Graphene 2017
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Electronic transport in a deformed graphene kirigami

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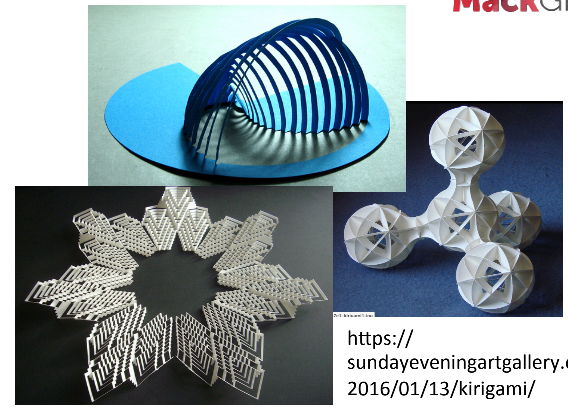
Graphene kirigami

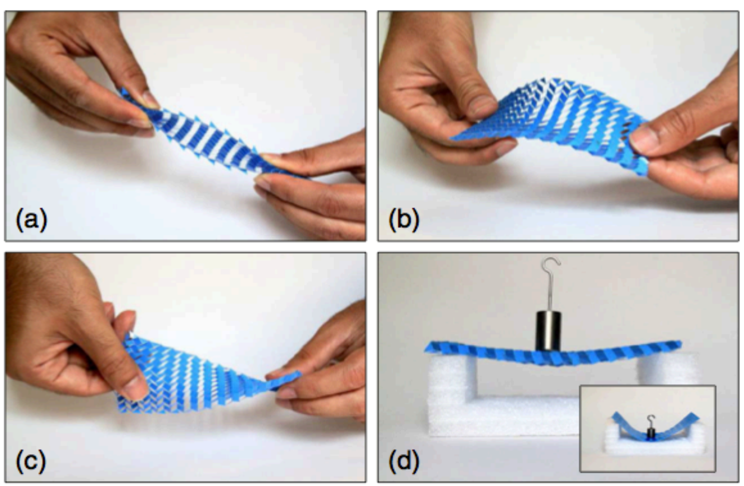
Kirigami (*kiru* “to cut”, *kami* “paper”) the Japanese art of papercutting is inspiring the design of new materials with configurable mechanical properties.



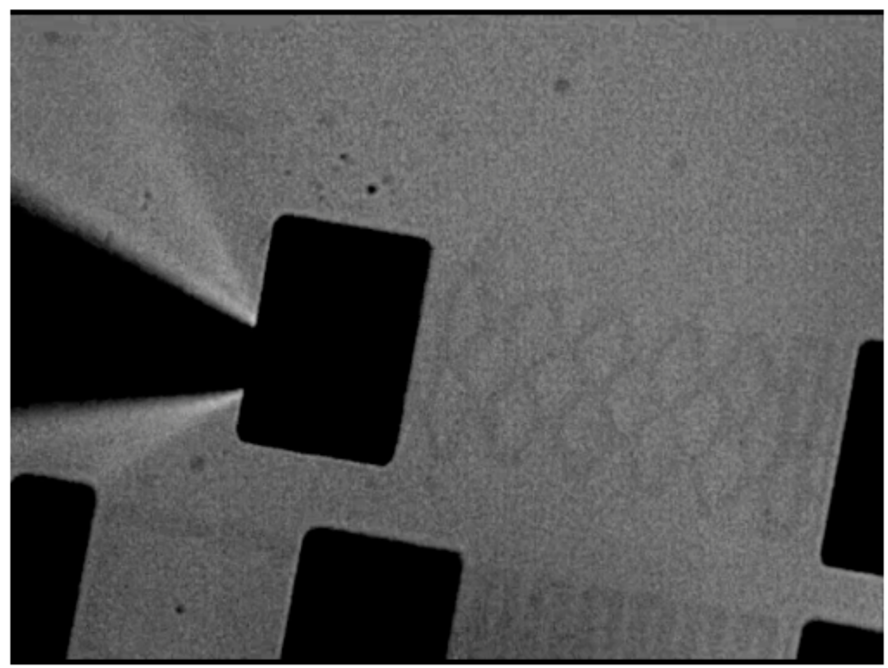
https://sundayeveningartgallery.com/2016/01/13/kirigami/

