Electronic Structure and Transport Properties of Graphene Grainboundaries

IWCN 2023

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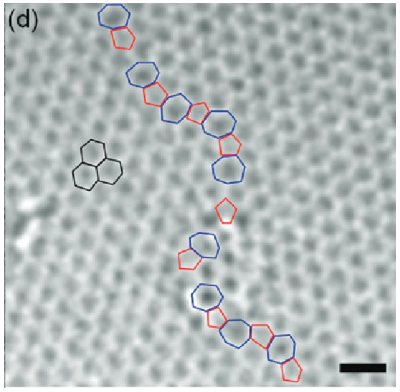
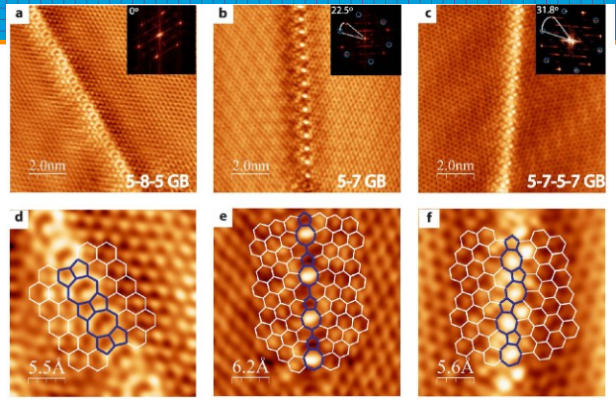
Dept. of Physics, Technical University of Denmark
NANOMADE, Mads Brandbyge's group

Introduction



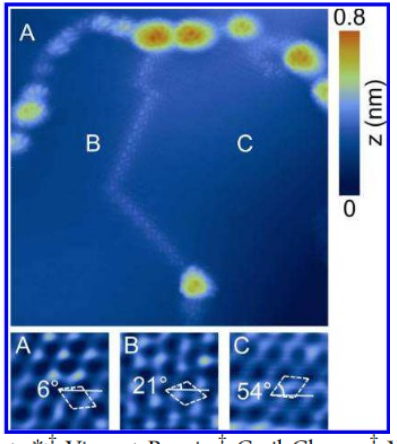
Kwanpyo Kim,[†,‡,∥] Zonghoon Lee,[§,⊥,∥] William Regan,[†,‡] C. Kisielowski,[§] M. F. Crommie,[†,‡] and A. Zettl[†,‡,*]

ACS nano, 2011, 5.3: 2142-2146



Bao Yang, Hai Xu, Jiong Lu, and Kian Ping Loh*

J. Am. Chem. Soc. 2014, 136, 34, 12041–12046



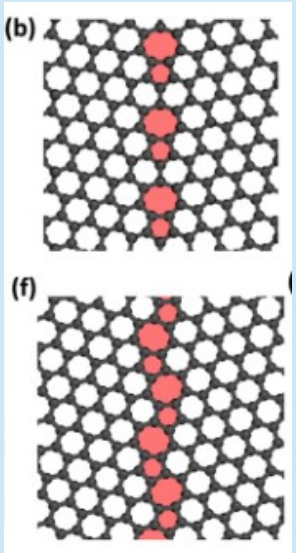
(15x15)nm^2

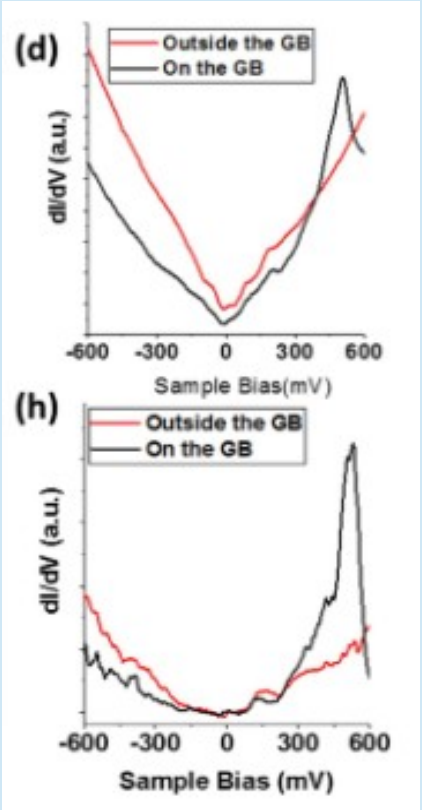
Yann Tison,[†] Jérôme Lagoute,*[,†] Vincent Repain,[†] Cyril Chacon,[†] Yann Girard,[†] Frédéric Joucken,[‡] Robert Sporken,[‡] Fernando Gargiulo,[§] Oleg V. Yazyev,[§] and Sylvie Rousset[†]

Nano letters 14.11 (2014): 6382-6386

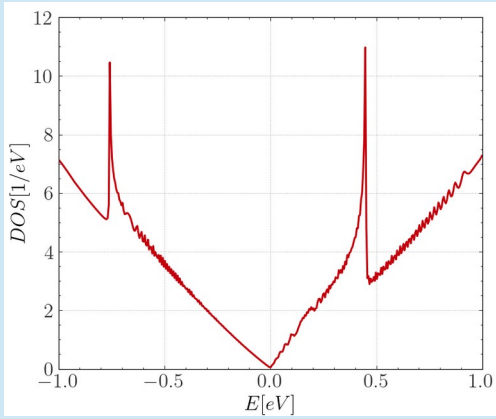
Grainboundaries: STM-Features

(5-7 & “Zigzag”)





STM sees peaks in DOS



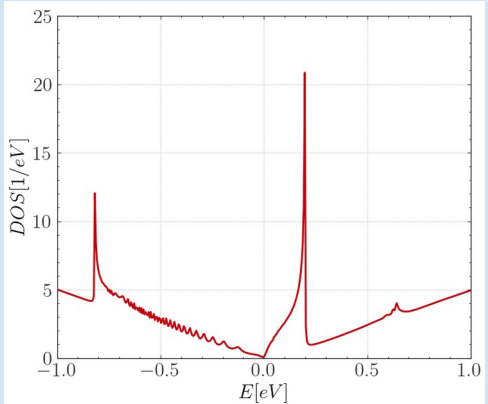
First approach:

