Emerging magnetism in boron-doped graphene nanoribbons

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Iago Pozo,[5] Diego Peña,[5] Thomas Frederiksen,[1,6] Aran Garcia-Lekue,[1,6]
Daniel Sánchez-Portal,[1,7] and Jose Ignacio Pascual[2,6]

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6 *IKERBASQUE, Basque Foundation for Science, Spain*
7 *Centro de Física de Materiales CSIC-UPV/EHU, Spain*

March 3, 2020

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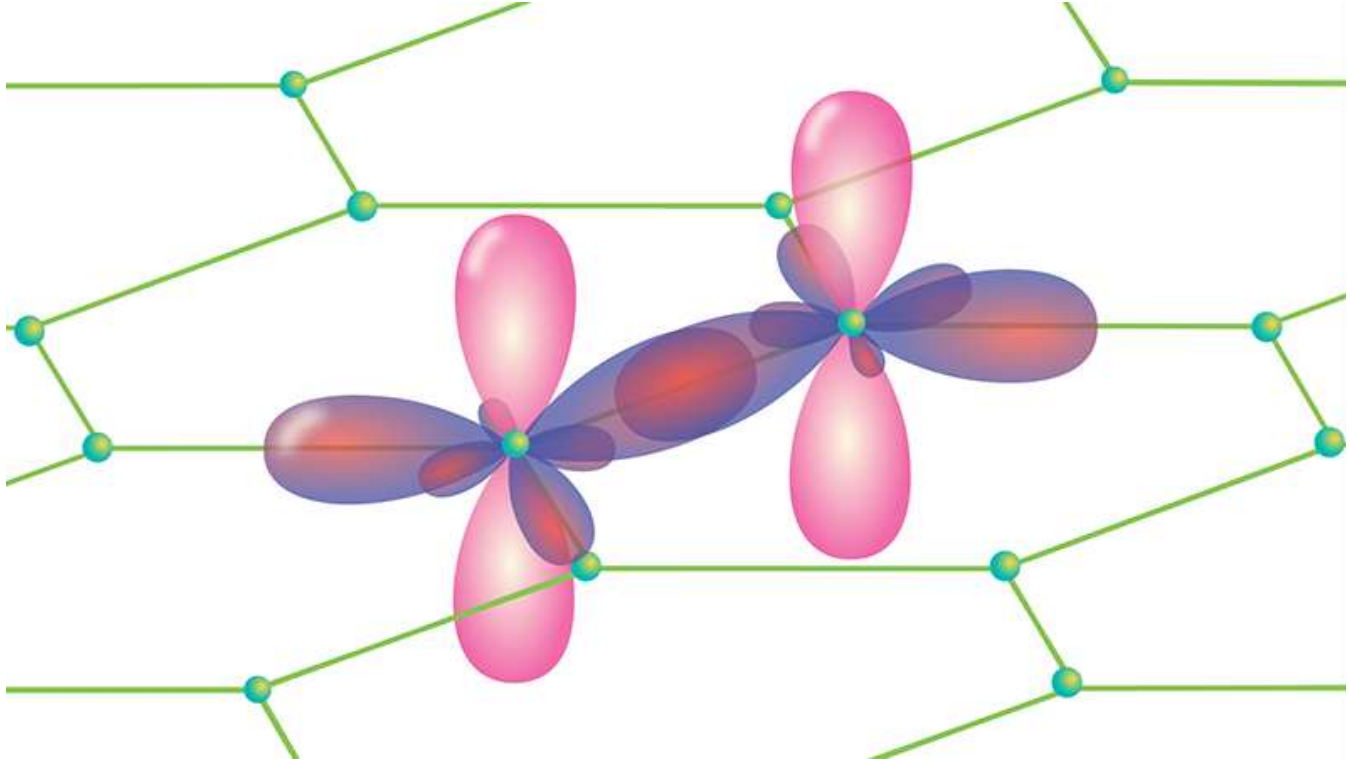
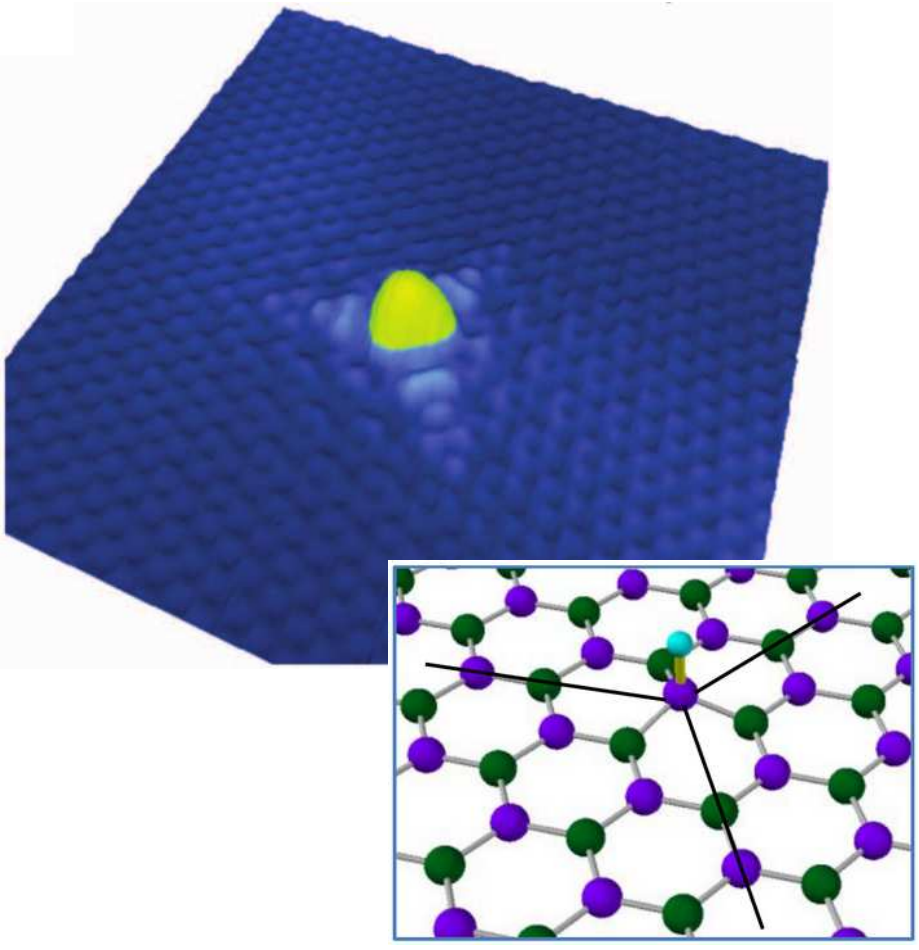
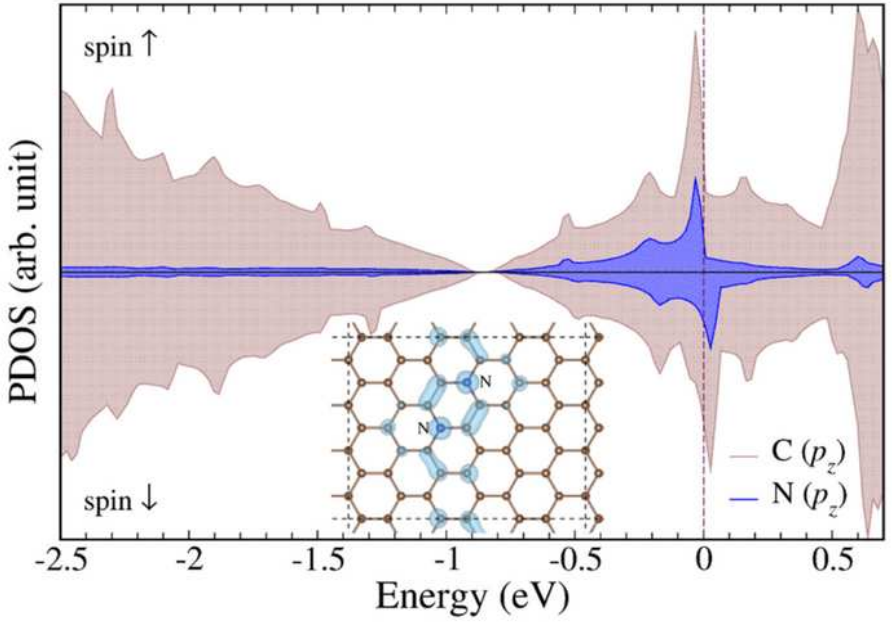
Magnetism in graphene