High stretchability.
High bendability
Good Self-Recoverability

At the nanoscale



Phys. Rev. Lett. 118, 084301 (2017)



Nature 524, 204–207 (2015)

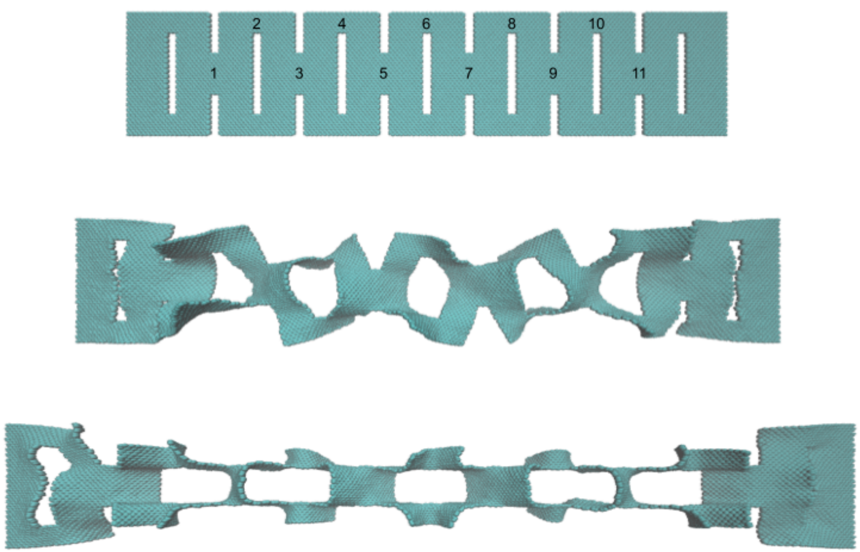
Graphene kirigami

How are the electronic states and the flow of current within the kirigami modified under deformation?

Molecular Dynamics

+

Tight binding



$$
\begin{aligned}
V_{pp\pi}(d_{ij}) &= t_0 e^{-3.37(d_{ij}/a-1)} \\
V_{pp\sigma}(d_{ij}) &= 1.7 V_{pp\pi}(d_{ij})
\end{aligned}
$$

$$t_{ij} = V_{pp\pi}\widehat{n}_i \cdot \widehat{n}_j + (V_{pp\sigma} - V_{pp\pi})\frac{(\widehat{n}_i \cdot \vec{d}_{ij})(\widehat{n}_j \cdot \vec{d}_{ij})}{d_{ij}^2}$$

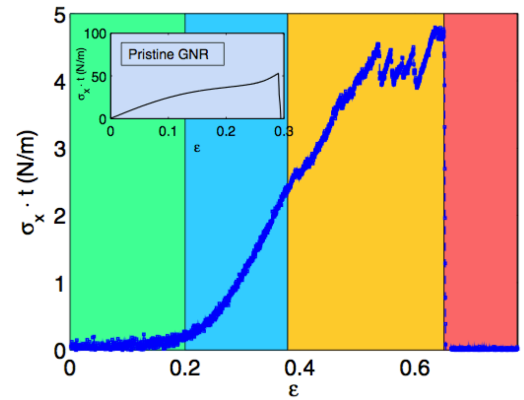
$$G^r = [G^a]^\dagger = [E + i\eta - H - \Sigma_p - \Sigma_q]^{-1}$$

$$G = \frac{2e^2}{h}\mathrm{Tr}[\Gamma_q G^r \Gamma_p G^a]$$

Mechanical properties

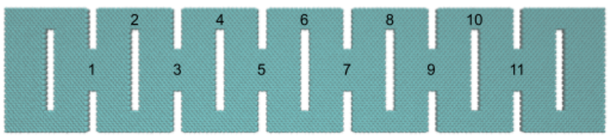
The graphene kirigami presents four deformation stages:

(i) Elongation with very little in-plane stress.
(ii) Elongation with stress.
(iii) Yielding.
(iv) Fracture.

