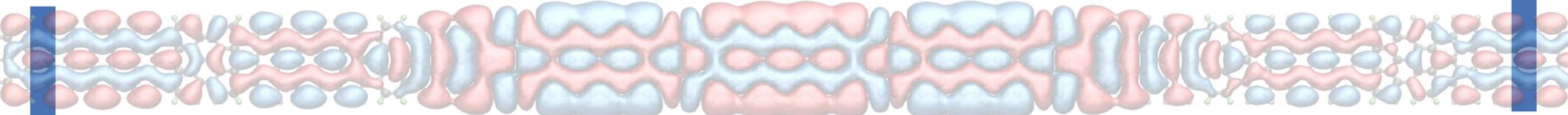


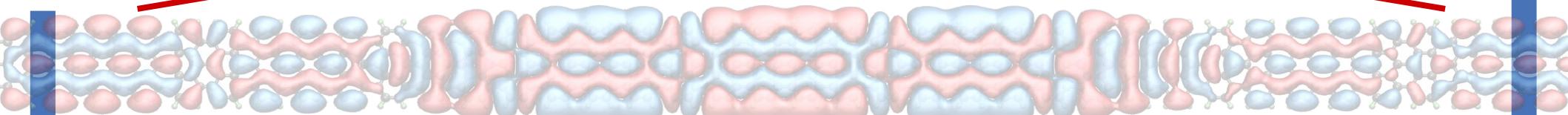
1-D Quantum Well States on Doped Graphene Nanoribbons Revealed by Transport Simulations



Pedro Brandimarte, Eduard Carbonell-Sanromà, Richard Balog, Martina Corso, Shigeki Kawaii, Aran Garcia-Lekue, Shohei Saito, Shigehiro Yamaguchi, Jose I. Pascual, and Daniel Sánchez-Portal

1-D Quantum Well States on Doped Graphene Nanoribbons

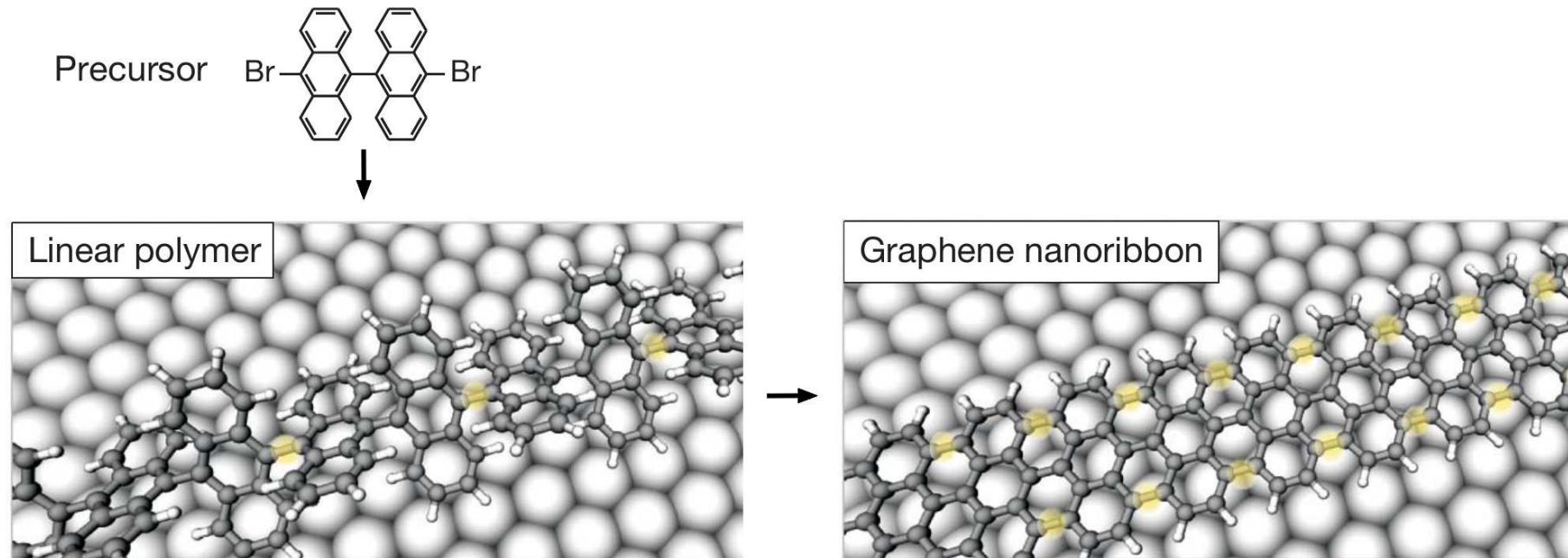
Revealed by Transport Simulations



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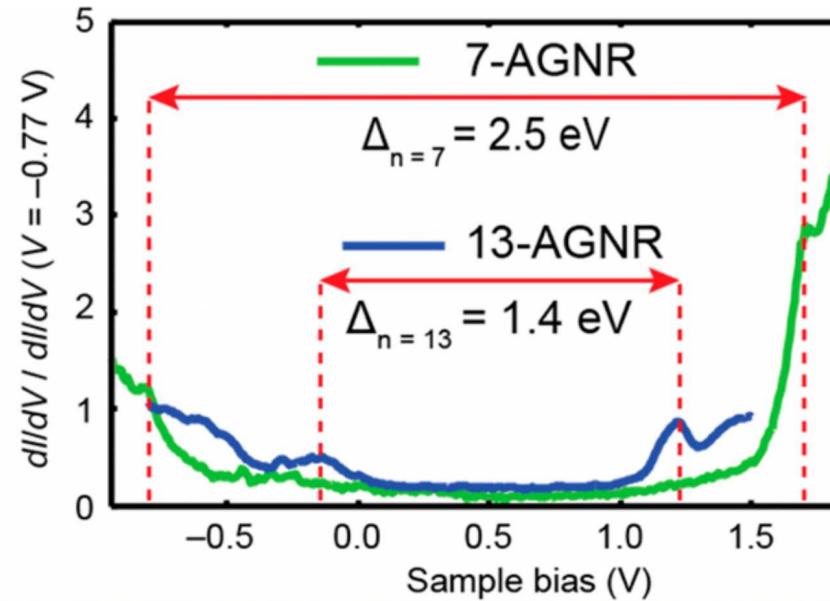
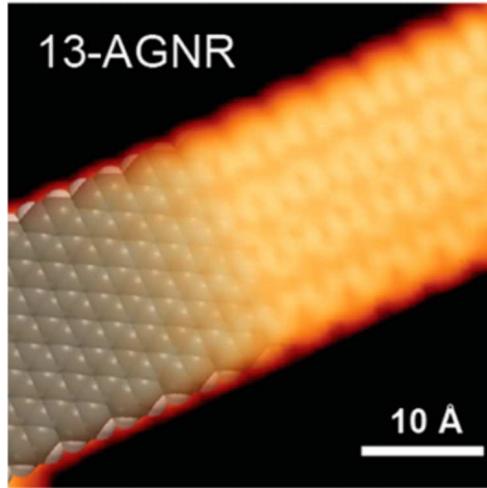
Graphene Nanoribbons (GNRs)

- Bottom-up fabrication of both AGNR and ZGNR by on-surface reaction.

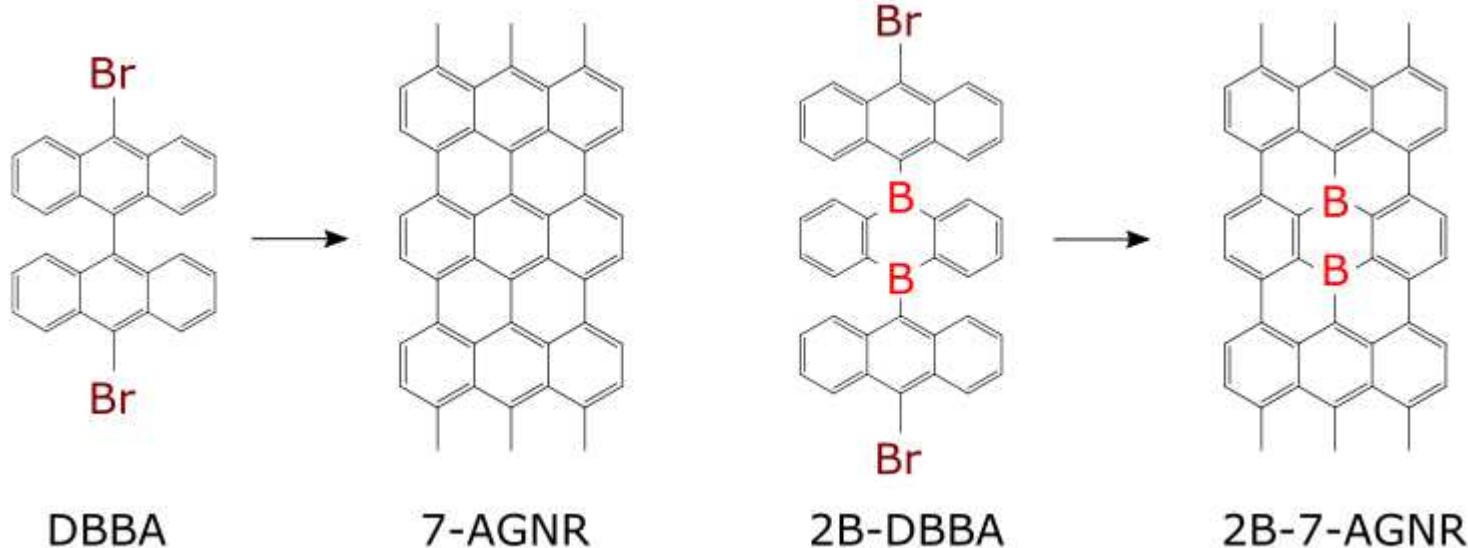


Graphene Nanoribbons (GNRs)

