Electronic Supplementary Material (ESI) for Physical Chemistry Chemical Physics.

Supplementary information: Inducing a topological transition in graphene nanoribbons superlattices by external strain

E. Flores,[1] José D. Mella,[1] E. Aparicio,[2] R. I. Gonzalez,[3,4] C. Parra,[5] E.M. Bringa,[2,3,*] and F. Munoz[6,4,†]

[1]*Departamento de Física, Facultad de Ciencias Físicas y Matemáticas, Universidad de Chile, Santiago, Chile*

[2]*CONICET and Universidad de Mendoza, Mendoza, 5500, Argentina*

[3]*Centro de Nanotecnología Aplicada, Facultad de Ciencias, Universidad Mayor, Santiago, Chile.*

[4]*Centro para el Desarrollo de la Nanociencia y la Nanotecnología, CEDENNA, Santiago, Chile*

[5]*Laboratorio de Nanobiomateriales, Departamento de Física, Universidad Técnica Federico Santa María, Valparaiso, Chile*

[6]*Departamento de Física, Facultad de Ciencias, Universidad de Chile, Las Palmeras 3425, 7800024 Ñuñoa Santiago, Chile*

1. FRACTURE PROCESS

In order to better understand the modulated AGNR fracture process, we include some MD snapshots in Figures S1 and S2.

* ebringa@yahoo.com
† fvmunoz@gmail.com

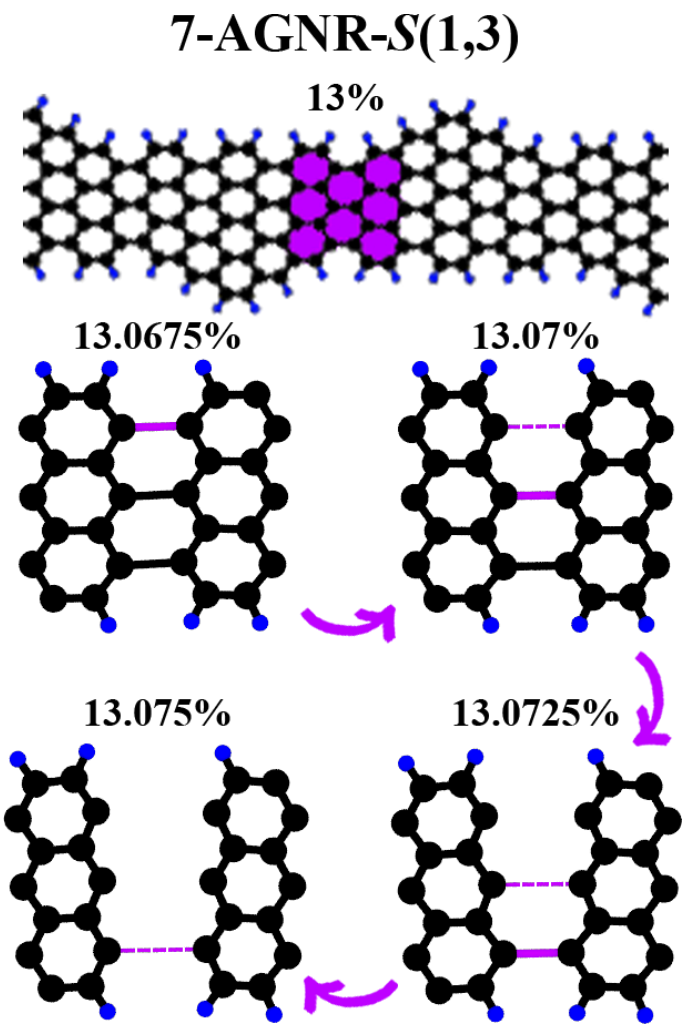

Figure S1. 7-AGNR-$S(1,3)$ superlattice at 13% strain when no bond has broken yet. Carbon atoms in black and hydrogen atoms in blue. The purple region marks the zone that will be involved in the fracture process. Detailed evolution of bond breaking in that purple region is presented as a function of strain, where purple thick bonds will break in the next snapshot and will be represented by dashed thin purple bonds.