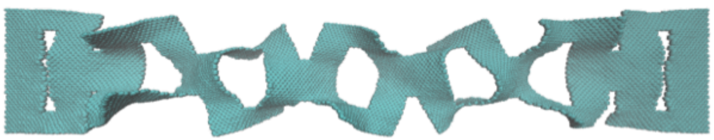


Phys. Rev. B 90, 245437 (2014)

0 %



15.5 %



34.7 %

Phys. Rev. B 93, 235408 (2016)

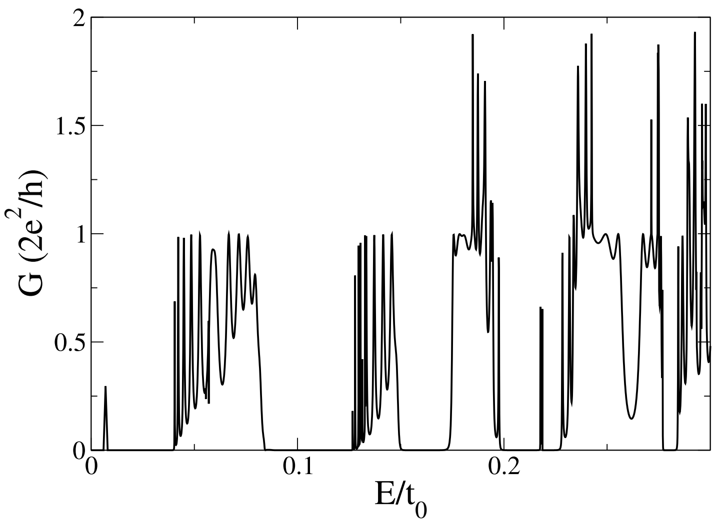
Horizontal and vertical segments twist and rotate and, as a result the kirigami elongates without significant modification of the average C-C bond length

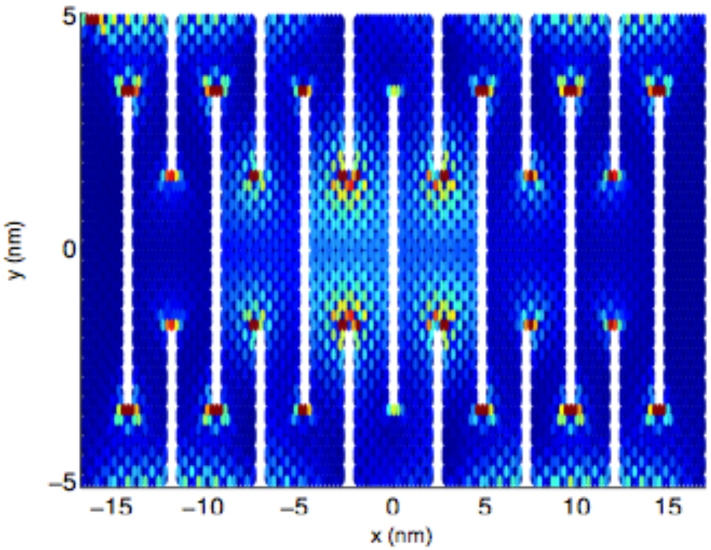
The kirigami is not capable of accommodating higher elongations only by twisting, further deformation occurs through stretching of the carbon bonds.

Transport properties

Localized states overlap creating in the conductance groups of 11 resonances for low energy and mini-bands for higher energies.

From the electron transport viewpoint the unstrained kirigami behaves as a superlattice of coupled quantum dots





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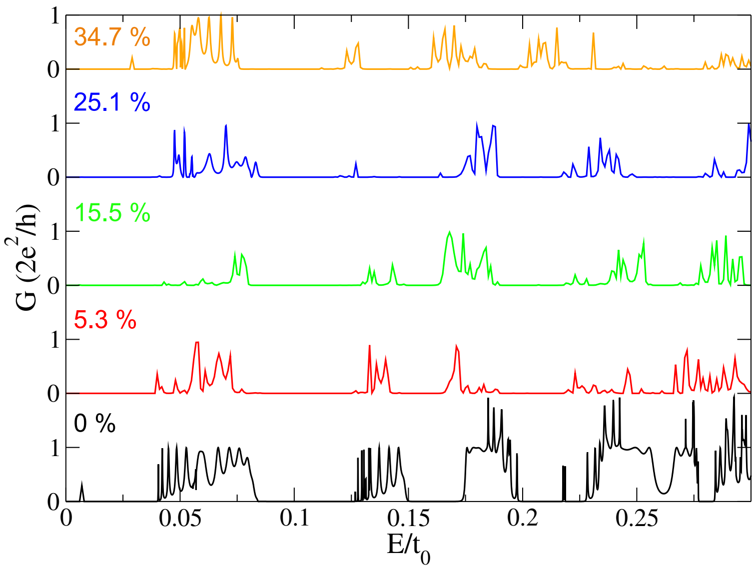
Assuming a 1D tight binding model the inter-dot coupling is estimated