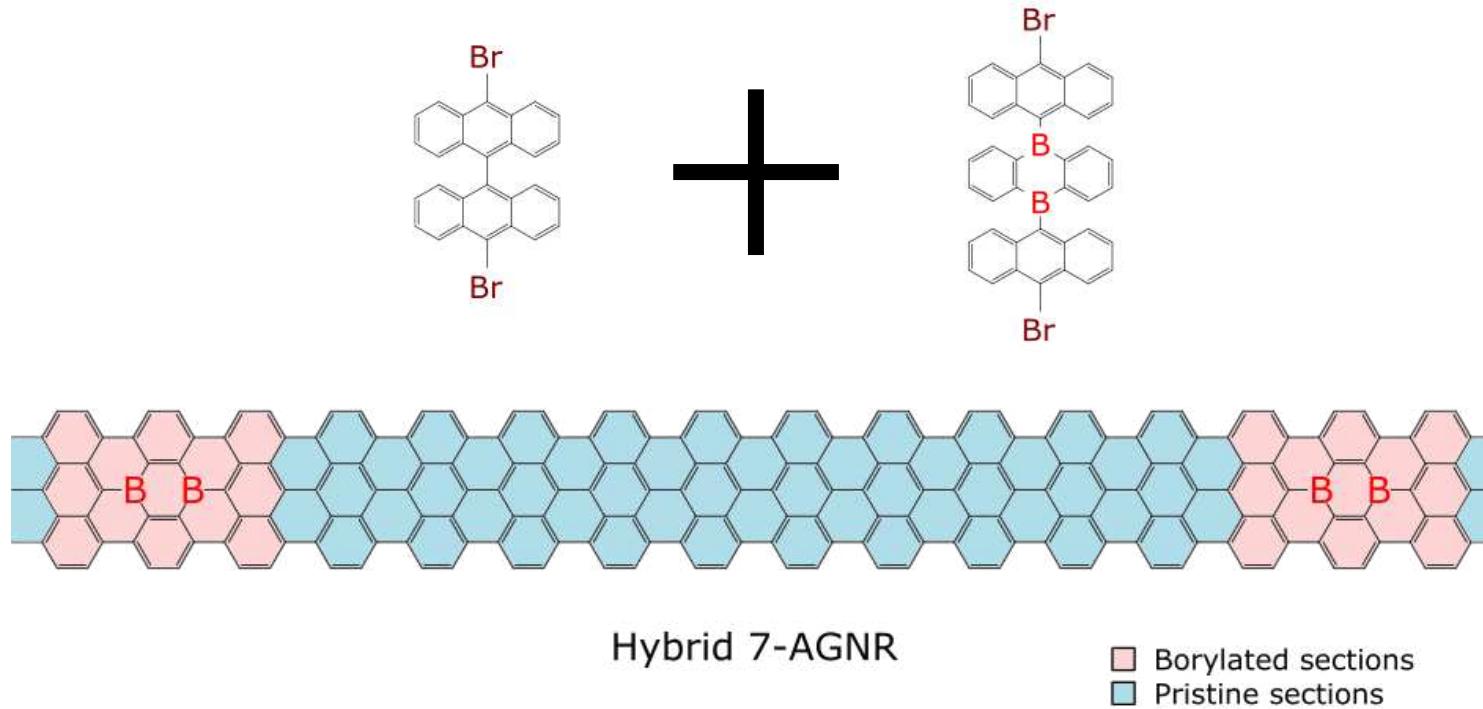
- Energy gap depending on their width and shape.



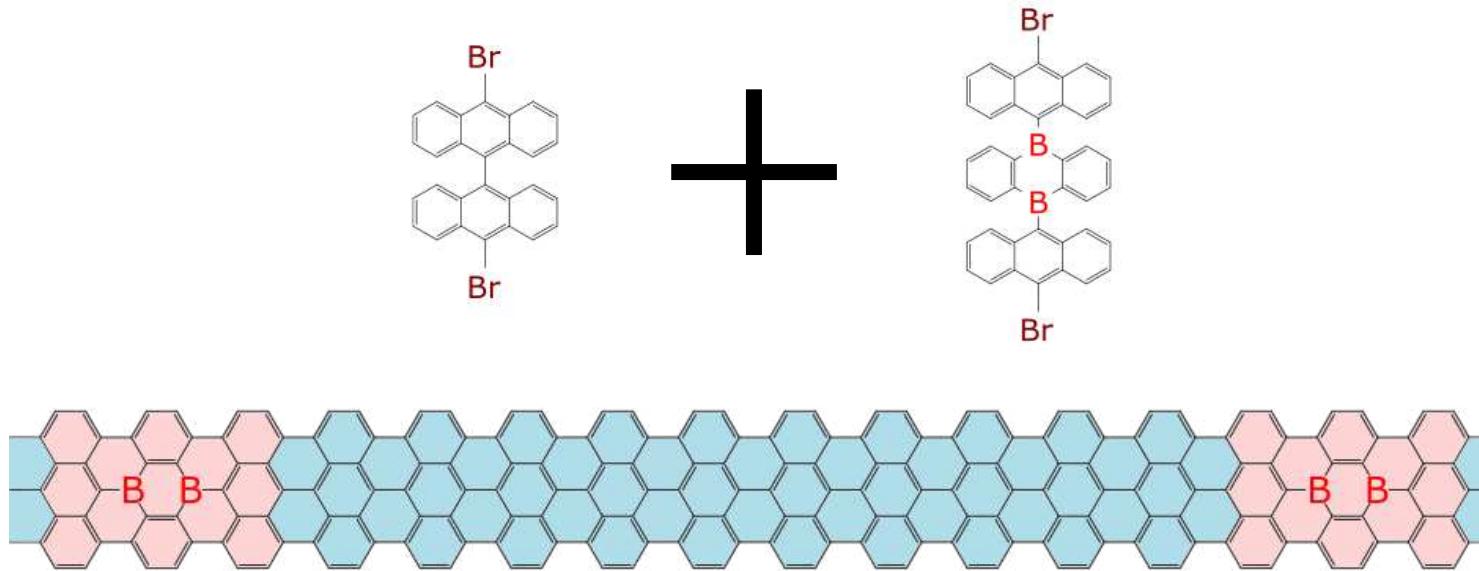
B-doped graphene nanoribbons



B-doped graphene nanoribbons



B-doped graphene nanoribbons

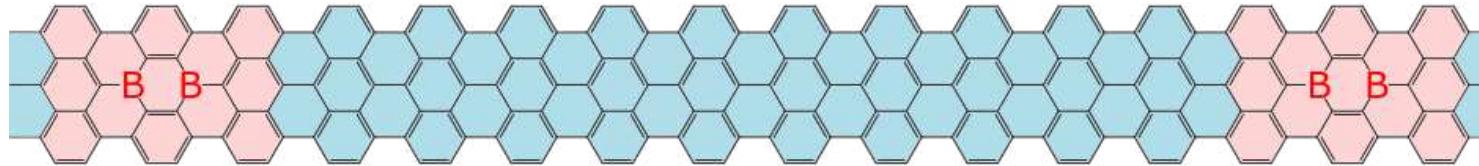
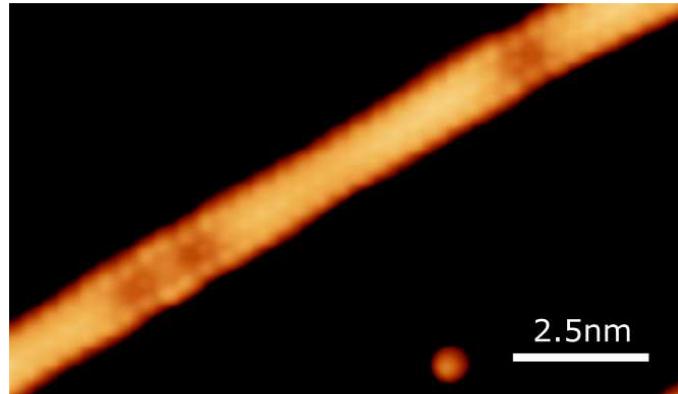