Tight-binding

+

Landauer

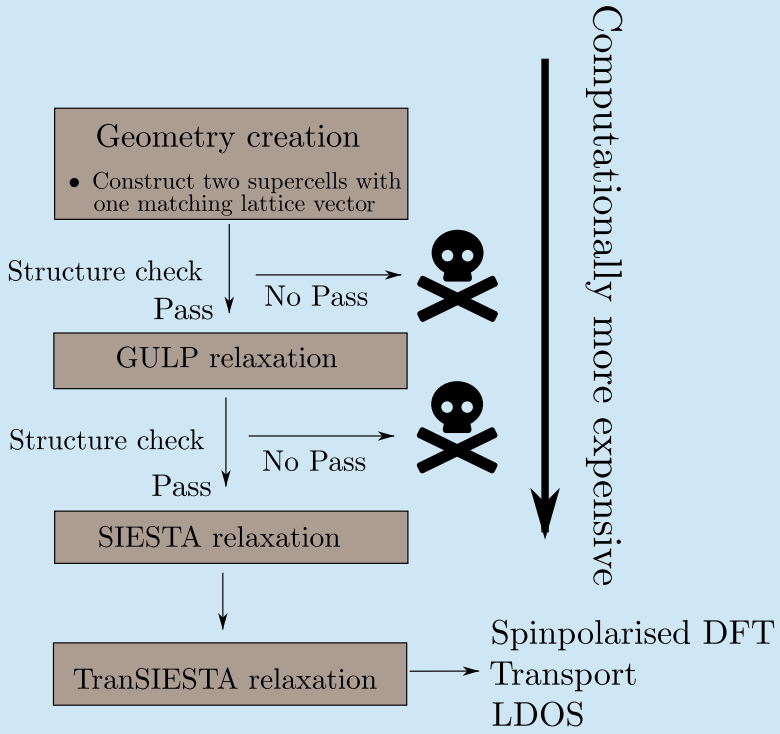
Transport



Adina Luican-Mayer[1,2], Jose E Barrios-Vargas[3], Jesper Toft Falkenberg[4], Gabriel Autès[5], Aron W Cummings[3], David Soriano[3], Guohong Li[1], Mads Brandbyge[4], Oleg V Yazyev[5], Stephan Roche[3,6] and Eva Y Andrei[1]

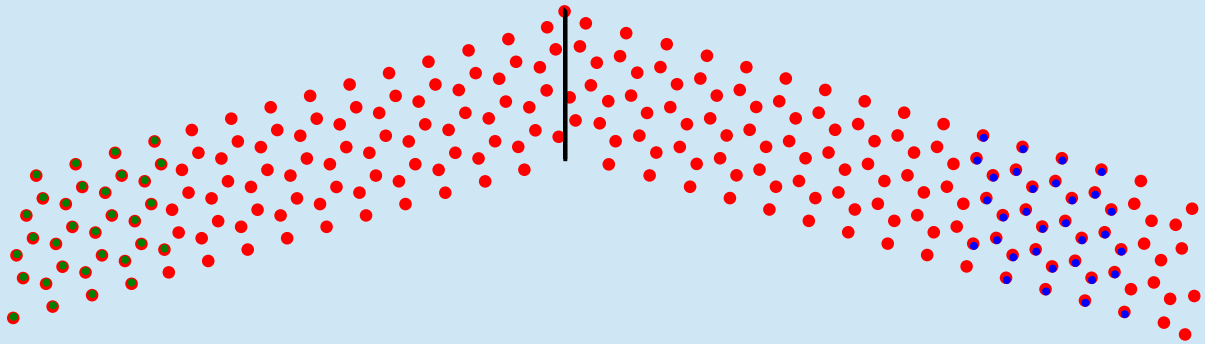
Scripting tools

Doing “high throughput” computation with Transiesta.....



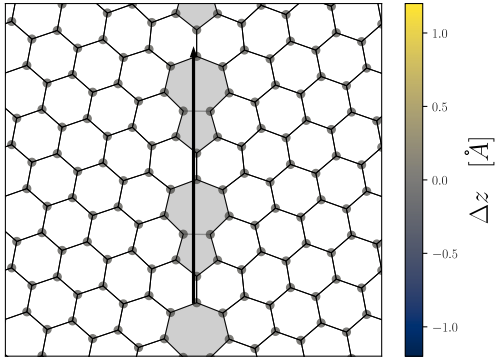
..... wrapped in python

```
import sisl
from Structures.Structures import load_GB_TS_relax as load_GB
from siesta_python.siesta_python import SiP
```