2. ELECTRONIC PROPERTIES

2.1. Penetration length of an edge state

The penetration length ε of an edge ($E = 0$) state into the AGNR goes as $\varepsilon \propto \Delta^{-}1$, with Δ the bulk band gap. Below we will show three ways to undertand it.

2.1.1. The SSH model

The finite SSH model can be described by the Hamiltonian

$$H = t \sum_{j=0}^{N-1} a_j^\dagger b_j + t \sum_{j=0}^{N-2} a_{j+1}^\dagger b_j + H.c., \tag{S1}$$

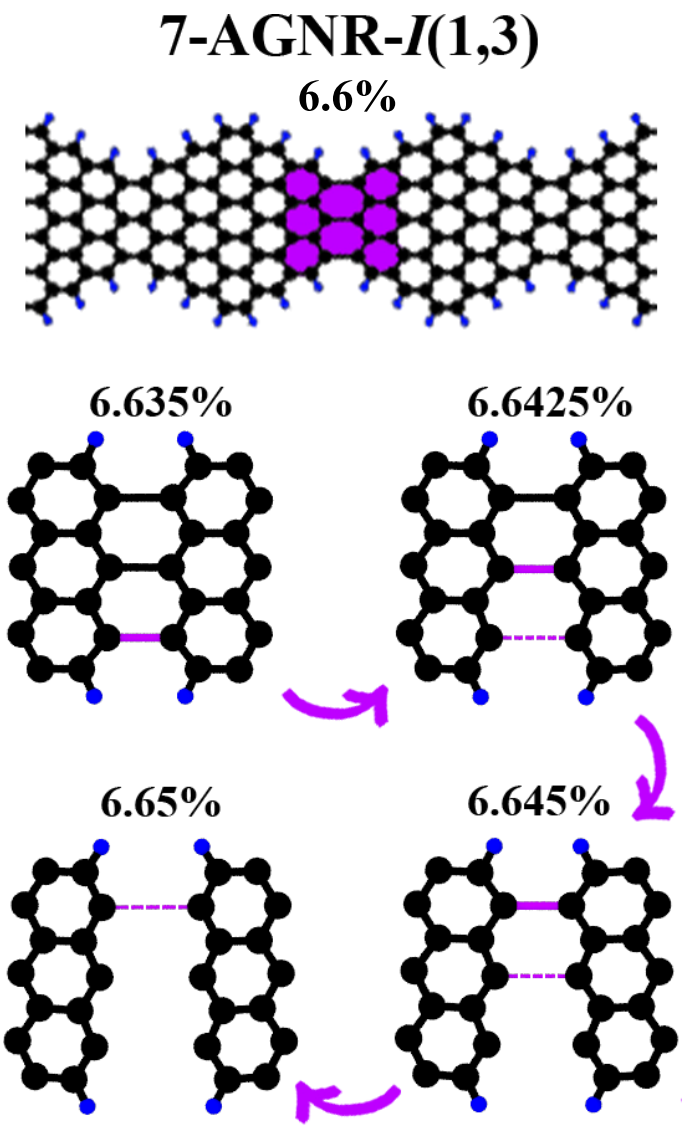

Figure S2. 7-AGNR-I(1,3) superlattice at 6.6% strain when no bond has broken yet. Carbon atoms in black and hydrogen atoms in blue. The purple region marks the zone that will be involved in the fracture process. Detailed evolution of bond breaking in that purple region is presented as a function of strain, where purple thick bonds will break in the next snapshot and will be represented by dashed thin purple bonds.