Hybrid 7-AGNR

■ Borylated sections
■ Pristine sections

E. Cabonell-Sanromà, P. Brandimarte *et al.* *Nano Letters* **17**, 50 (2017).

B-doped graphene nanoribbons

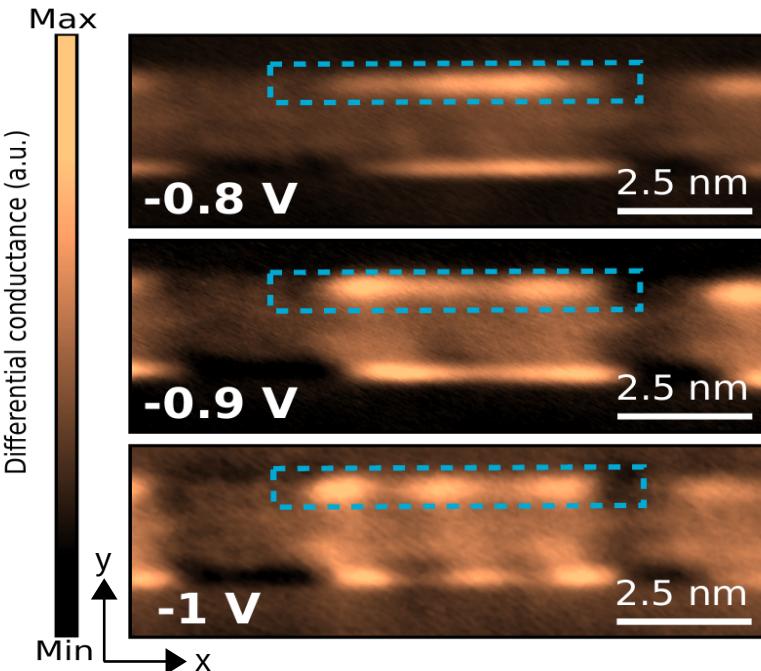
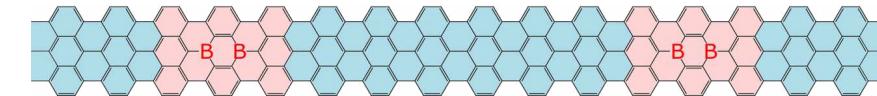


Hybrid 7-AGNR

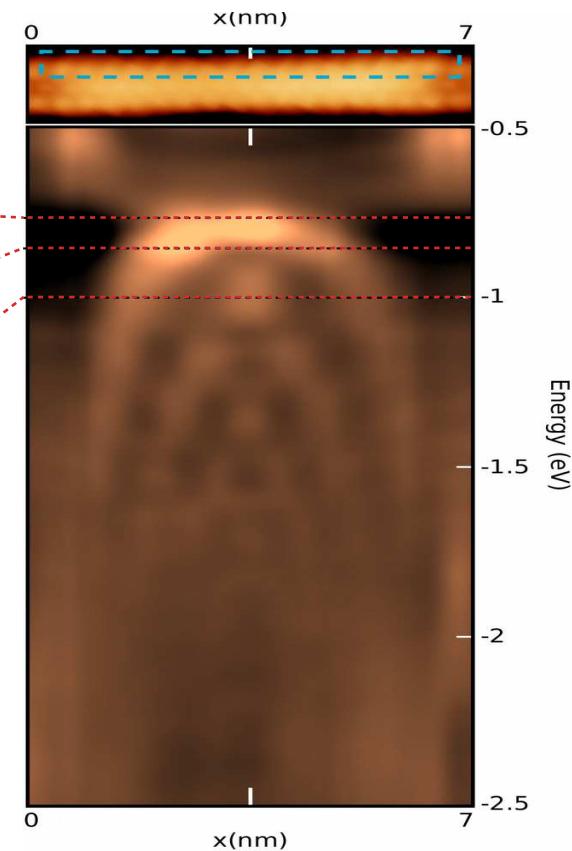
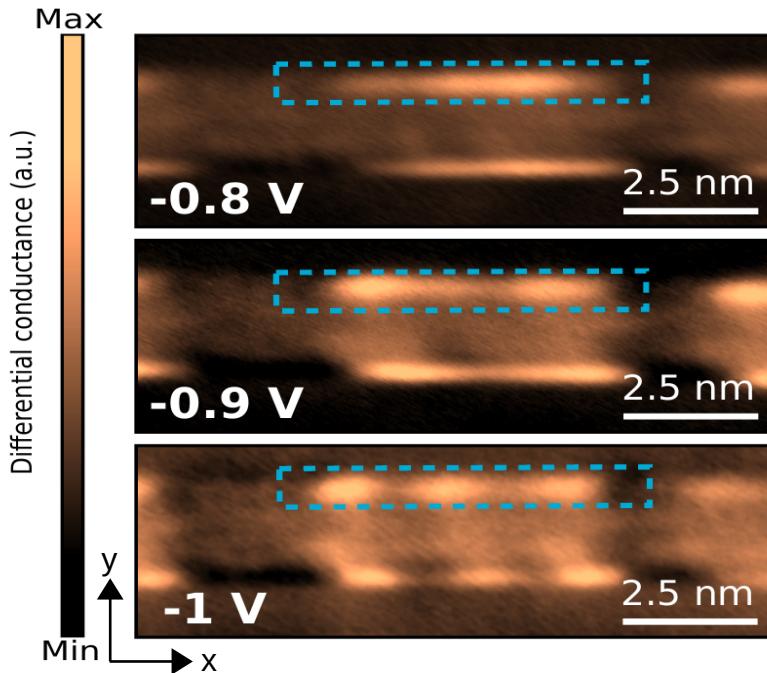
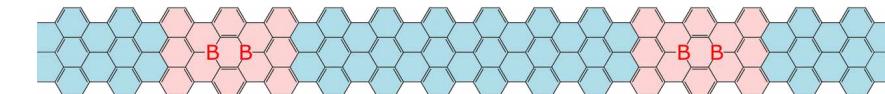
■ Borylated sections
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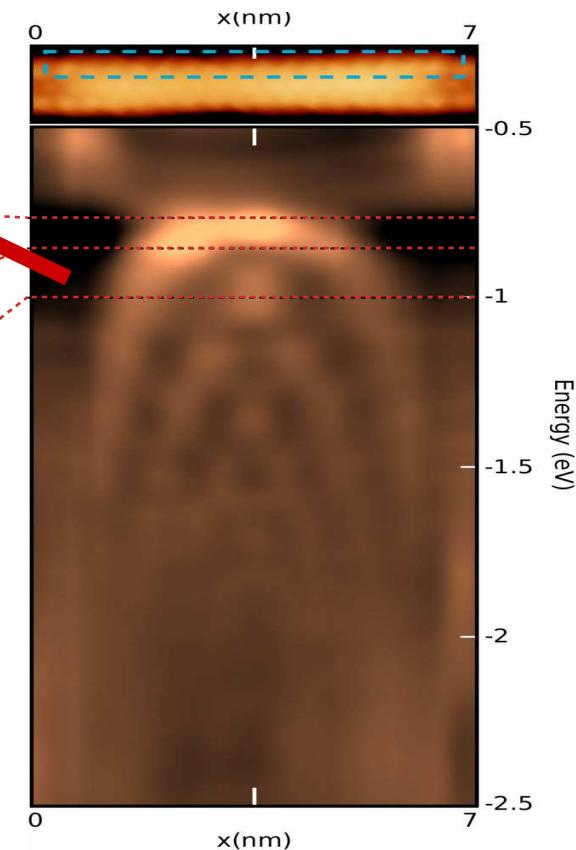
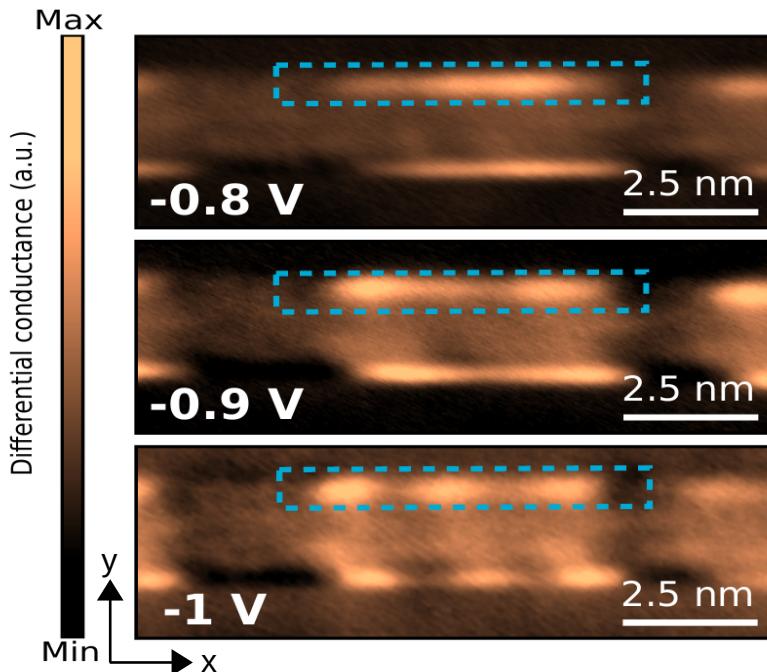
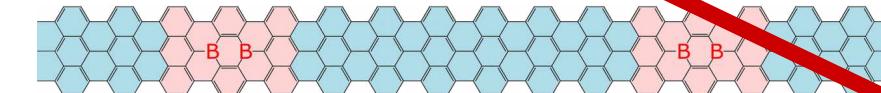
B-doped graphene nanoribbons