J. Proctor. *Physics* **12**, 104 (2019).

Magnetism in graphene

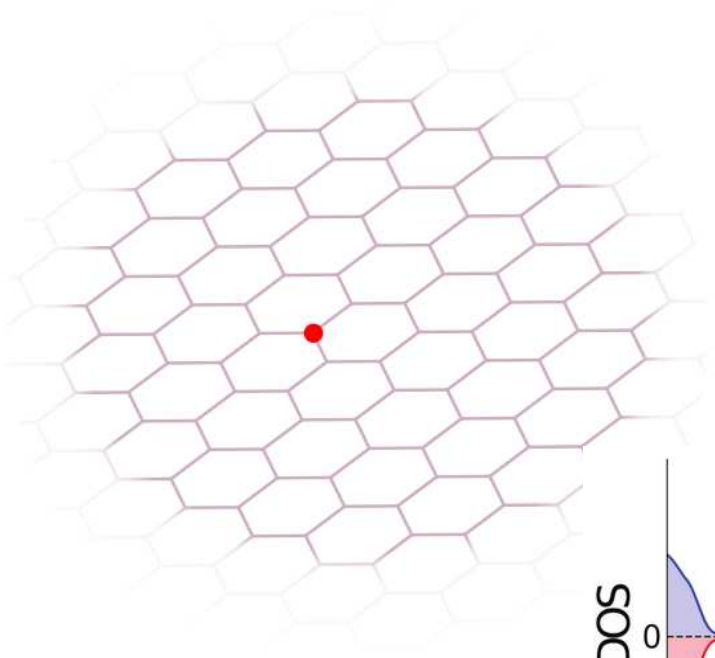


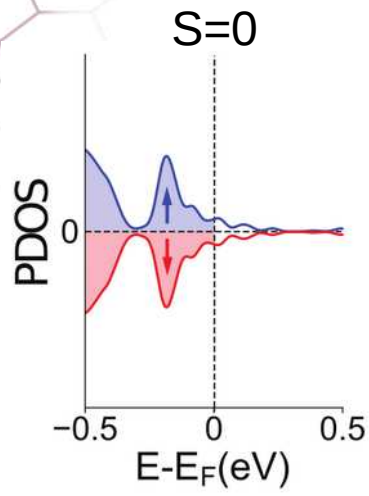


H. Gonzalez-Herrero *et al*. *Science* **352**, 6284 (2016).

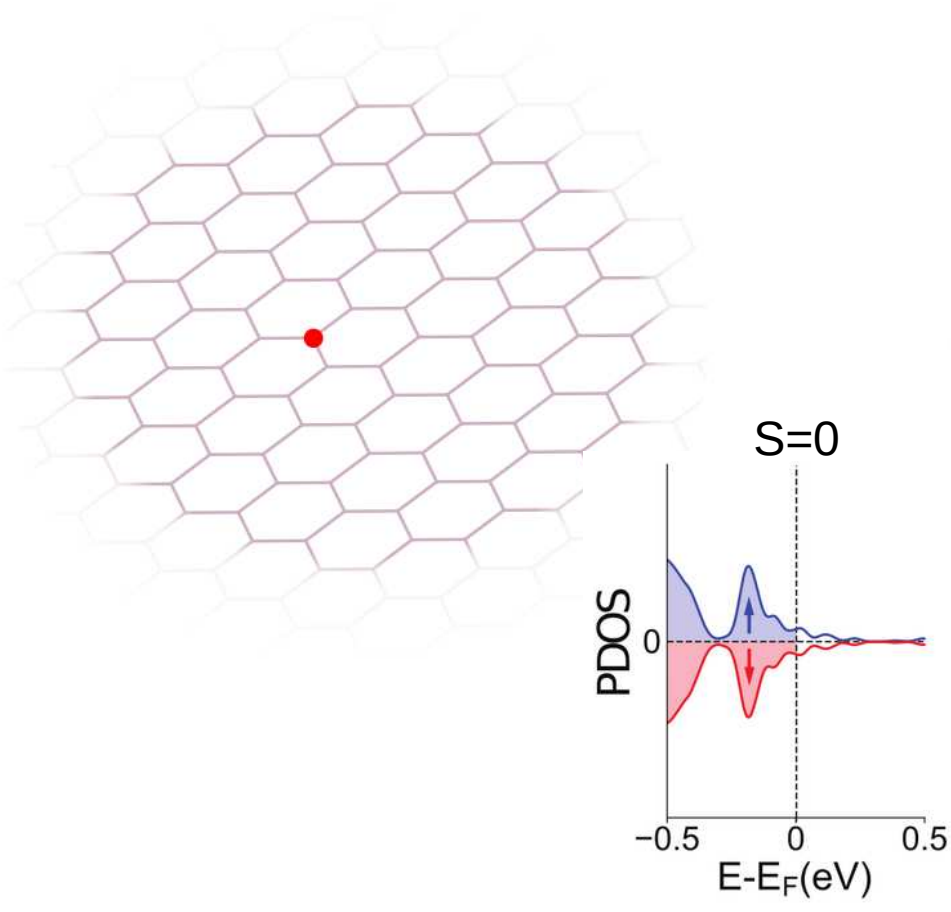
P. Błoński *et al*. *J. Am. Chem. Soc.* **139**, 3171 (2017).

