic electrodes that alter the GNR excitonic properties (31). Indeed, because the synthesis of these GNRs is performed directly on metallic surfaces, which in turn causes luminescence quenching, the intrinsic emission properties of atomically precise GNRs remain almost unexplored territory.

Here, we build on a strategy that involves using a scanning tunneling microscope (STM) tip to transfer individual seven-atom-wide armchair edge GNRs (7-AGNRs) from the bare part of a Au(111) surface to a neighboring thin insulating NaCl layer (32). Using STM-induced luminescence (STML), we then address the fluorescence properties of single GNRs that are isolated from any contact with metallic electrodes. Our STML data reveal a sharp emission line at an energy that is lower than the excitonic emission expected for an infinitely long ribbon and that is traced back to dark excitons that involve topological states localized at the GNR termini. This emission line is accompanied by a rich and complex vibronic emission spectrum.

Luminescence from decoupled GNRs

Recent STML works have demonstrated that the fluorescence properties of individual organic molecules can be excited when they are sufficiently decoupled from a metallic substrate (33–38). A common strategy consists of evaporating the molecule on a thin insulating layer of oxide or salt that is adsorbed on a metal surface. This efficient approach is, however, not suited to long organic structures such as GNRs whose synthesis requires a catalytic reaction step at the surface of metallic substrates (39). In Fig. 1, we detail our method to measure the luminescence properties of single GNRs with subnanometer-scale precision. We first follow the usual on-surface synthesis approach (Fig. 1A) to form seven-atom-wide and m-atom-long AGNRs ([7, m]AGNRs) on a Au(111) surface from a 10,10-dibromo-9,9'-bithiophene (DBBA) precursor (I) and subsequently evaporate NaCl so as to form three-monolayer-thick (3ML) NaCl islands on Au(111) [see section I of (40)]. An STM image of the substrate after such a preparation (Fig. 1B) shows a clean NaCl island (bottom left) and several [7, m]AGNRs of different lengths and orientations located on the bare gold area. In Fig. 1C, we schematically explain how the tip of the STM is used to transfer a [7, m]AGNR adsorbed on the gold surface onto a NaCl cluster (32) [see section II of (40) for details]: (i) The tip approaches a [7, m]AGNR extremity until contact is reached. A weak bond between the last tip atom and the reactive ribbon terminus allows the ribbon to be lifted by retracting the tip by a few nanometers. (ii) The tip is then laterally displaced on top of a NaCl cluster where (iii) the ribbon is released by applying a voltage pulse of 3.5 V amplitude and 30-ms width. Figure 1D shows an STM image of a [7, 28]AGNR that was deposited on 3ML NaCl using this method. No modification of the ribbon can be observed in this image (41), indicating that the procedure does not affect the structure of the GNR.

In Fig. 1E, we display an STML spectrum that was acquired for the STM tip located at the position marked by a black dot in Fig. 1D. This spectrum reveals an intense and complex signal composed of sharp lines of an excitonic nature that are absent for ribbons directly adsorbed on Au(111) [see section III of (40) for details]. This attests to the success of our decoupling procedure. In this STML spectrum, one first identifies an intense 0-0 line at ±1.45 eV (855 nm), with a sub-meV spectral width (Fig. 1F), followed by several features of weaker intensities assigned to vibronic emission. Whereas the vibronic peaks at high energy (~1000 cm⁻¹) are reminiscent of Raman-like patterns that are frequently observed in STML spectra (33, 36, 42, 43), the series of equally spaced peaks at low energy (~500 cm⁻¹) is unusual; we discuss this later. The energy of the 0-0 line (hv = 1.45 eV, where h is Planck’s constant and v is frequency) is intriguingly low, because the lowest excitonic transition is expected at ±2 eV for a [7, m]AGNR (22). However, no fluorescence contribution is observed at energies higher than the one of the 0-0 line, irrespective of the voltage bias used (up to 2.8 V) or of the GNR length.