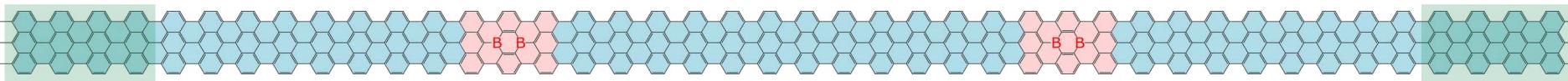
B-doped graphene nanoribbons



B-doped graphene nanoribbons



Transport simulation setup



Density-Functional Theory (DFT)

+

Non-Equilibrium Green's Function (NEGF)

TranSIESTA

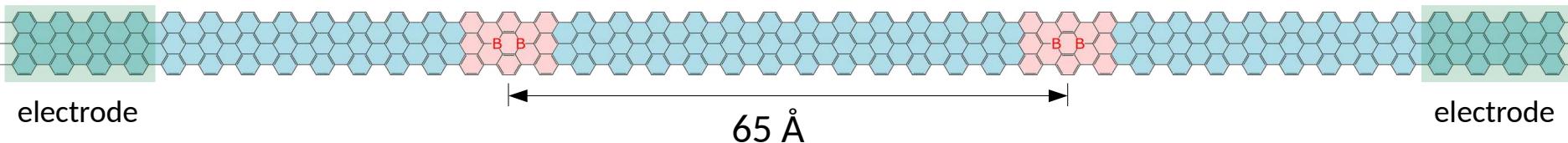
J. M. Soler *et al.* *J. Phys. Condens. Matter.* **14**, 2745 (2002).

M. Brandbyge *et al.* *Phys. Rev. B* **65**, 165401 (2002).

N. Papior *et al.* *Comp. Phys. Commun.* **212**, 8 (2017).

E. Cabonell-Sanromà, P. Brandimarte *et al.* *Nano Letters* **17**, 50 (2017).

Transport simulation setup



Density-Functional Theory (DFT)

+

Non-Equilibrium Green's Function (NEGF)

TranSIESTA

Simulation characteristics:

- 756 atoms;
- double- ζ (5040 orbitals);
- vdW (optB88);
- real space grid cutoff: 250 Ry;
- forces < 10 meV/Å.

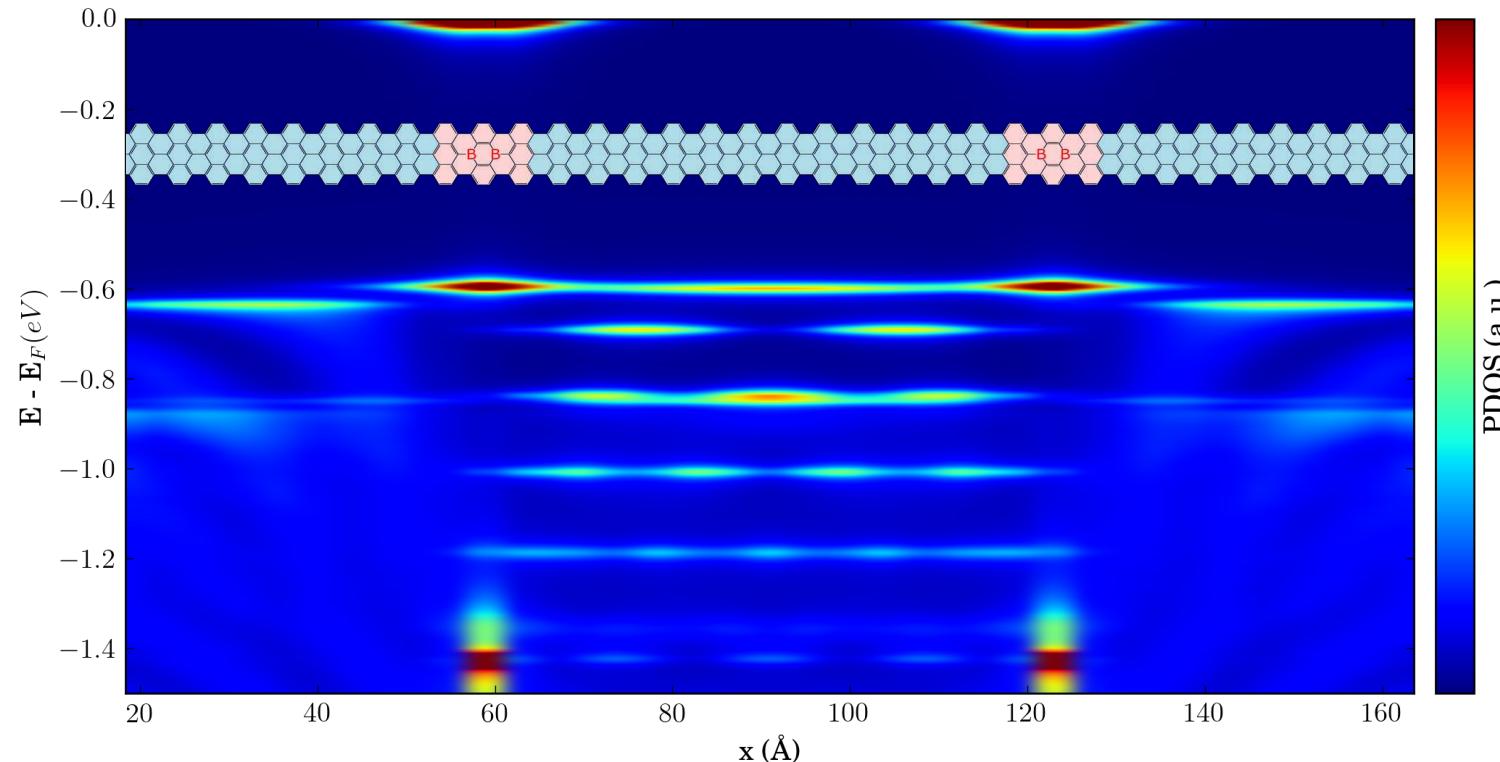
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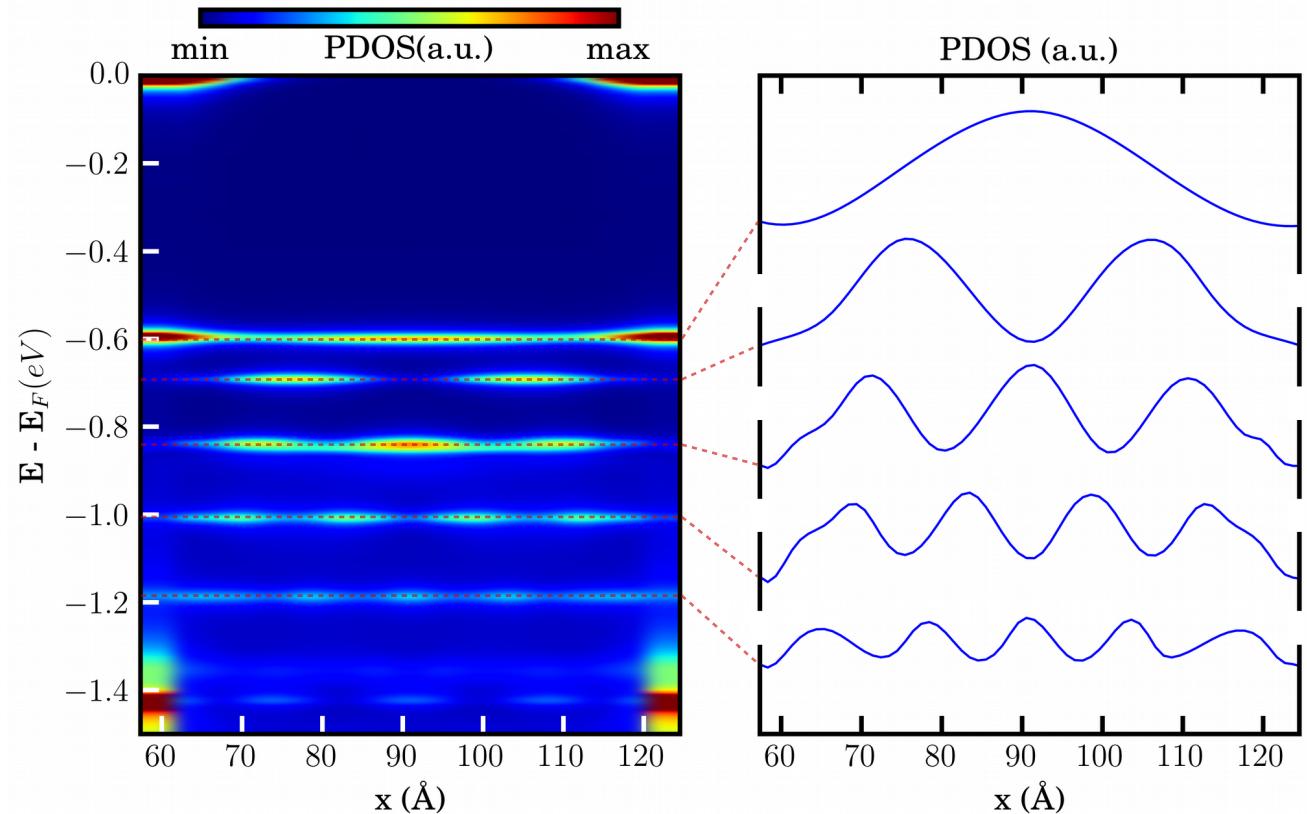
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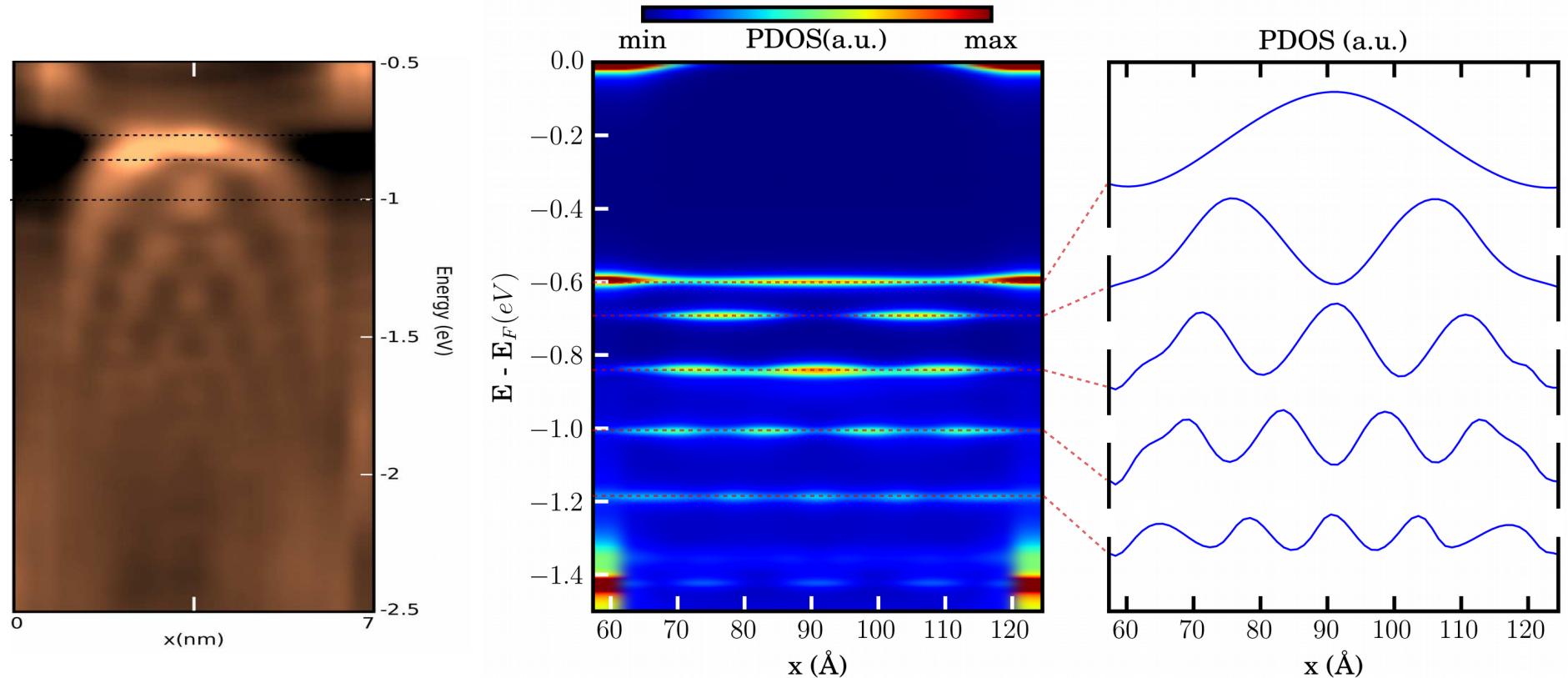
DOS projected on each ribbon “row”