with t, v the intracell and intercell hopping constants. In the non-trivial phase ($v > t$), the localized state on the left is

$$\Psi_L^\dagger = \alpha \sum_{j=0}^{N-1} (-1)^j e^{-\frac{j}{\varepsilon}} a_j^\dagger, \tag{S2}$$

with α a normalization constant, and the penetration length $\varepsilon = \ln^{-1}(v/t)$. From this relation follows $e^{1/\varepsilon} = \frac{v}{t} = 1 + \frac{\Delta}{2t}$. If ε is big enough to truncate a series expansion, we get: $\frac{1}{\varepsilon} = \frac{\Delta}{2t}$. Even though the SSH model is not the closest to an AGNR, it is fairly simple and illustrate our point that $\varepsilon \propto \Delta^{-1}$.

2.1.2. A simple estimation with graphene

In graphene, the dispersion relation near a the K point is

$$E = t\sqrt{k_x^2 + k_y^2}, \tag{S3}$$

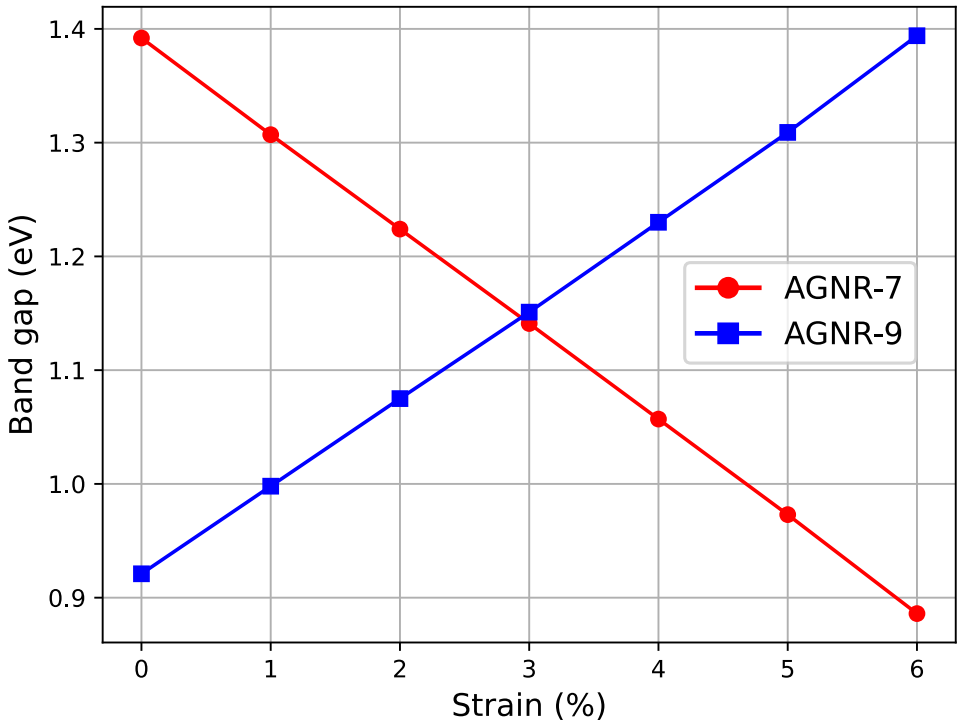

Figure S3. Evolution of the band gap as a function of strain. The AGNRs are relaxed (the only constraint is the strain). The 7-AGNR and 9-AGNR belong to different topological phases, hence their band gaps have the opposite behavior with strain.

If it is finite along y (*i.e.* a generic GNR), k_y will be quantized, according to its boundary conditions. We will still use the symbol k_* to denote its minimum value. A wave along x can be written (assuming separability) as:

$$\Psi(x,y) = f(y)e^{-ik_x x}, \tag{S4}$$

with $k_x = t^{-1}\sqrt{E^2 - t^2k_*^2}$. In particular, if we have a solution with $E = 0$, k_x becomes imaginary, *i.e.* a localized wave:

$$\Psi(x,y) = f(y)e^{-x\varepsilon}, \tag{S5}$$

where $\varepsilon^{-1} = ik_x = |k_*|$. Since the band gap of this generic GNR is $\Delta = 2t|k_*|$, it follows the relation $\varepsilon = \frac{2t}{\Delta}$.