Influence of topological end states on optical properties

To identify the origin of the 0-0 line, we display in Fig. 2A a series of STML spectra recorded along the main axis of a decoupled [7, 24]AGNR. With the exception of a peak at 677 cm⁻¹ (discussed later), all spectral contributions fade rapidly when the tip is moved away from the ribbon terminus. A differential conductance (dIdV, where I is current and V is voltage) spectrum recorded at a GNR terminus (red spectrum in Fig. 2B) reveals electronic states at V = −0.6 and 1.9 V, which correspond to localized states of a topological nature (44) that are absent from spectra recorded at the center of the [7, 24]AGNR (blue spectrum in Fig. 2B). These topological end states result from the unsaturated electronic structure of the sp²-hybridized carbon atoms located at

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the center of the zigzag (7, 24)AGNR termini (32). The similar spatial dependencies of the optical and electronic (dI/dV) signals (i.e., intense at the GNR extremities and weak in the middle) suggest that the end states are involved in the fluorescence process. To confirm this hypothesis, we investigated the STML properties of a decoupled ribbon (Fig. 2C) that has the central carbon atom of one of its termini bonded to two hydrogen atoms (labeled as “CH2 terminus”). This configuration, which naturally occurs for a fraction of the (7, m)AGNRs synthesized on Au(111) surfaces, is known to saturate the ribbon electronic structure, leading to a sp3 hybridization of the central carbon atom and to the absence of topological state on this side (45, 46). The STML spectrum (in red) acquired at this CH2 terminus reveals broad emission resonances similar to the plasmonic emission that is measured with the same tip on top of the Au(111) substrate (in black). By contrast, the spectrum acquired at the opposite CH terminus (in blue) reveals an excitonic emission signature. All these observations indicate a prominent role of the topological end states in the fluorescence process.

To elucidate the role of these end states, we performed time-dependent density-functional theory (TDDFT) calculations of a (7, 16)AGNR whose left edge is “saturated,” as described above. Owing to the open-shell nature of the electronic structure of this half-saturated ribbon, the ground-state density is obtained from a spin-unrestricted doublet DFT calculation. We plot the corresponding frontier Kohn-Sham orbitals and their ground-state occupations for both spin channels in Fig. 2D. The three orbitals on the left are shown for the majority spin (up), and those on the right for the minority spin (down). The Kohn-Sham energies that correspond to these orbitals are schematically shown in the center. The pair of occupied orbitals (bottom) is reminiscent of the valence band of infinite GNRs; conversely, the two unoccupied orbitals (top) correspond to the GNR conduction band. The ground state and a higher-lying excited state D4 shown in the center of the ribbon in this excitation, its transition density (D0 → D4) is shown in the right side of Fig. 2E, which also demonstrates that the excitation is localized on the ribbon’s nonsaturated terminus.

Interestingly, the oscillator strength of this dark state can be activated through efficient coupling with the picocavity plasmon confined at the tip, as was suggested in previous works (34, 48) and as we further detail in section V of (40). We therefore assign this transition to the experimentally observed 0-0 peak at 1.45 eV. This assignment is also consistent with the particularly narrow width of the 0-0 line that reflects the long-lived nature of the D4 dark state. Conversely, the same spin-dependent transition channels can also interfere constructively and give rise to a bright transition between the ground state and a higher-lying excited state D4 (1.82 eV). Because of the involvement of an orbital localized close to the nonsaturated end of the ribbon in this excitation, its transition density (D0 → D4) is also localized on this terminus (right side of Fig. 2E). Other dark excitations appear in the TDDFT calculations between D1 and D4 and are discussed in section IV of (40).