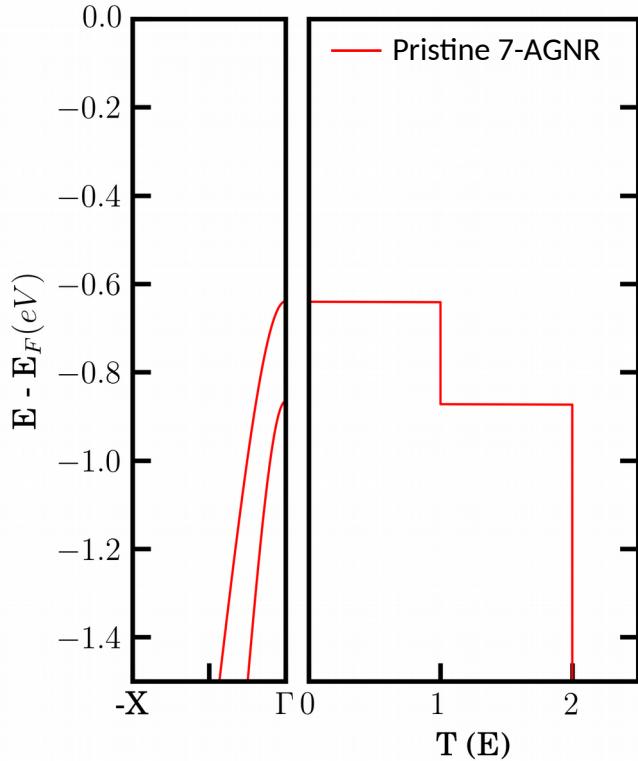
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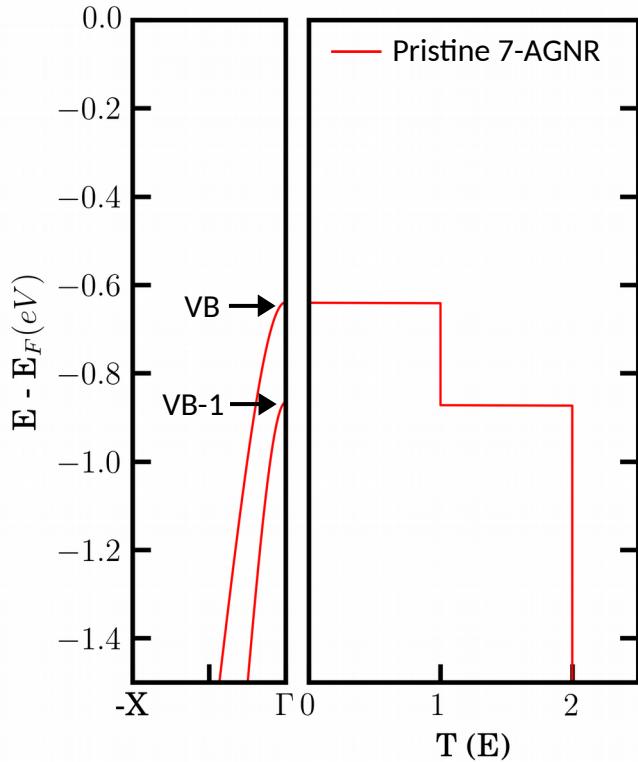
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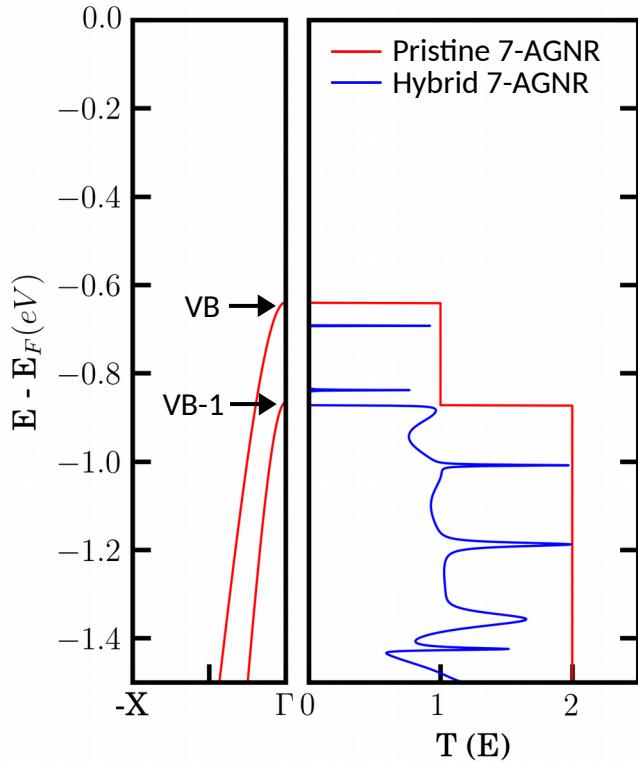
Zero bias transmission