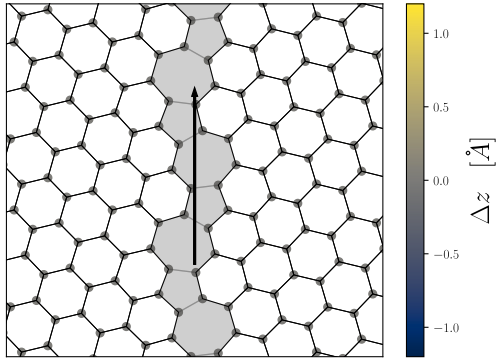


Some examples

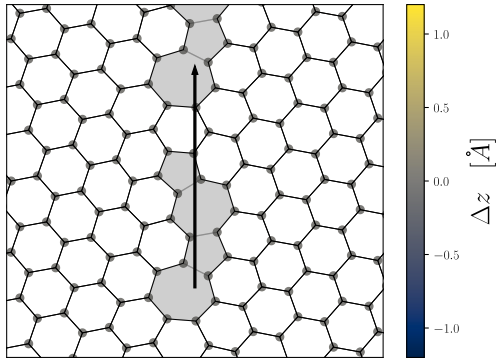
21.78°



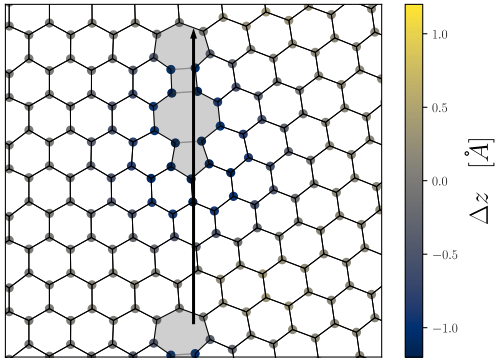
32.21°



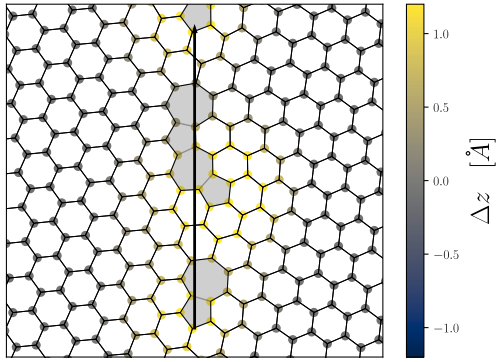
21.78°



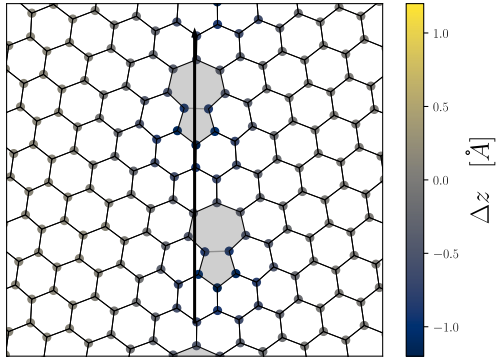
8.21°



17.59°



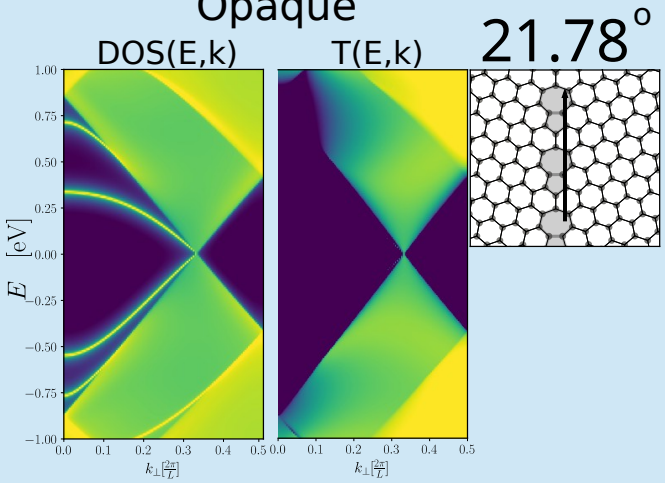
43.57°



Qualitative Classification

Qualitative Classification

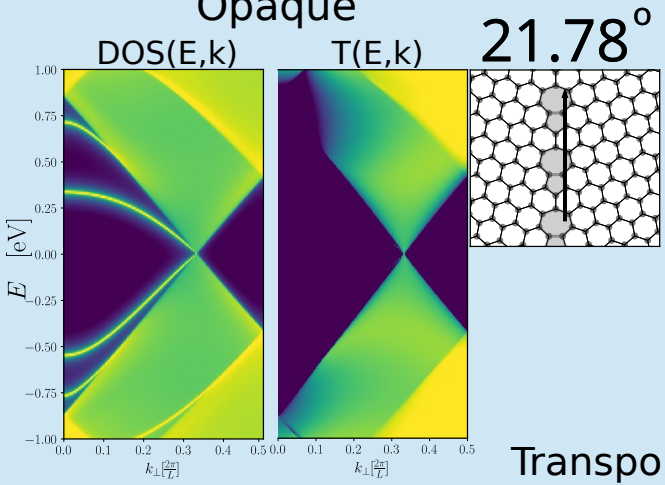
Opaque



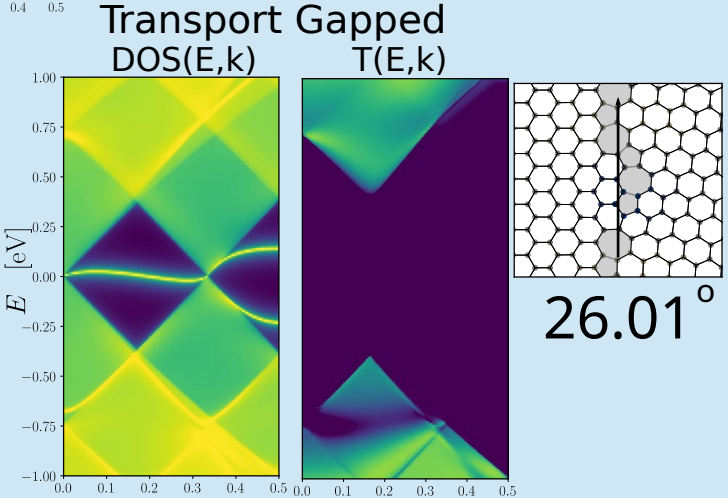
Log-plots!

Qualitative Classification

Opaque



Transport Gapped

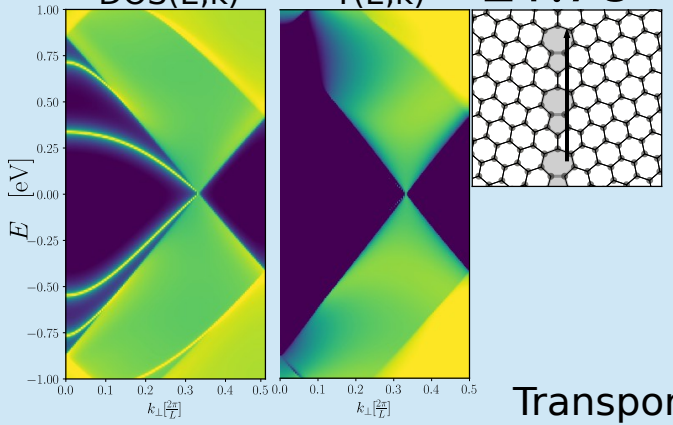


Log-plots!

Qualitative Classification

Opaque

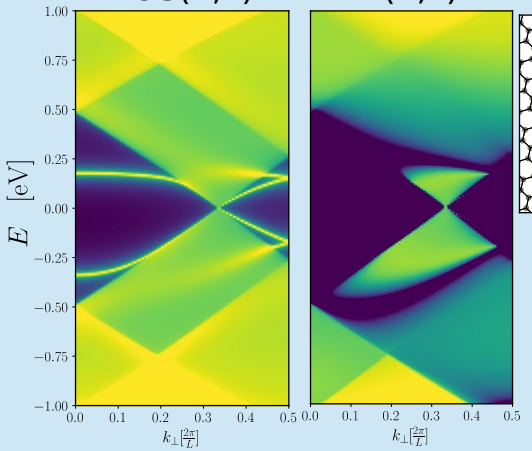
DOS(E,k) T(E,k)



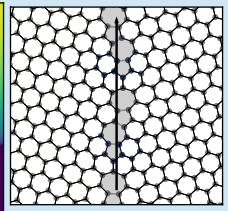
21.78°

Destructive Interference

DOS(E,k) T(E,k)

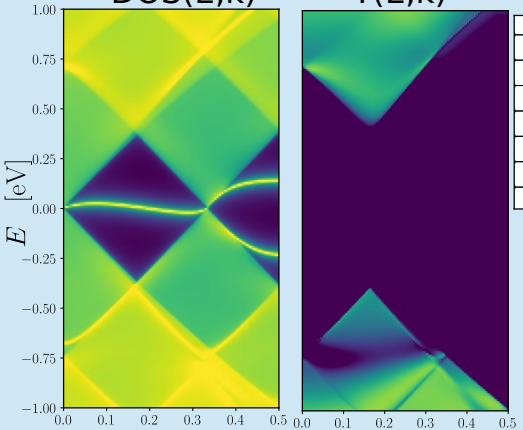


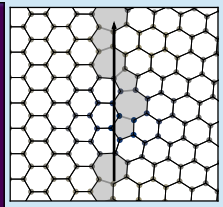
25.28°



Transport Gapped

DOS(E,k) T(E,k)





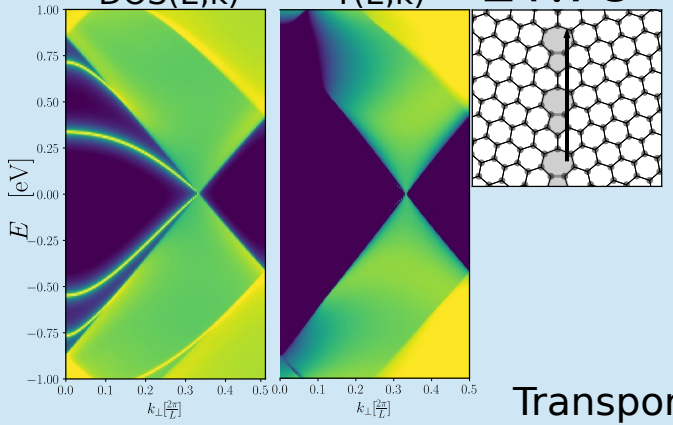
26.01°

Log-plots!