Building on our TDDFT calculations and experimental observations, in Fig. 2F, we propose a model based on a many-body representation of the GNR states to explain the mechanisms of the reported GNR fluorescence. If one considers only what happens on one side of the ribbon, the (7, m)AGNR on NaCl/Au(111) is in a neutral ground state of doublet character, D0. At a negative voltage of ≈−0.6 V, an electron can tunnel from the (7, m)AGNR to the
Fig. 2. Local excitonic emission from (7, m)AGNRs. (A) STML spectra (V = 2.7 V, I = 200 pA, t = 300 s) acquired over the line running along the long axis of a decoupled (7, 24)AGNR, an image of which is shown in the inset (V = 2.3 V, l = 3 pA). (B) dI/dV spectra acquired in the center (blue) and at one extremity (red) of the (7, 24)AGNR imaged in (A). The blue and red asterisks in the inset images mark the tip positions used to record the dI/dV spectra. Constant height dI/dV maps that were acquired at voltages corresponding to dI/dV resonances are displayed in the insets. The voltage dependency of the 0-0 emission efficiency appears as black squares overlaid on the red spectrum. (C) STM image (V = −2.5 V, I = 5 pA) (top) and sketch (middle) of a decoupled (7, 20)AGNR with one CH terminus (i.e., leading to a sp² carbon atom) and one CH₂ terminus (i.e., leading to a sp³ carbon atom). STM spectra (V = 2.0 V) acquired on each terminus (as marked with asterisks in the top STM image) and on top of the bare Au(111) are shown at the bottom. The gray shading represents the raw data, and the solid lines represent the smoothed data. (D) Frontier Kohn-Sham orbitals and their corresponding ground-state occupations for both spin channels. The color represents the phase (sign) of the wave function visualized as an isosurface (red is negative, and blue is positive). (E) Transition electron density associated with the D₀ → D₁ (left) and D₀ → D₂ (right) transitions calculated using TDDFT. The transition density, which is the oscillating component of the electron density that is associated with the electronic transition, is shown as an isosurface, where the color represents the sign (phase) of the density. (F) Fluorescence excitation model: At sufficiently high positive voltage (1.85 V), the GNR can be transiently driven to its negative charge state (S₀⁻) by charge tunneling from the tip to one of its topological end states. Subsequent tunneling of this charge to the substrate may leave the GNR in one of the excited neutral states (D₀ to D₄) that nonradiatively relax to the lowest-lying state D₁. The molecule eventually relaxes to its ground state D₀ by emitting a photon. This simple scheme assumes a negligible voltage drop over the line running along the long axis of a decoupled (7, 20)AGNR, an image of which is shown in the inset (V = 1.9 eV) that is higher than those of the excited states (D₁ to D₄), S₀ → D₁ to D₄ transitions may occur. The fact that eventually only the D₁ → D₀ emission is observed in the experiment indicates fast nonradiative transitions from D₁ (τ ≈ 2) to the lowest excited dark state D₁ and explains why the fluorescence of the 7-AGNR appears intrinsically low in usual photoluminescence measurements (28). The bias onset of the D₁ → D₀ emission ([V = 1.85 V; black squares in Fig. 2B and section VI in (40)] matches the voltage that is required to tunnel into the S₀⁻ state, consistent with the proposed mechanism.

Luminescence of confined acoustic vibronic modes of the GNRs

A notable advantage of GNRs over usual chromophores is that one can envisage tuning their optoelectronic properties by changing their length. In Fig. 3, we investigate how this parameter affects the STML properties of (7, m)AGNRs by studying ribbons made of 4 [(7, 16)AGNR] to 15 [(7, 60)AGNR] DBBA units (Fig. 3A). For all these (7, m)AGNRs, the energy of the 0-0 line remains essentially constant [see section VII of (40) for more details], in agreement with TDDFT simulations [section IV of (40)] and with the observation of an optical transition determined by excitons localized at the ribbon termini. The series of vibronic peaks at low energy (<500 cm⁻¹) presents a different behavior. As shown in Fig. 3B, the energy separation between successive peaks decreases with ribbon length; for the (7, 60)AGNR, separating the peaks from each other becomes difficult. Additionally, the number of peaks in the comb increases up to 10 for the longest ribbons. These behaviors reflect the confinement of acoustic modes, hereafter referred to as longitudinal acoustic modes (LAMs), in the GNRs that act as one-dimensional boxes of controllable length. The first-order LAM (α) was identified in Raman measurements that were performed on ensembles of length-selected AGNRs (49); here, we report the higher-order modes and monitor their dispersion as a function of the GNR length. In Fig. 3C, we report the evolution of the energy separation between successive vibronic lines as a function of the number of carbon atoms, m, in the long axis of the ribbons. As expected, Fig. 3C reveals a linear dispersion of the modes with a slope corresponding to the speed of sound (v = 18.7 km s⁻¹) in GNRs and graphene (49-51). Notably, DFT simulations [blue triangles in Fig. 3C; see also section IV of (40)] of the different (7, m)AGNRs reproduce almost perfectly the dispersion observed in our STML spectra. This confirms the vibronic peak assignment and allows us to represent the first three LAMs (α, β, and γ in Fig. 3D) for a (7, 16)AGNR.