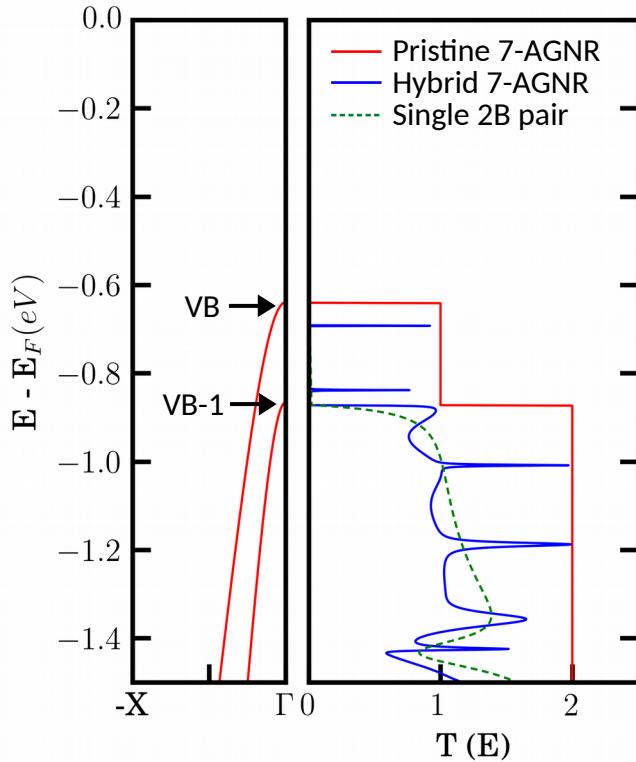
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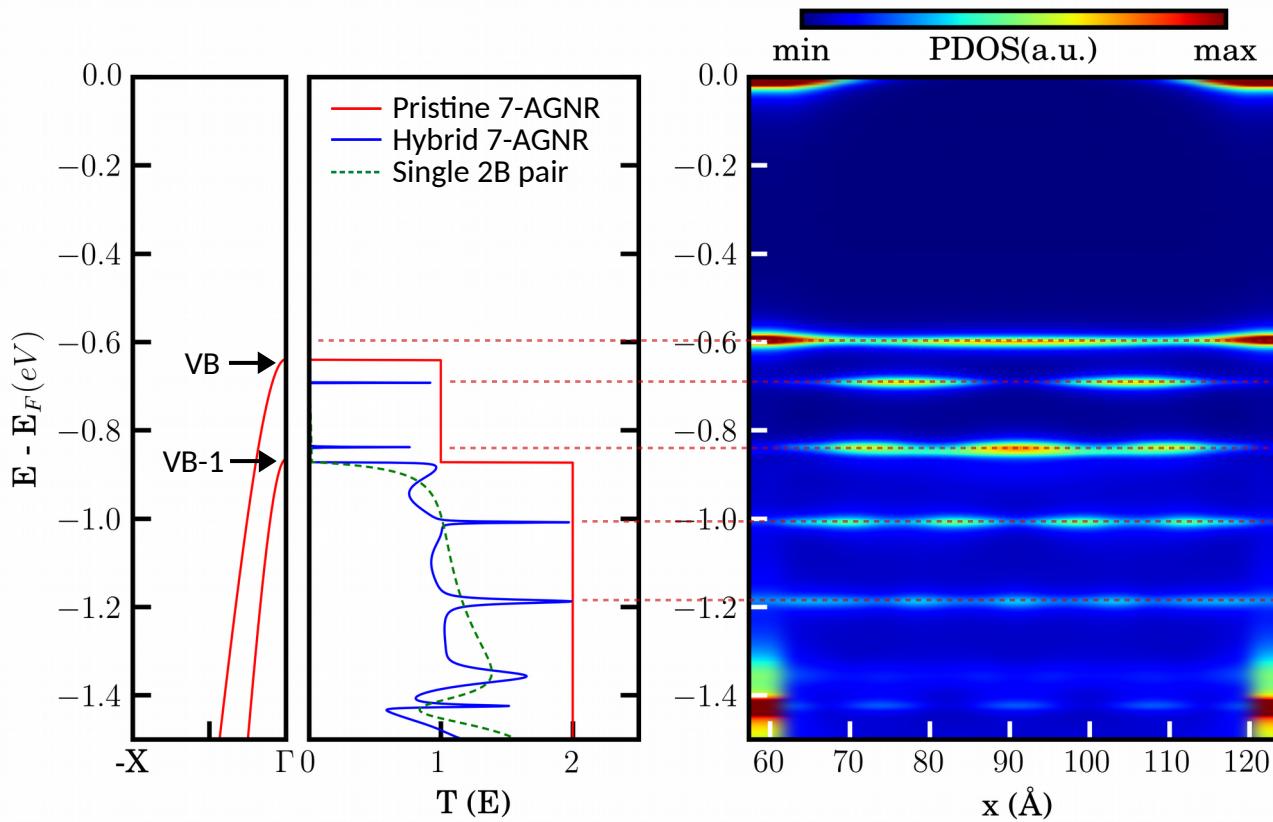
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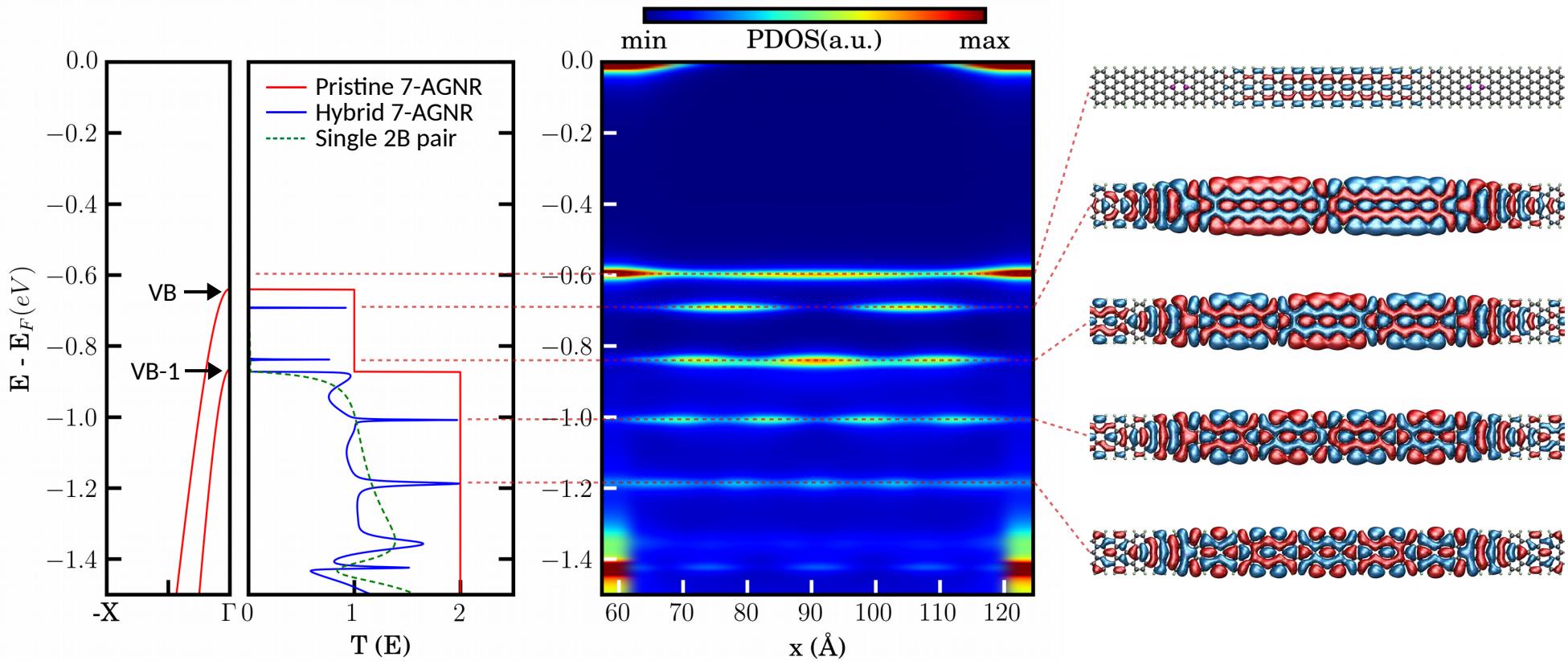
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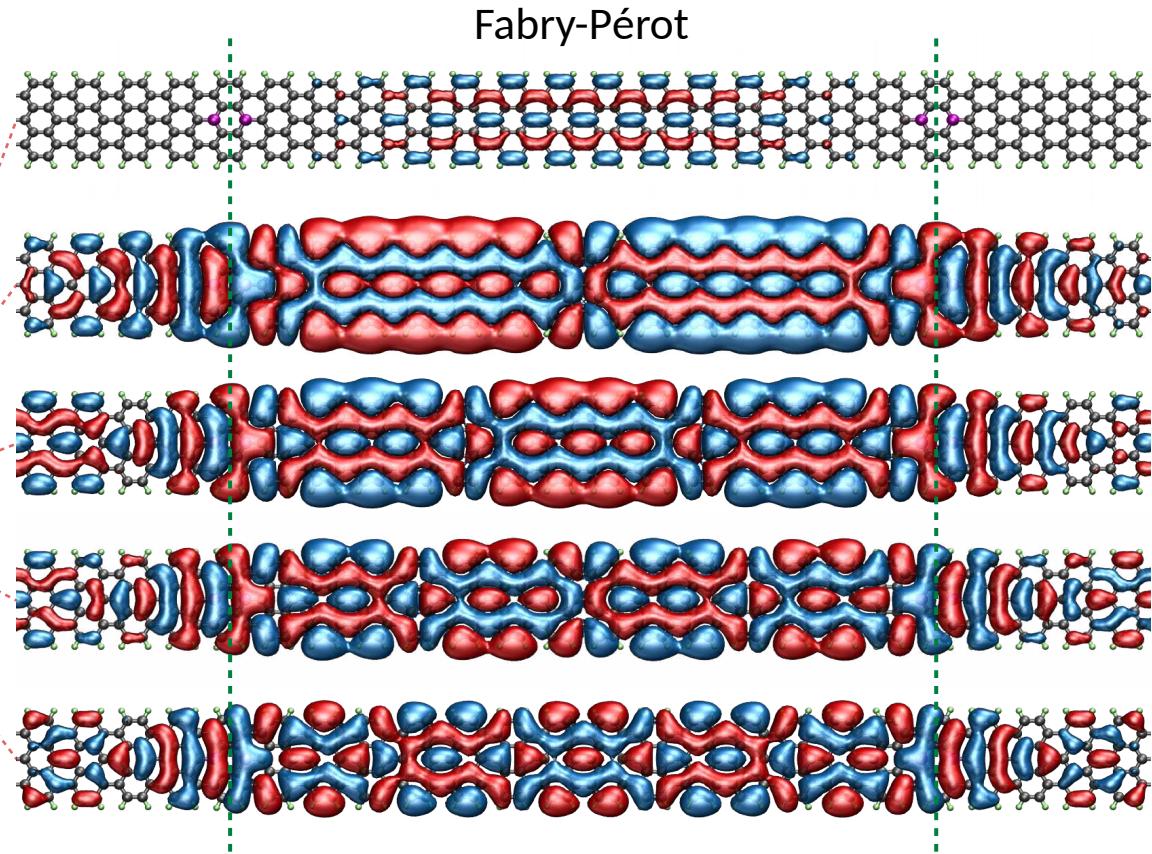
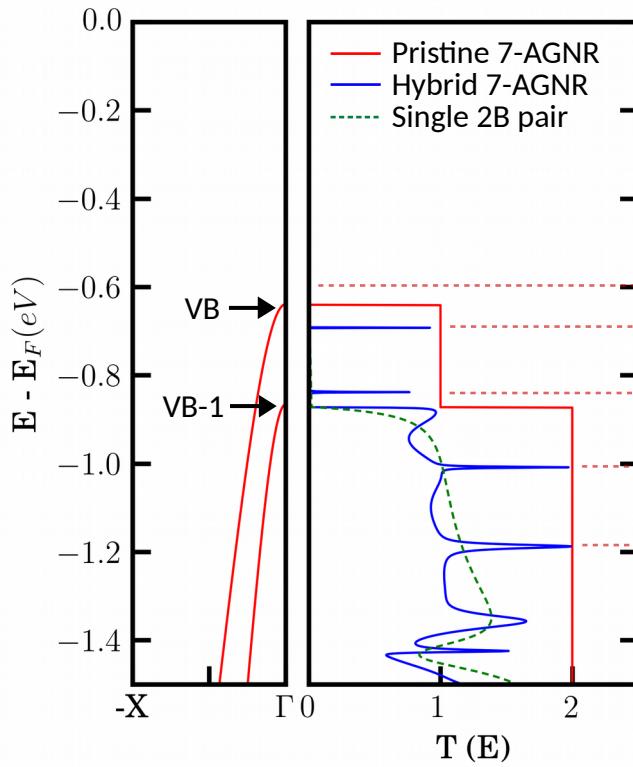
Zero bias transmission