$$E_n = -2\gamma \cos\left(\frac{n\pi}{N+1}\right), \qquad n = 1, 2, \ldots, N,$$

$$\gamma \approx 0.01 t_0$$

Transport properties

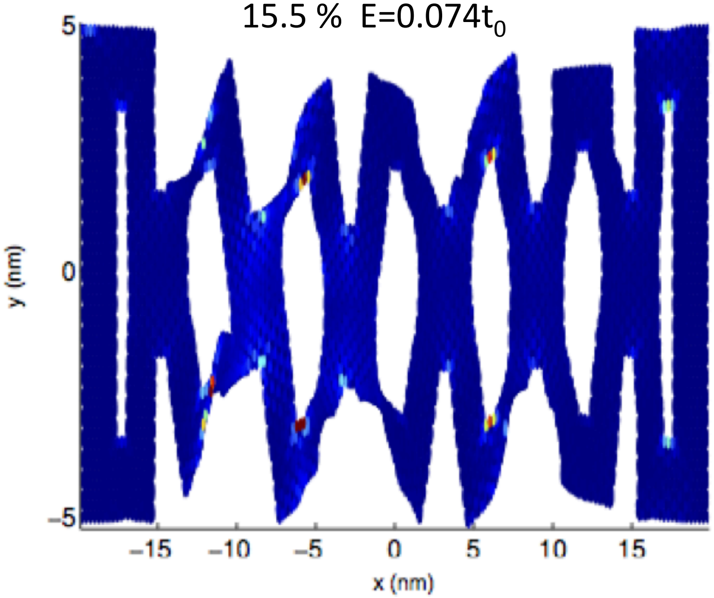


Under tensile load in stage 1 (5.3 and 15.5%):

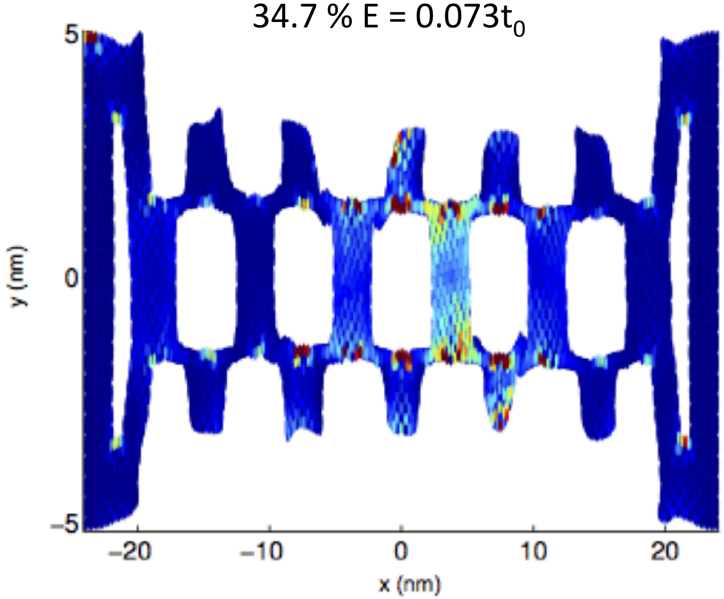
- the kirigami elongates and becomes distorted, which significantly perturbs the overlap between the localized states.
- The conductance is progressively reduced.

Unexpectedly, resonant transmission is revived when the kirigami enters stage 2 of deformation (25.1 and 34.7%).