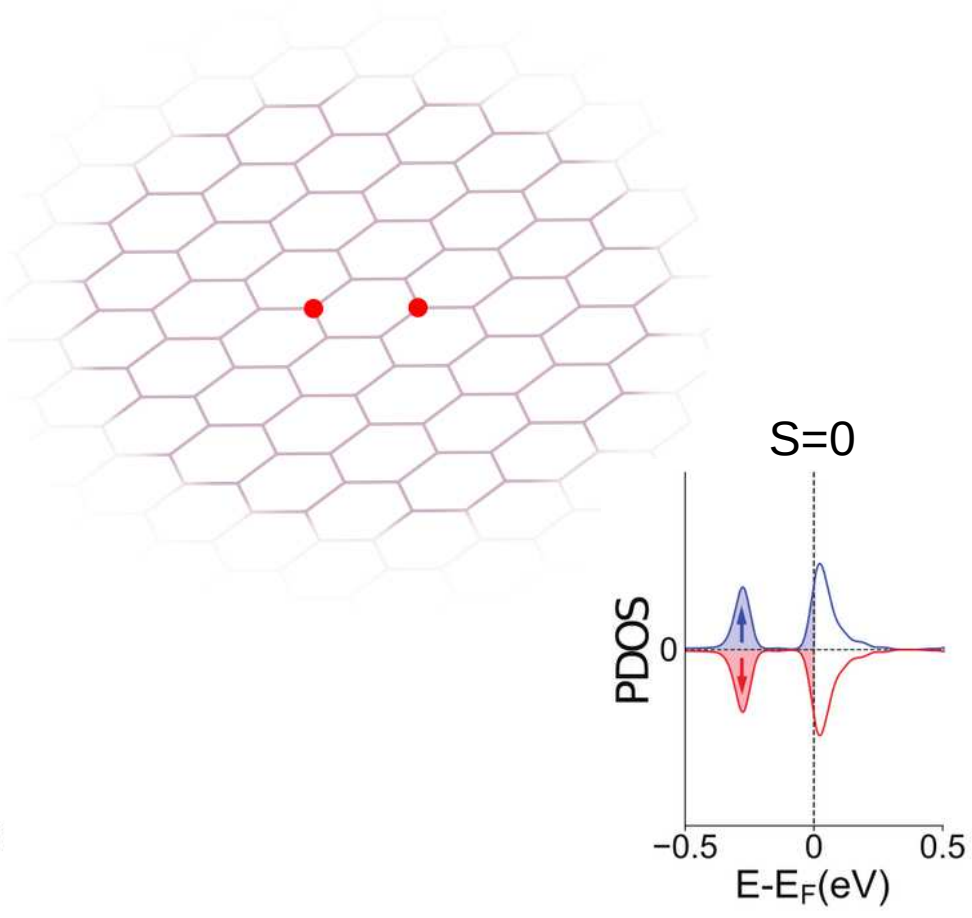
Boron-doped graphene





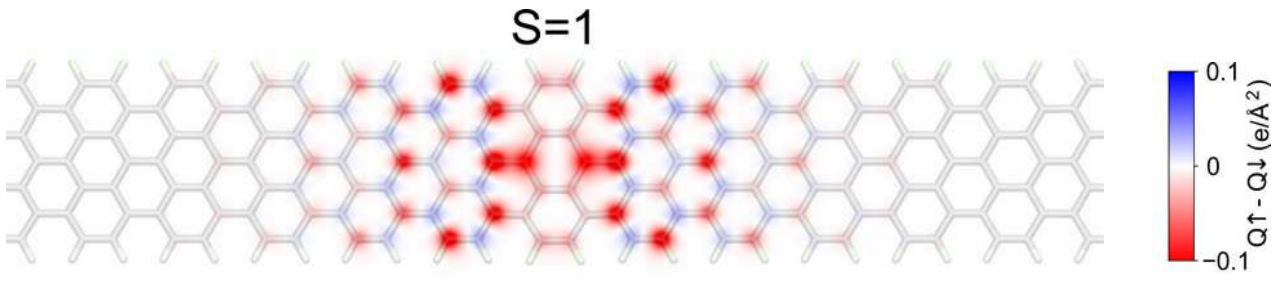
Boron-doped graphene





R. Faccio *et al*. *J. Phys. Chem. C* **114**, 18961 (2010).