2.1.3. *Penetration length of a zig-zag GNR*

An exact expression for the edges states in zigzag terminated graphene (*i.e.* periodic along the y-axis) was found by Fujita *et al.*[S1]:

$$\psi_m \propto \cos^{-2m}\left(\frac{k}{2}\right), \tag{S6}$$

where m is the index of the site since the border, and k is wavevector from the periodic direction. The penetration length, ε is:

$$\varepsilon^{-1} = \ln\left[\cos^2\left(\frac{k}{2}\right)\right]. \tag{S7}$$

If we are interested in edge states with $E \approx 0$, the values of k of interest are close to π, or $k = \pi - \delta_y$. After some algebra, we find

$$\frac{1}{\varepsilon} \approx \delta_y \tag{S8}$$

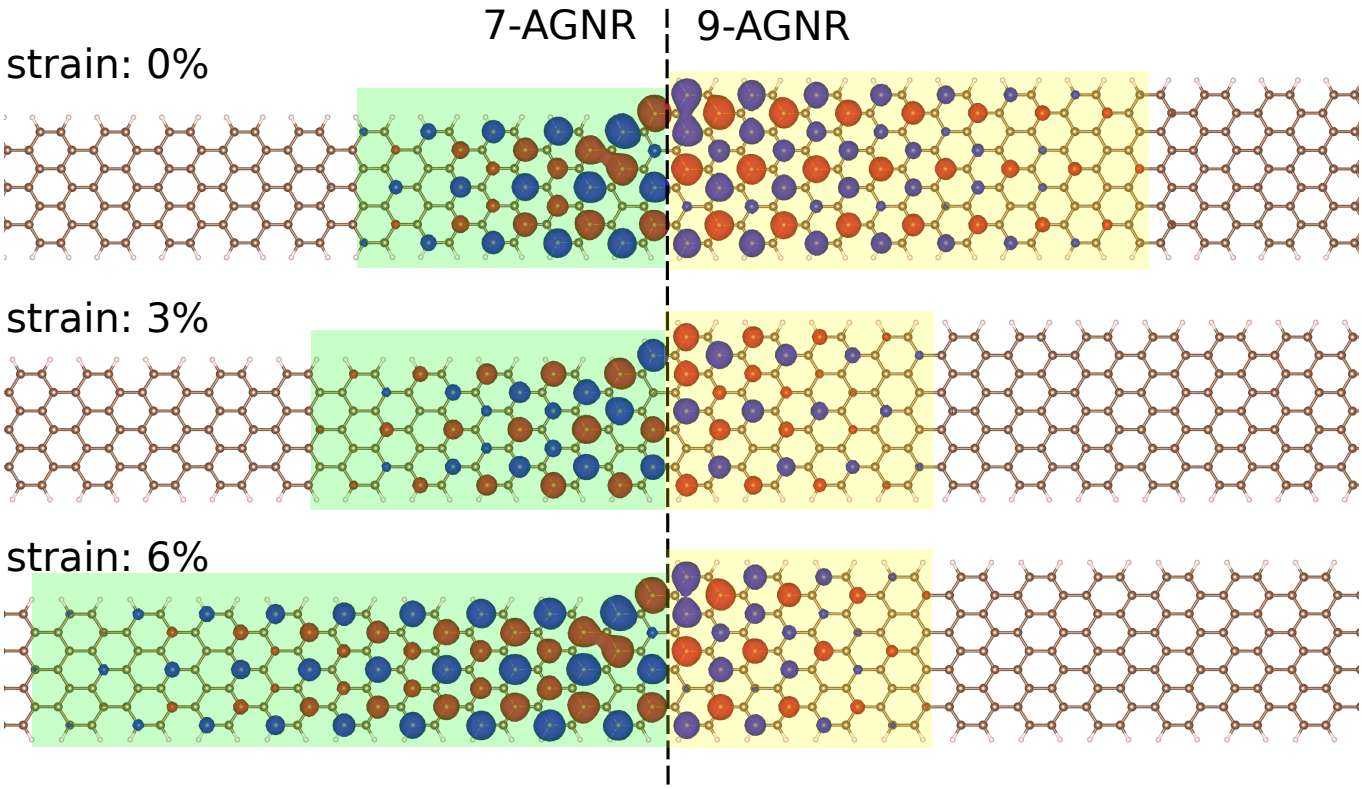

Figure S4. Localization of the interface wave function as a function of the applied strain. There is a clear correspondence between the *local* band gap of the N-AGNR and the