15.5 % $E=0.074t_0$



34.7 % $E = 0.073t_0$



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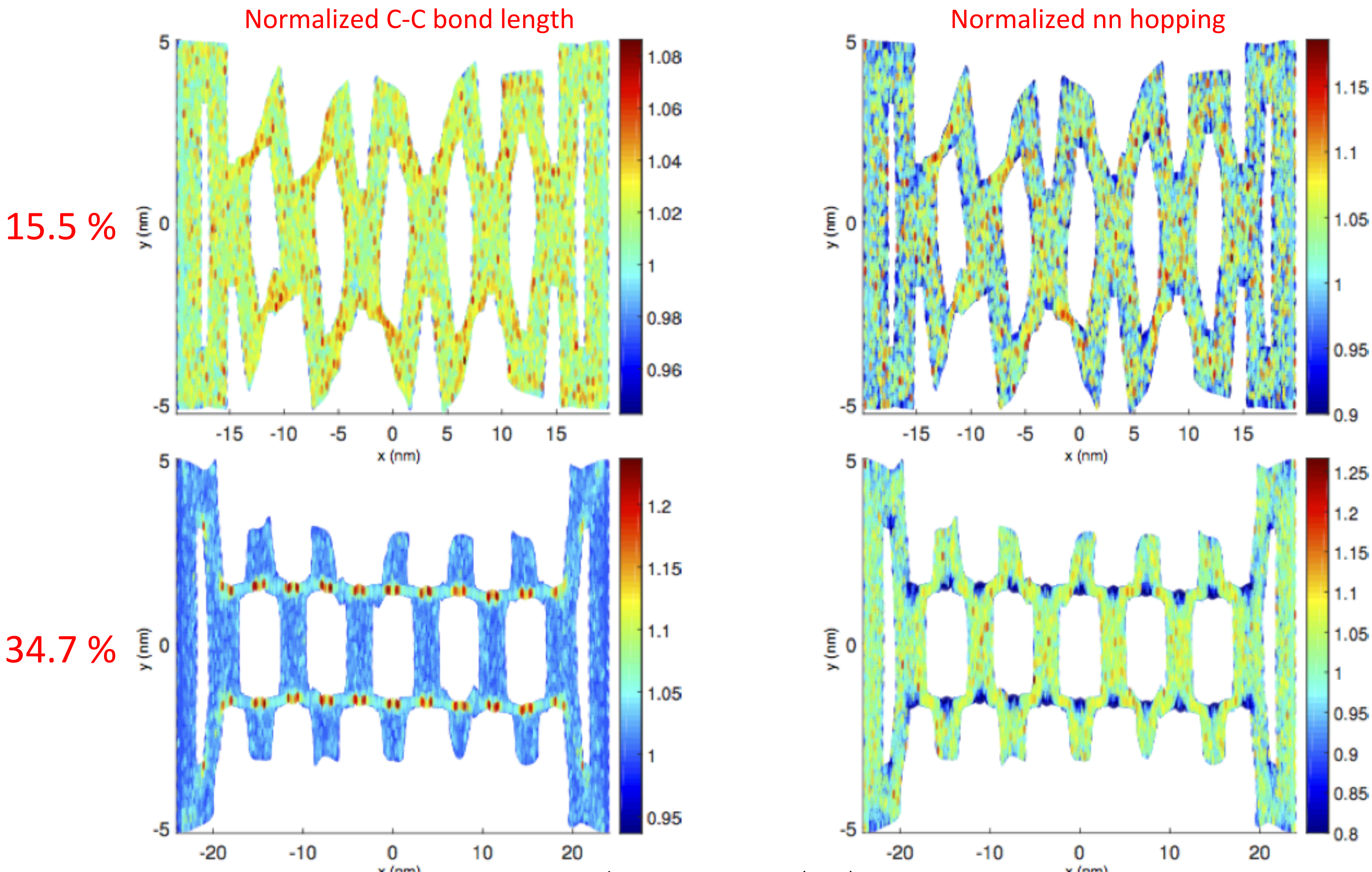
Transport properties

Nearly periodic strain barriers created during deformation stage 2 reinforce electron confinement.