Qualitative Classification

Opaque

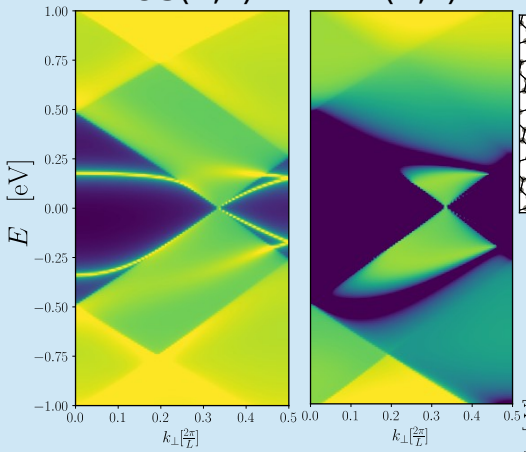
DOS(E,k) T(E,k)

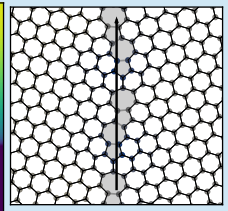


21.78°

Destructive Interference

DOS(E,k) T(E,k)

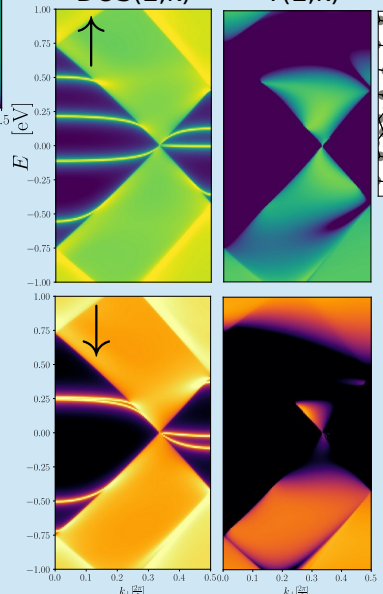


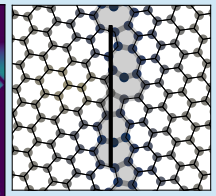


25.28°

Spinpolarised

DOS(E,k) T(E,k)

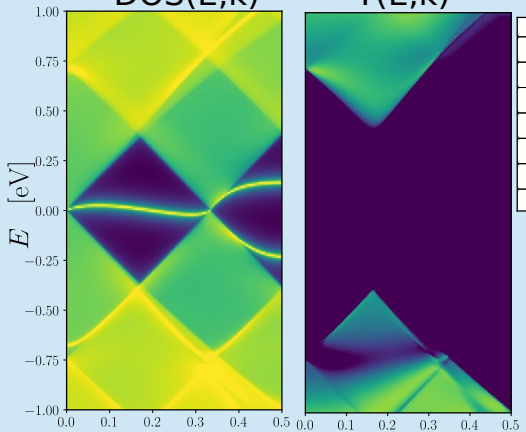


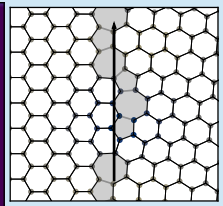


17.89°

Transport Gapped

DOS(E,k) T(E,k)

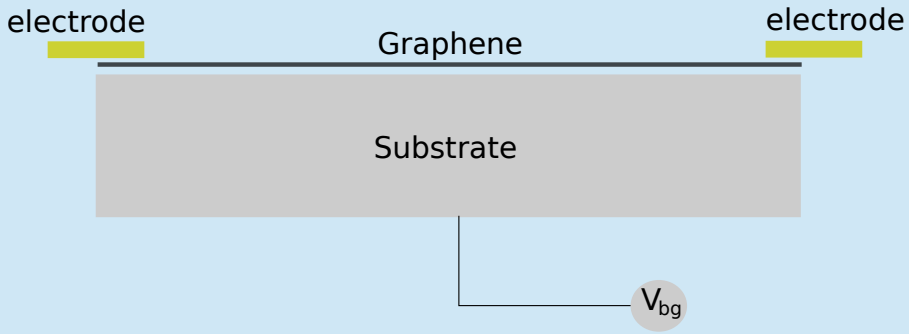




26.01°

Log-plots!

Gating

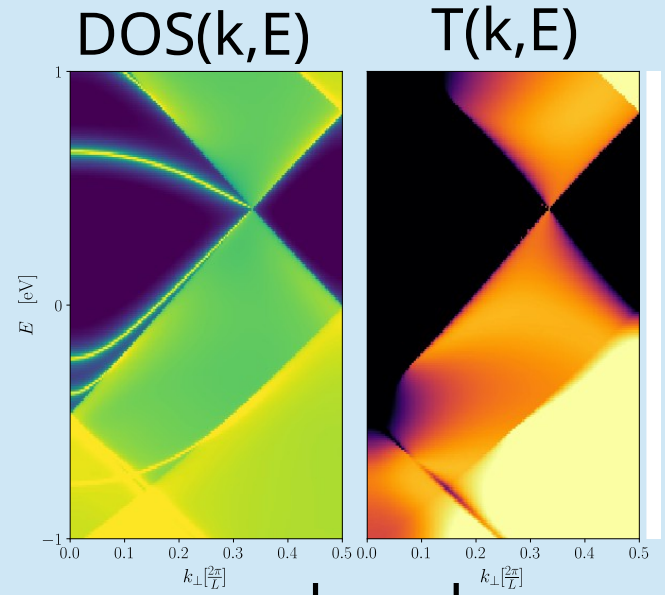


Backgate tunes the Fermi level of graphene

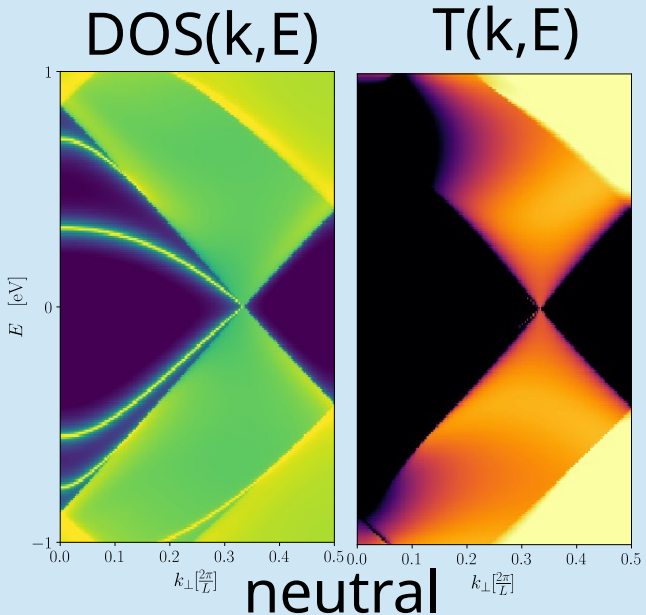
Mix extra charge into the pseudopotential in the DFT calculation.