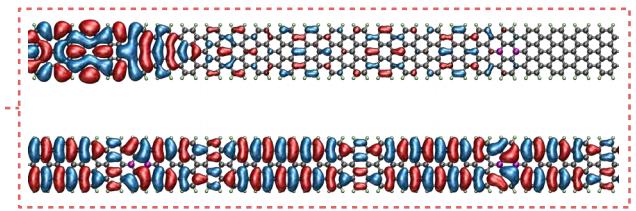
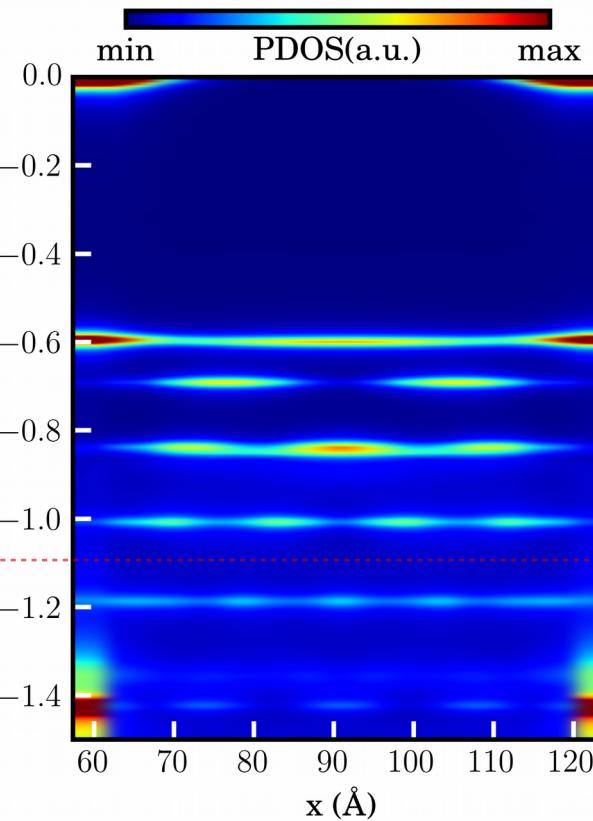
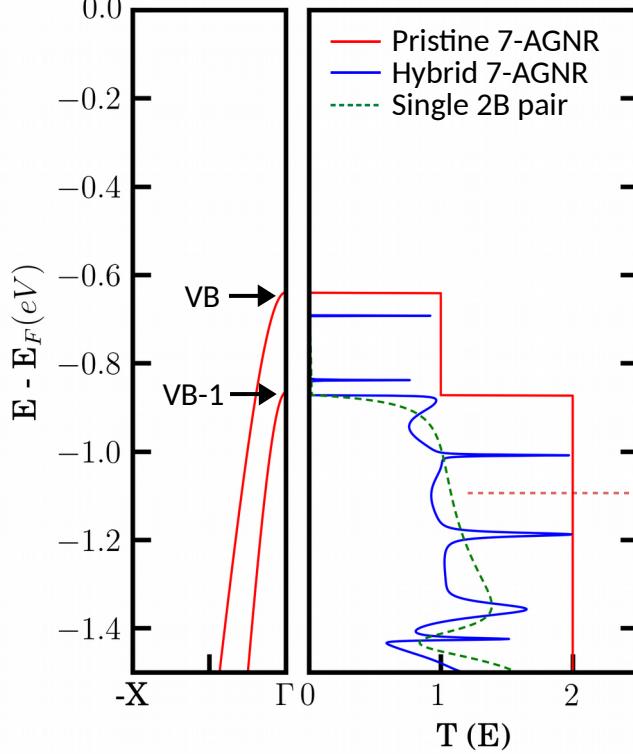
Scattering states