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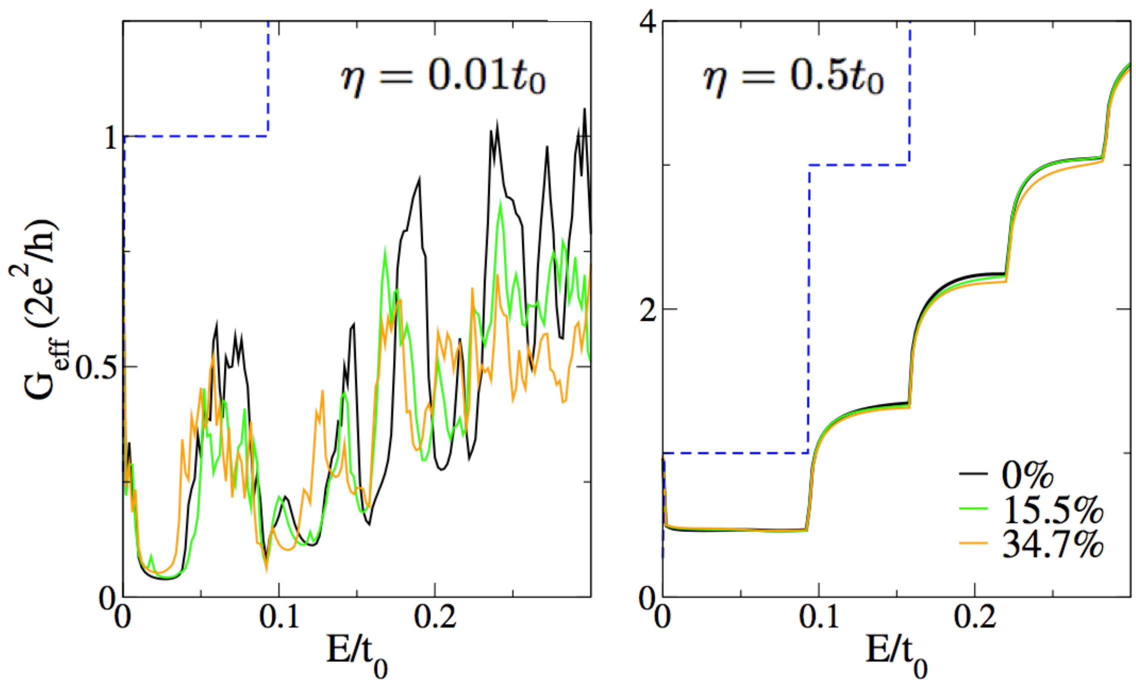
Transport properties

To address the robustness of the strain modulation of the conductance in a more realistic scenario, we added dephasing processes through the Büttiker-probe model.

- We are not interested in the particular physical mechanism (impurities, phonons or electrons) behind the destruction of quantum coherence, we fix the self-energy of each Büttiker-probe to:

$$\sum_{\phi} = i\eta \qquad \tau_{\phi} = \frac{\hbar}{2\Gamma_{\phi}} = \frac{\hbar}{4\eta} \qquad l_{\phi} = \sqrt{D\tau_{\phi}}$$



Dephasing destroys resonant transmission and mini-bands structure.

$$\eta = 0.01t_0 \Rightarrow l_{\phi} \approx 42 \ \ nm > L$$

$$\eta = 0.5t_0 \Rightarrow l_{\phi} \approx 6 \ \ nm \approx w$$

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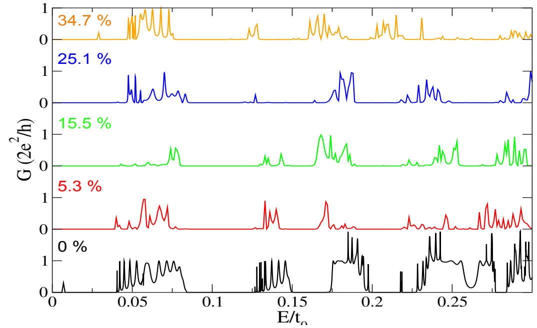
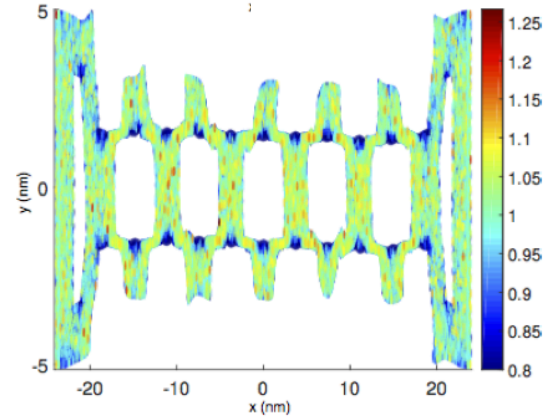
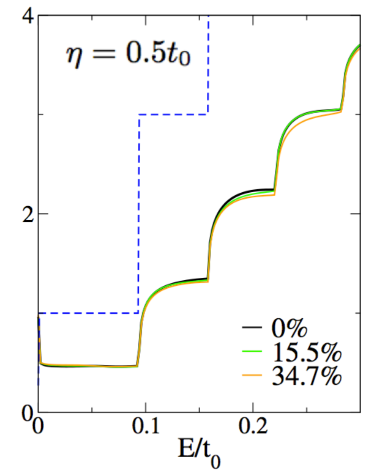
Take-home message