Bellaiche, L., and David Vanderbilt.
Physical Review B 61.12 (2000): 7877

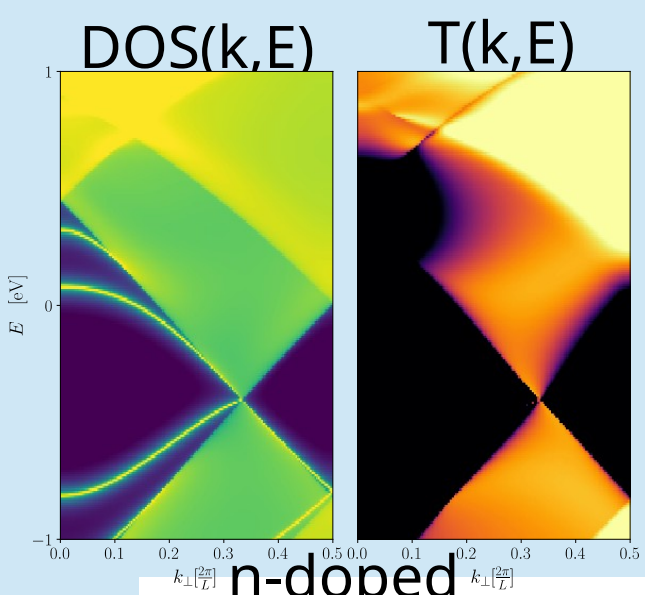
Gating: Opaque GB



p-doped



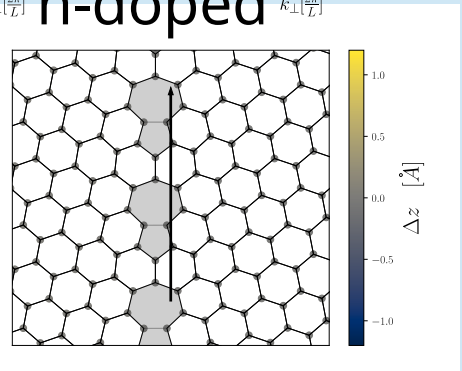
neutral



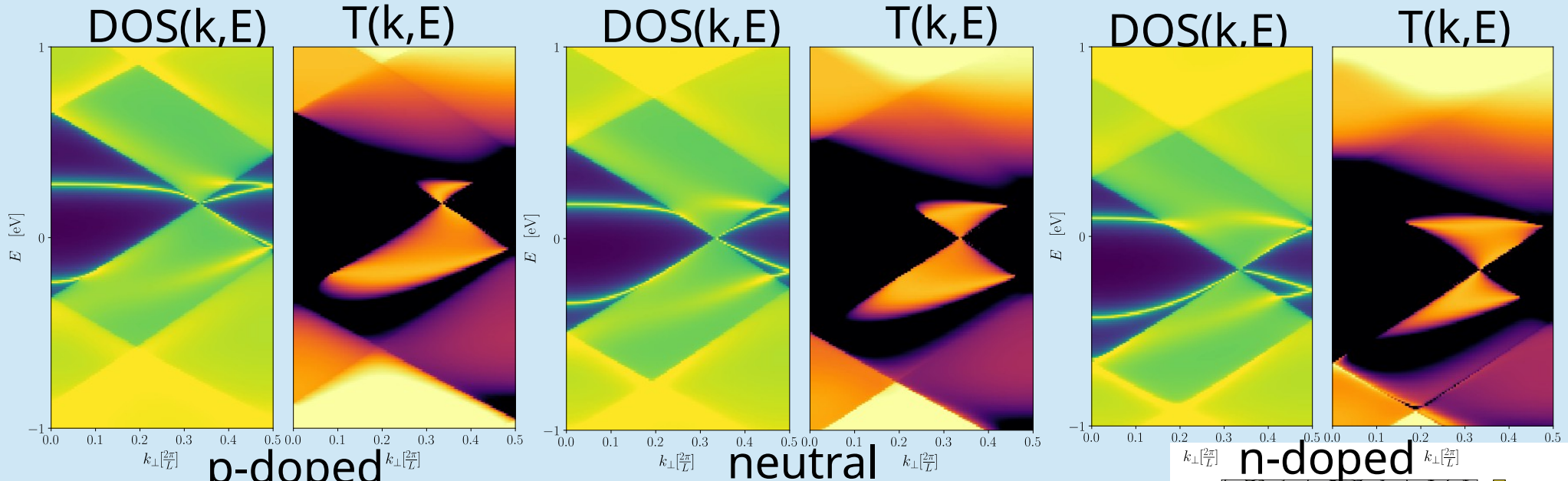
n-doped

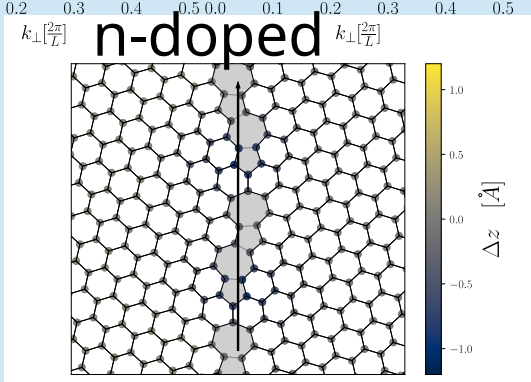
Band deformation

Little change in transmission



Gating: Destructively interfering GB