Interestingly, the envelope of the vibronic comb is very similar for all ribbons, showing attenuated emission for the peaks closest to the 0-0 line, a maximum intensity reached for peaks from 100 to 200 cm⁻¹, and a slow decay at higher energy. At the same time, the maximum intensity of the vibronic peaks reaches only up to 50% of the 0-0 line intensity. In a Franck-Condon picture, multiple excitations of the same vibrational mode would also result, as in Fig. 3, in regularly spaced vibronic peaks (33). However, the overall shape of the vibronic comb (i.e., a dominant 0-0 line and vibronic peaks whose intensity increases and later decreases with detuning from the 0-0 line) cannot be reconciled with a Franck-Condon distribution. The data of Fig. 3 therefore indicate that each vibronic peak of the comb corresponds to single excitations of LAMs of different orders. Besides, only modes that have even symmetry (such as α and γ) have...
been predicted to be optically active in far-field Raman spectroscopy (49) because only those result in a change of polarizability. This selection rule is clearly not respected in our experiments because all the modes, regardless of their parity, appear intense in the spectra. This somewhat surprising behavior can be attributed to the localization of the exciton to only one end of the GNR (i.e., lowering the symmetry of the system), an effect that we associate with the interaction with the tip in our experiment. This results in a net oscillator strength for modes of both even and odd symmetries. Moreover, fitting the relative intensities of the LAMs with a Franck-Condon model [section VIII of (40)] allows us to retro-engineer the effective deformation that is associated to the exciton creation. These data suggest that the exciton confinement is even stronger than expected from the gas-phase TD-DFT calculations, which likely also reflects the presence of the tip. The overall emerging picture is that of emitters strongly localized at the topological ends of the GNRs and Franck-Condon–coupled to delocalized acoustic modes of the ribbon structure. Here, the spectroscopic vibronic pattern reflects an end-localized deformation in the excited state with respect to the ground-state geometry.

**High-energy vibronic peaks**

Lastly, we discuss the length-dependency of the high-energy (>500 cm$^{-1}$) vibronic peaks (Fig. 4). This spectral section is characteristic of the probed material and is often referred to as the fingerprint region. In contrast to the low-energy peaks, the most-intense peaks here do not shift with ribbon length. With the exception of the 677-cm$^{-1}$ peak, all these peaks can be identified based on a comparison with calculations of the vibronic activities (Fig. 4A) and literature (52). The 1238-cm$^{-1}$ peak can be assigned to in-plane bond-bending vibrational modes of the C–H bonds at the GNR edges. The 1348- and 1610-cm$^{-1}$ peaks are the so-called D and G modes, respectively, which are associated to $E_{2g}$ and $A_{1g}$ deformations of the carbon rings that are found in all vibronic spectra of sp$^2$ carbon materials. Their intensity ratio D/G is generally used to determine the presence of defects in meso- and macroscopic scale systems; a low ratio indicates an overall good structural quality of the material (53). At the level of an individual ribbon, this ratio may be used to tag the bonding motive of the carbon atoms that surround the exciton. More precisely, the D mode that is a second-order process in graphene becomes first-order in the case of GNRs (52), which explains its high intensity in our STML spectra.

The 677-cm$^{-1}$ peak, whose intensity varies with tip position differently from the rest of the spectra (Fig. 2A), is not reproduced by simple Franck-Condon simulations. Our closed-shell DFT calculations for ribbons of various lengths consistently reveal a normal mode at 692 cm$^{-1}$ that we tentatively associate with the experimental peak at 677 cm$^{-1}$. This mode presents a single antinode and is of odd symmetry (see the C–H$_{2g}$ mode in Fig. 4B, where IR refers to infrared active). We therefore suggest that this vibrational mode promotes nonadiabatic coupling (i.e., Herzberg-Teller active modes) between the localized exciton and higher-lying delocalized excitons, which explains the nonvanishing intensity of the 677-cm$^{-1}$ peak for the tip located on top of the middle of the GNR (Fig. 2A). Furthermore, in the experimental spectra, weak vibronic combs on the low-energy side of the 677- and 1348-cm$^{-1}$ peaks that reproduce the shape and energy separation reported in Fig. 3 can also be distinguished. These peaks are therefore interpreted as combination