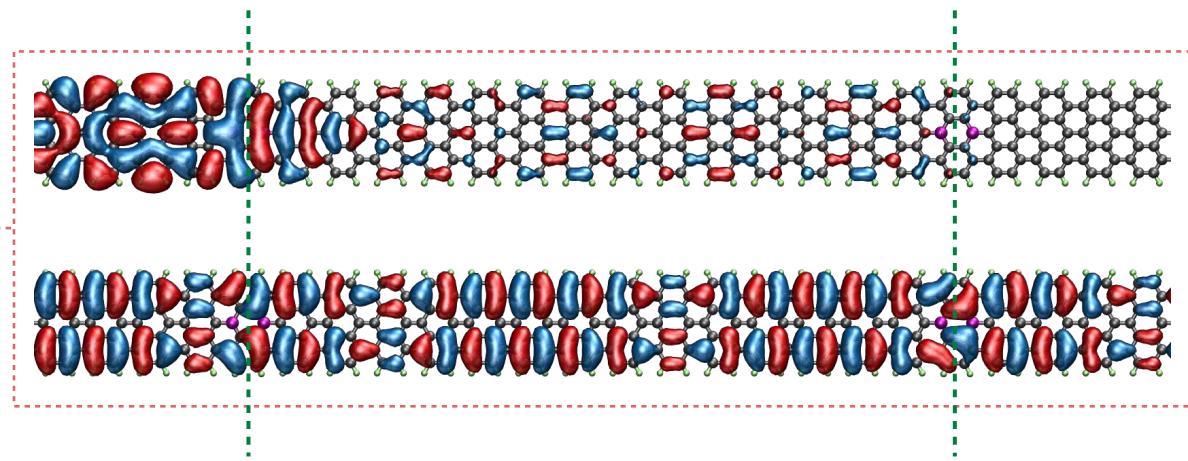
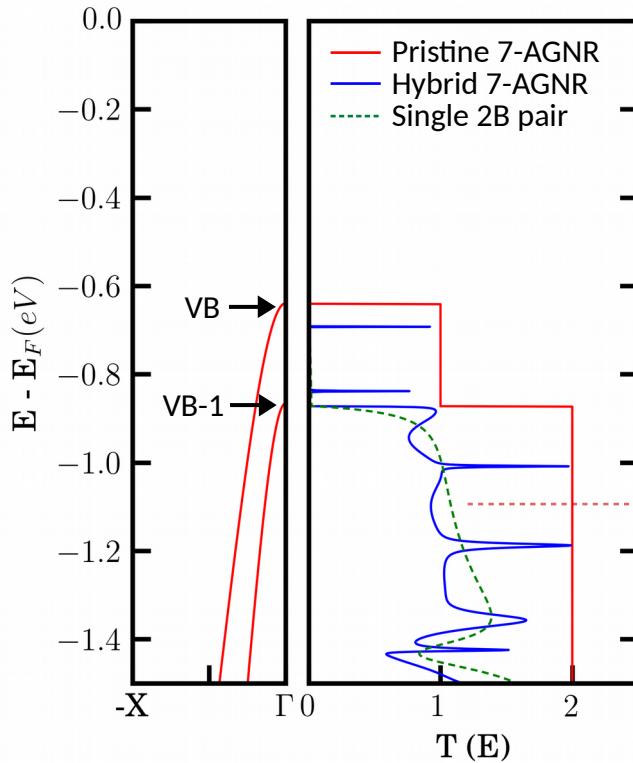
Scattering states



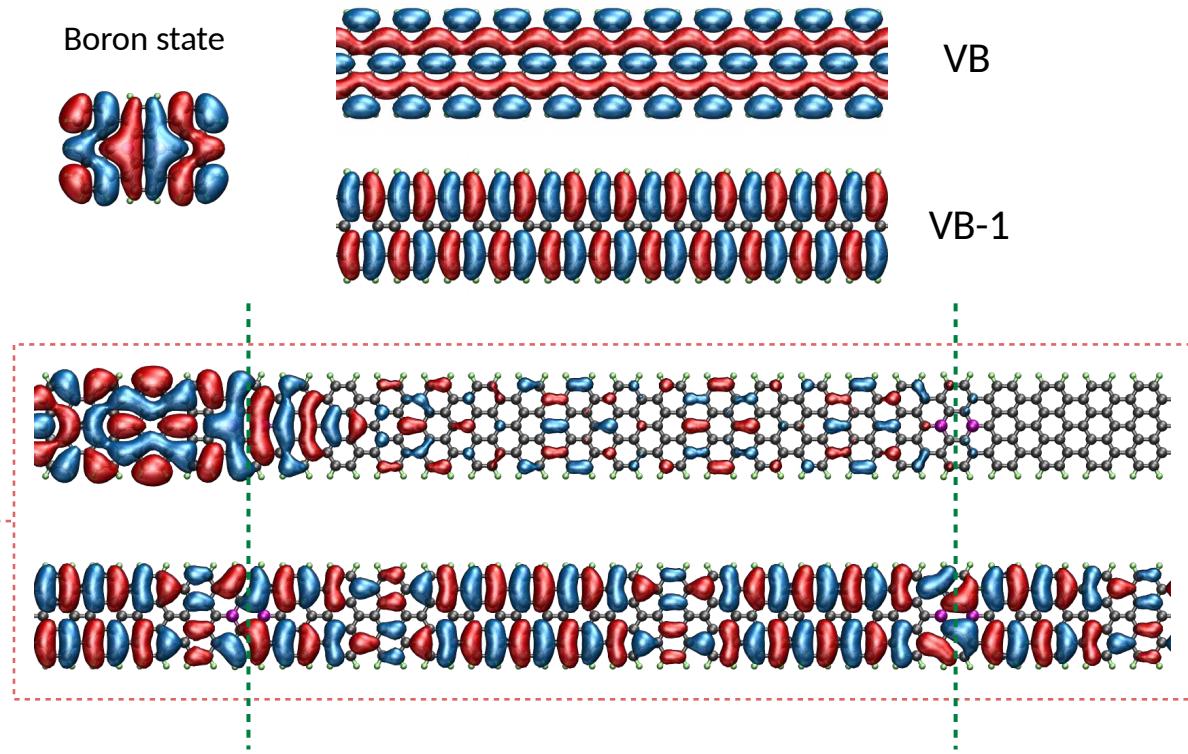
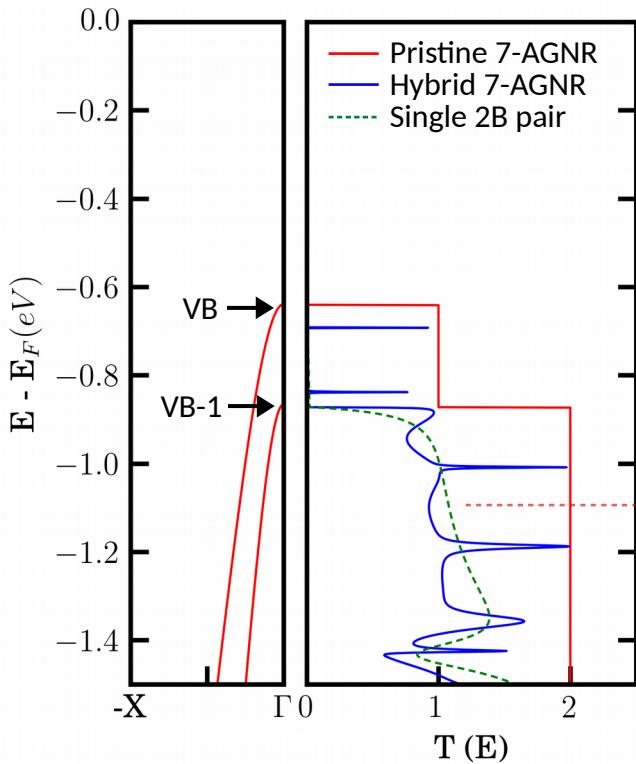
Scattering states



Band selectivity



Band selectivity



Conclusion

1-D Quantum Well States on Doped Graphene Nanoribbons ~~Revealed~~ by Transport Simulations Understood

- Transport simulations can **reproduce** observed quantum well states.
- The theoretical analysis **reveal a band selectivity** mechanism.



Universidad Euskal Herriko
del País Vasco Unibertsitatea



Thank you!



GOBIERNO
DE ESPAÑA

MINISTERIO
DE ECONOMÍA
Y COMPETITIVIDAD



CSIC
CONSEJO SUPERIOR DE INVESTIGACIONES CIENTÍFICAS

Experiment:

Eduard Carbonell-Sanromà
Richard Balog
Martina Corso
Shigeki Kawaii
Shohei Saito
Shigehiro Yamaguchi
Jose I. Pascual

Theory:

Aran Garcia-Lekue
Daniel Sánchez-Portal

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