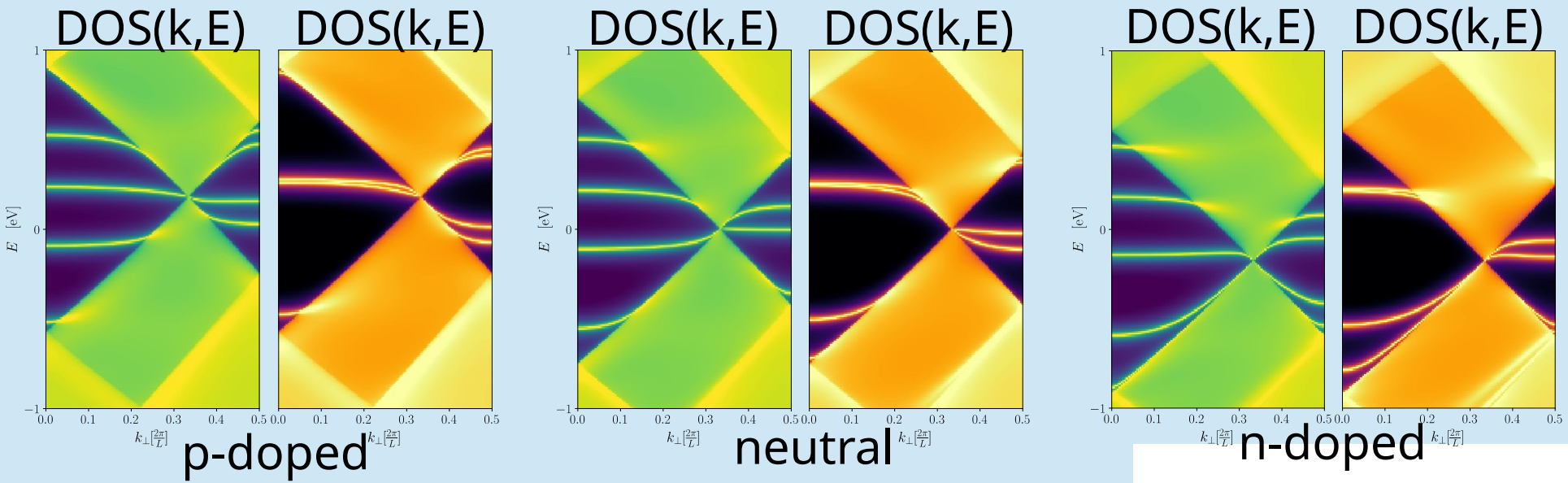




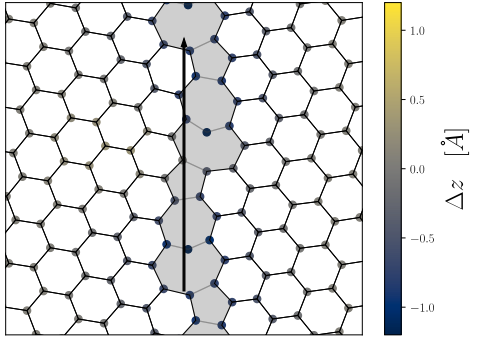
Significant changes in QP bands

Pushing band into Dirac Cone → Higher Transmission

Gating: Spinpolarized



Significant changes in QP bands

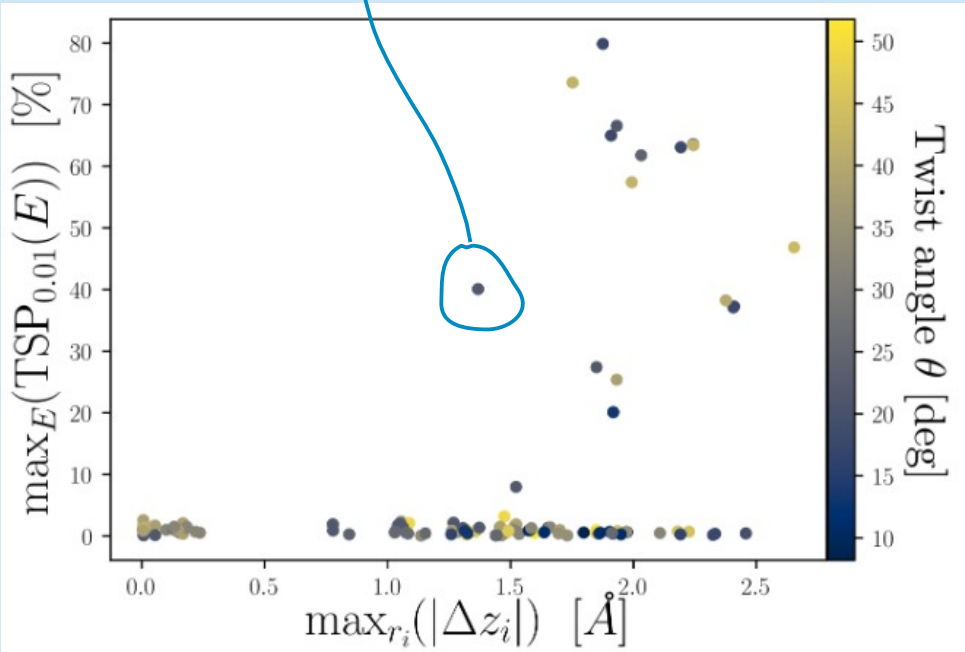


Spinfiltering

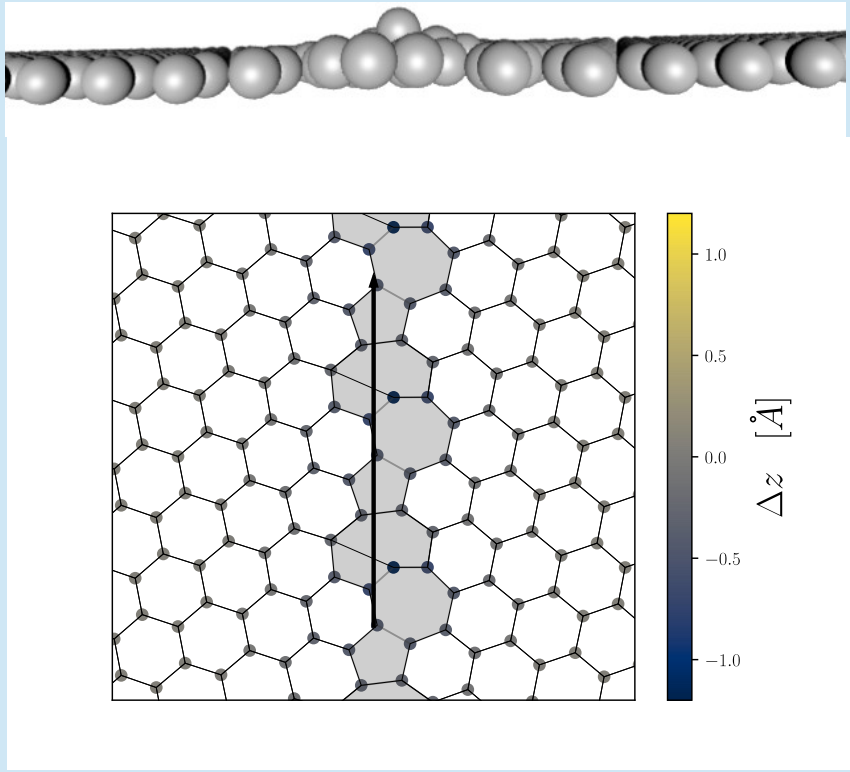
Spinfiltering measure:

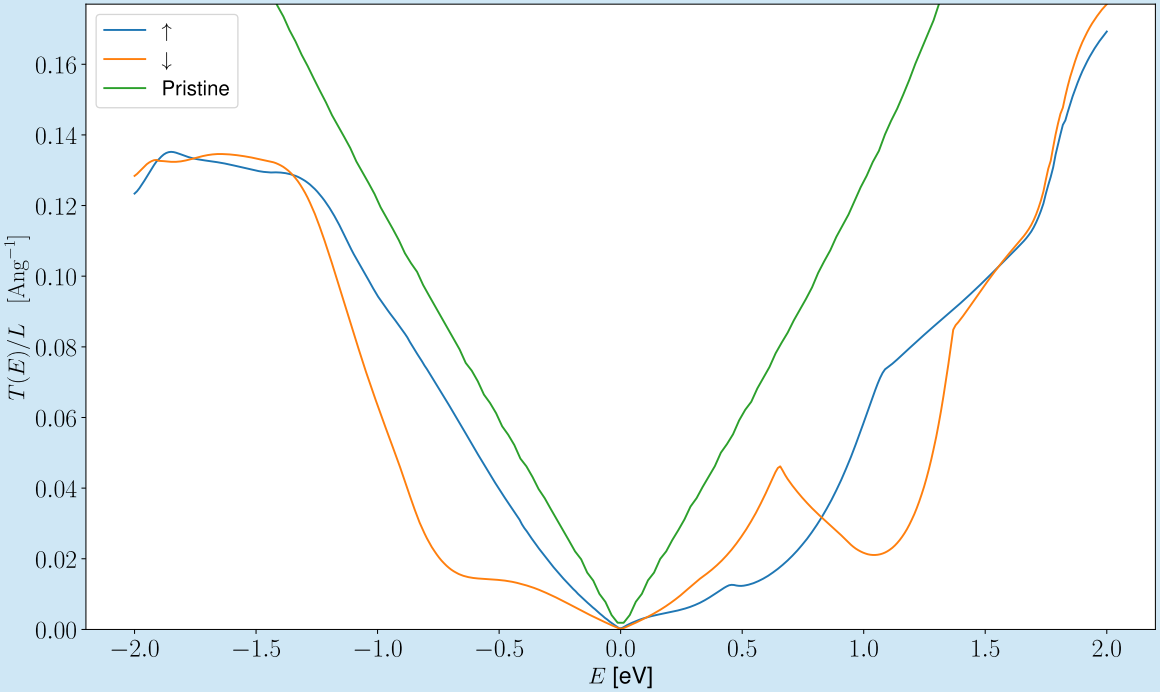
$$\mathrm{TSP}_\delta(\epsilon) = \frac{T_\uparrow(\epsilon) - T_\downarrow(\epsilon)}{T_\uparrow(\epsilon) + T_\downarrow(\epsilon) + \delta}$$

Lets have a look at this



Spinfiltering





Quasiparticles: Lifetimes

Solve: $[H_d + \frac{1}{2}(\Sigma(\epsilon) + \Sigma^\dagger(\epsilon))]\psi^{QP} = \epsilon\psi^{QP}$

$$\tau \sim \frac{2\hbar}{|\langle\psi^{QP}|\Sigma(\epsilon) - \Sigma^\dagger(\epsilon)\,|\psi^{QP}\rangle|}$$

Quasiparticles: Lifetimes

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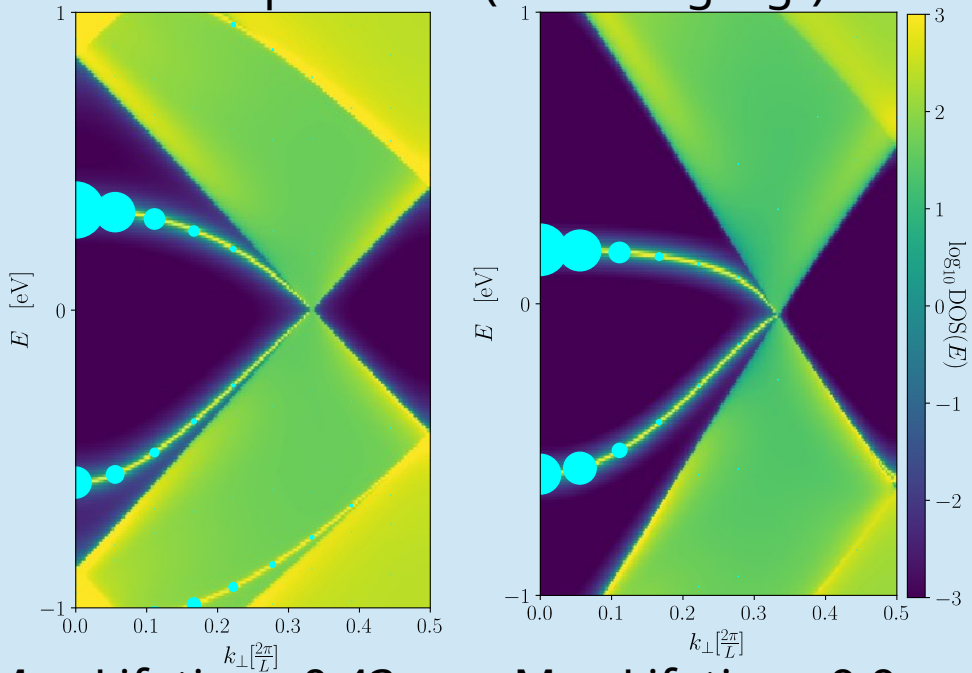
From Experiment (5-7 & “Zigzag”)



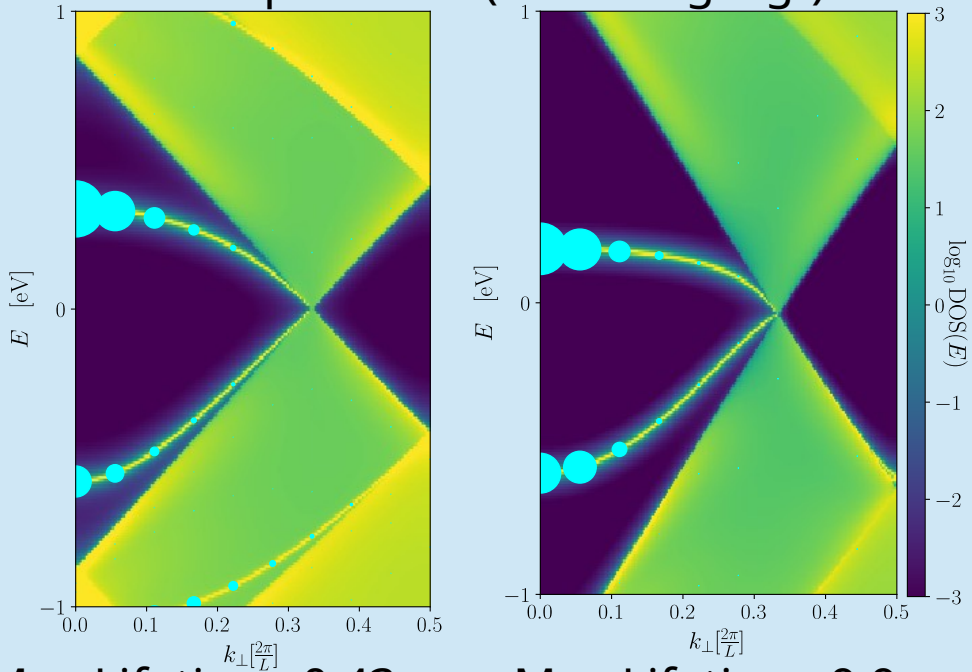
Max Lifetime: 0.43ns Max Lifetime: 9.9ns

Quasiparticles: Lifetimes

Solve: $[H_d + \frac{1}{2}(\Sigma(\epsilon) + \Sigma^\dagger(\epsilon))]\psi^{QP} = \epsilon\psi^{QP}$

$$\tau \sim \frac{2\hbar}{|\langle\psi^{QP}|\Sigma(\epsilon) - \Sigma^\dagger(\epsilon)\,|\psi^{QP}\rangle|}$$