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**Fig. 3. Coupling of excitons with longitudinal acoustic modes for (7, m)AGNRs of increasing length.** (A) STM images (−2 V < $V$ < −3 V) of decoupled (7, m)AGNRs. (B) STML spectra (2.3 V < $V$ < 2.7 V) acquired from the ribbons in (A). The vertical bars indicate equally spaced peaks. The first three peaks are labeled $\alpha$, $\beta$, and $\gamma$. The gray shading represents the raw data, and the solid lines represent the smoothed data. (C) The experimental (red dots) and calculated (blue triangles) average energy separation, $\Delta E$, between successive vibronic peaks as a function of $m$. For clarity, the error bars, which are smaller than the size of the dots, are not shown. L refers to the ribbon length. (D) The first three LAMs ($\alpha$, $\beta$, and $\gamma$) calculated by DFT [see section IV of (40)] for a (7,16)AGNR. The red arrows indicate the normalized atomic displacement profile (the arrow lengths were scaled by a factor of 10).

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**Fig. 4. Fingerprint region of the (7, m)AGNR vibronic spectra.** (A) High-energy region of the STML spectra (2.3 V < $V$ < 2.7 V) acquired from the same ribbons imaged in Fig. 3A. The gray shading represents the raw data, and the solid lines represent the smoothed data. (B) DFT calculation of the main modes identified in the spectra in (A). A visual representation of the high-frequency vibrational modes calculated for the (7, 16) ribbon (only half a ribbon is shown) that can be tentatively assigned to the vibronic peaks obtained from the spectra in (A) is shown. The vectors that indicate the vibrational modes (normalized atom displacements) have been scaled by a factor of 10 for the C–H$_{2g}$, D, and G modes and by a factor of five for the C–H mode.
bands that replicate the low-energy vibronic progression.

Conclusions and outlook

Our atomically resolved fluorescence measurements reveal sharp (>0.6 meV) emission from a long-lived dark exciton localized at the topological ends of (7, m) AGNRs. These localized emitting centers are coupled to one-dimensional acoustic phonon modes that are delocalized over the whole ribbon. Emission centers localized in insulators and/or semiconductors, such as color centers or defects in solids (54), are often used as single- or entangled-photon sources of particular interest for quantum sensing and quantum technology applications. An advantage of the topologically localized centers in GNRs over more conventional solid-state quantum emitters is that the number and the position of the photon sources can be tailored through chemical engineering of the short and long edges of the GNR, which thus provides an efficient path to tune intersublevel coupling and control the classical and quantum emission properties. An obvious next step will be to identify the single-photon source character of the emission at the topologically localized centers and to characterize their performance. In addition, each topological end state of (7, m) AGNRs hosts an unpaired electron and is therefore spin-polarized, thereby providing organic nanoscale solutions for quantum schemes that combine electronic, magnetic, and photonic degrees of freedom. These GNRs can also be viewed as ideal atomically controlled platforms to identify, with atomic-scale spatial accuracy, the role of exciton-phonon coupling on the (de)coherence of the quantum units. Eventually, the two ends of the GNR could be functionalized with specifically chosen chromophores (55) to determine whether delocalized acoustic phonon modes can affect the coherent coupling between the chromophore dipoles (34, 56), as does electronic-vibrational mixing in light-harvesting complexes.

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Data and materials availability: All data needed to evaluate the conclusions in the paper are present in the paper or the supplementary materials. For all figures presented in this study are available on Zenodo (59). The following software was used: COMPASS 5.6, ACCD module to calculate the plasmonic potential of the tip, Gaussian 16 version C.01 to perform ab initio calculations on the GNRs, and Matlab 2021a for data postprocessing. License information: Copyright © 2023 the authors, some rights reserved; exclusive license American Association for the Advancement of Science. No claim to original US government works. https://www.sciencemag.org/about/science-licenses-journal-article-reuse

SUPPLEMENTARY MATERIALS

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Materials and Methods

Supplementary Text

Figs. S1 to S8

Table S1

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