localization of the electronic state along each segment: the smaller the band gap the larger the localization. To avoid a non-uniform strain along the sample only the ground-state structure was relaxed. The isovalue is 0.005, and the shaded regions are just a guide to the eye.

Our case of interest is the penetration of the states from zigzag edges in an AGNR, not graphene. This imposes a quantization of the values of k allowed, and also gives rise to a band gap, then $\frac{1}{\varepsilon} \approx \frac{\Delta}{2t}$.

[S1] M. Fujita, K. Wakabayashi, K. Nakada, and K. Kusakabe, Peculiar localized state at zigzag graphite edge, Journal of the Physical Society of Japan **65**, 1920 (1996).

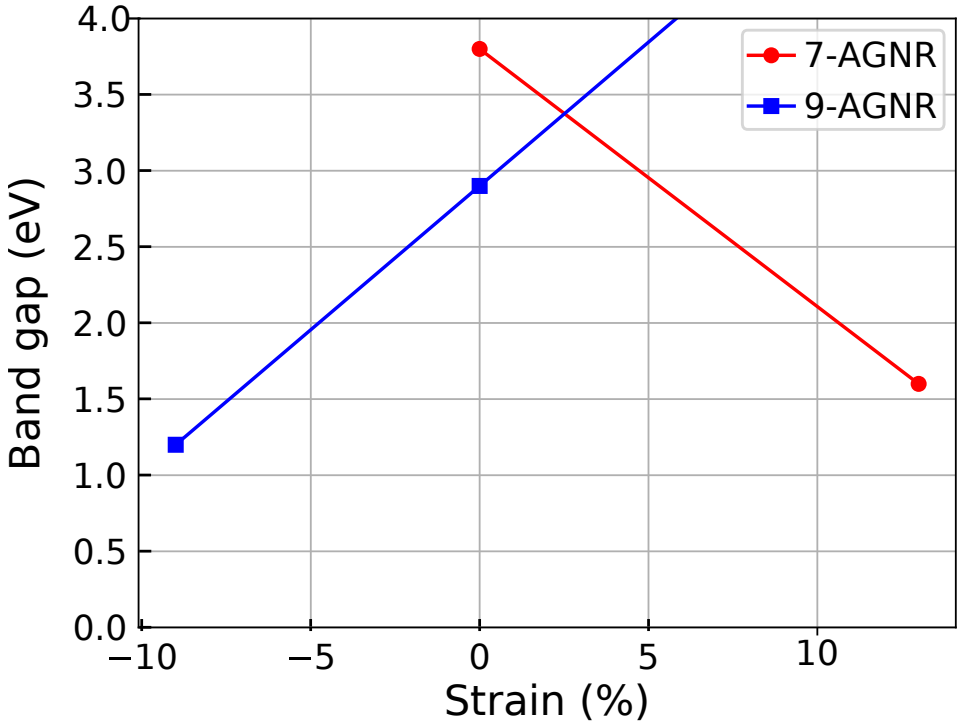

Figure S5. Similar to Fig. S3, but the evolution of the band gap as a function of the strain is estimated from GW calculations. See the main text for details.