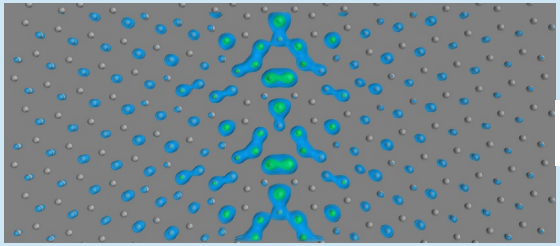
From Experiment (5-7 & "Zigzag")



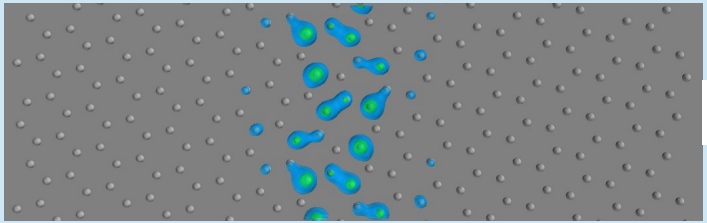
Max Lifetime: 0.43ns

Max Lifetime: 9.9ns

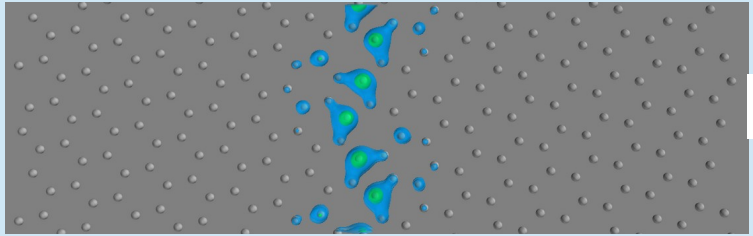
5-7 , E=-0.32eV, k=1/6



Zigzag, E=0.21eV, k=0.056

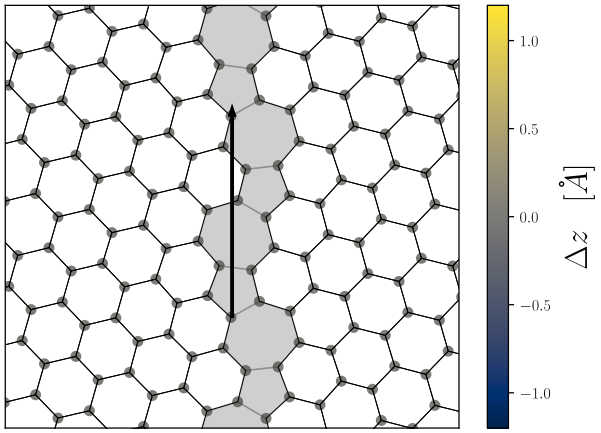


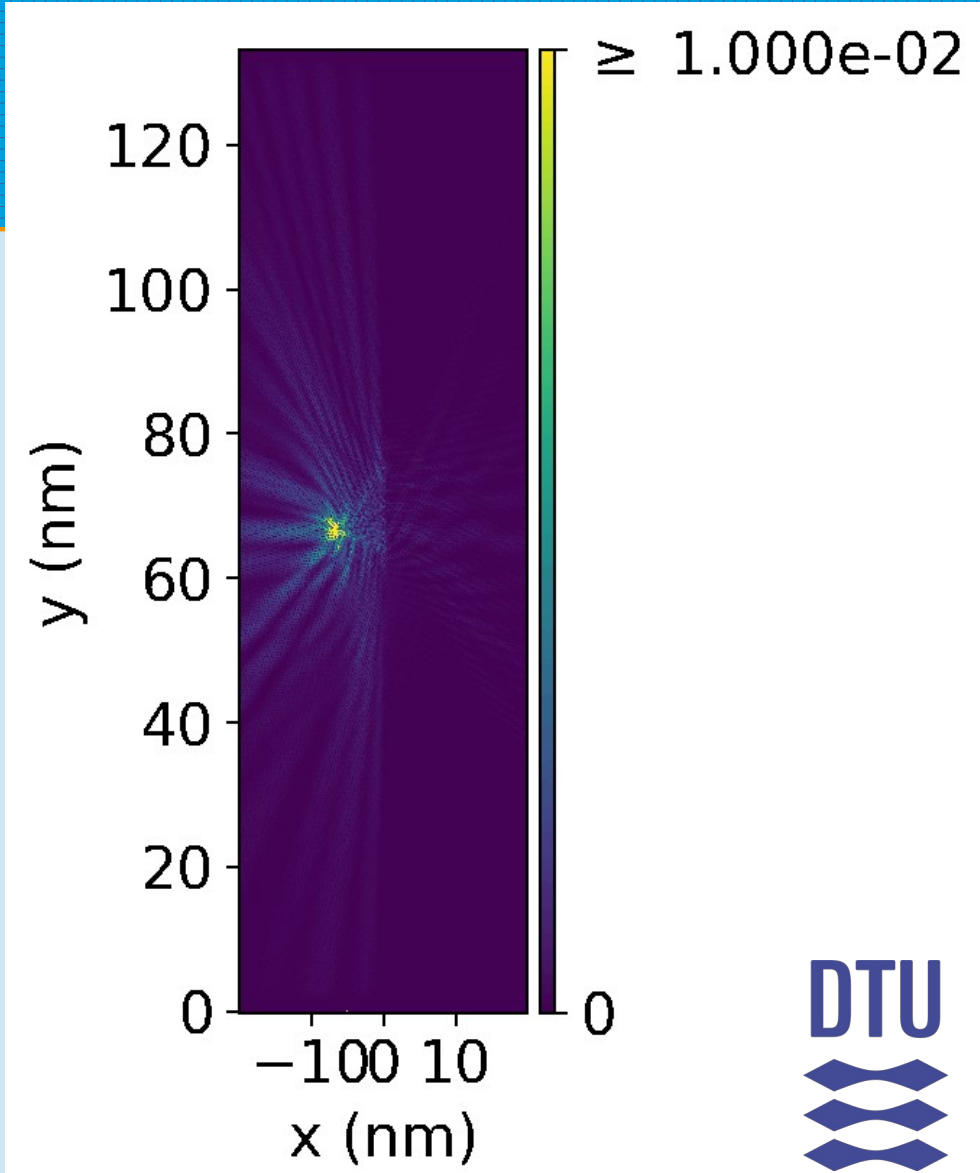
Zigzag, E=-0.54eV, k=0.056



Current flow, TB

Inject electron on a site
Scanning energies (-2, 2)eV





In Conclusion

Periodic GBs: quasiparticle states

- Localized
- Bandstructure
- Strong gate-dependence / tunability
- Out-of-plane buckling → Spin polarization + Spin filtering

Electron transmission

- QP Intersection with Dirac Cone → Enhanced Transmission

Work in progress

A.B Lorentzen,
P. Bøggild,
A.P. Jauho,
M. Brandbyge

Funding: DET FRIE FORSKNINGSRÅD
DANISH COUNCIL FOR
INDEPENDENT RESEARCH