- The undeformed kirigami behaves as a system of coupled quantum dots.
- Mechanical deformations during stage 1 disturb the overlap between localized states reducing conductance.
- During stage 2, strain barriers along the links between kirigami segments restore electronic confinement and resonant tunnelling.
- The Effect of mechanical deformation on the conductance is washed out when the phase-relaxation length is smaller than the typical lengths of the kirigami







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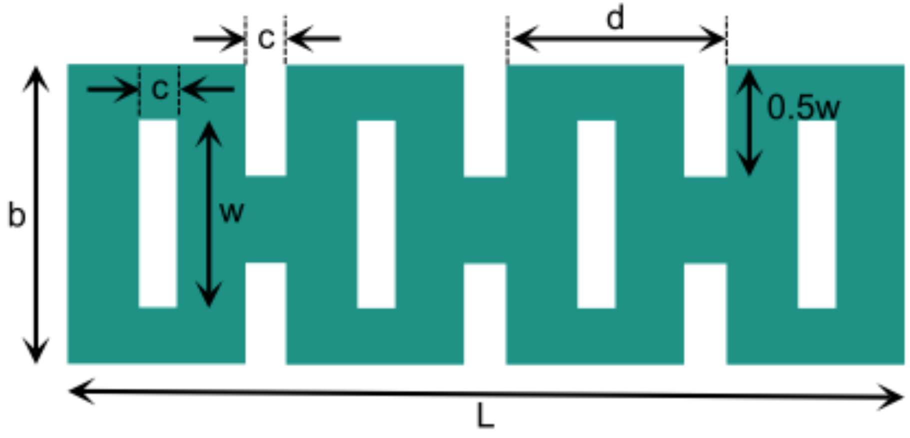
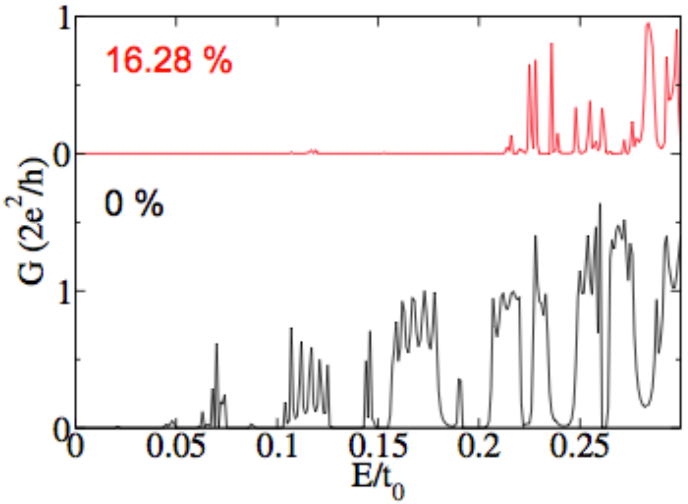
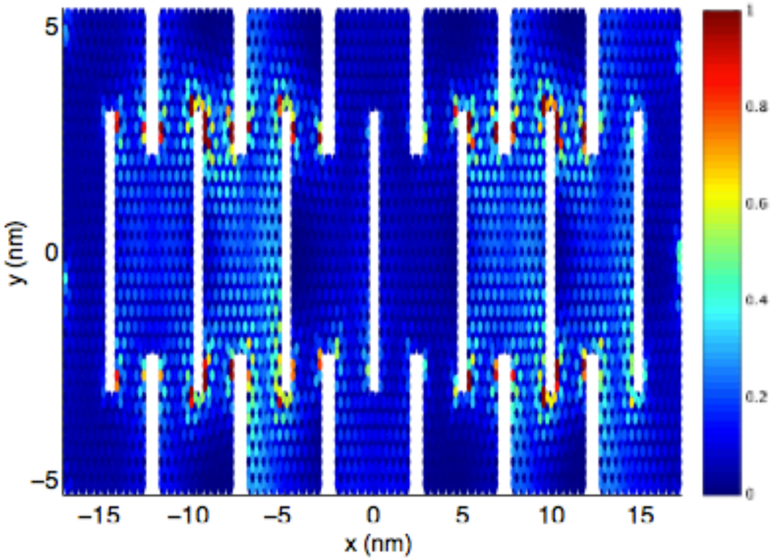
Appendix







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