Boron-doped GNR



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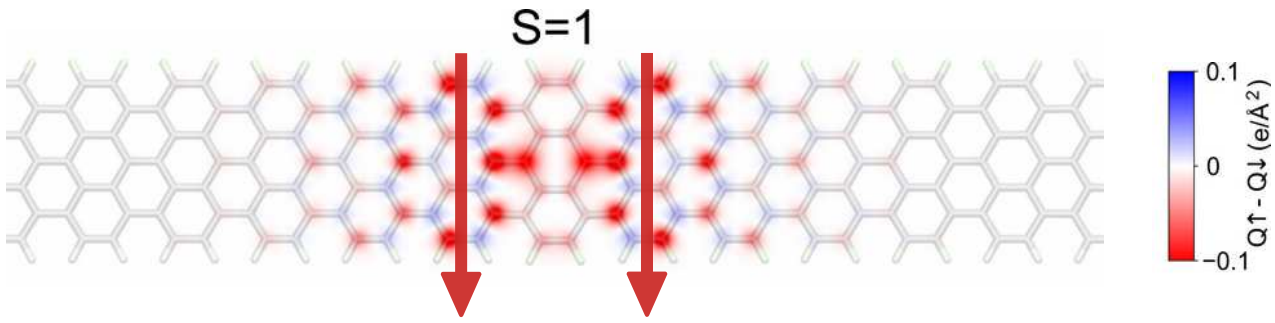

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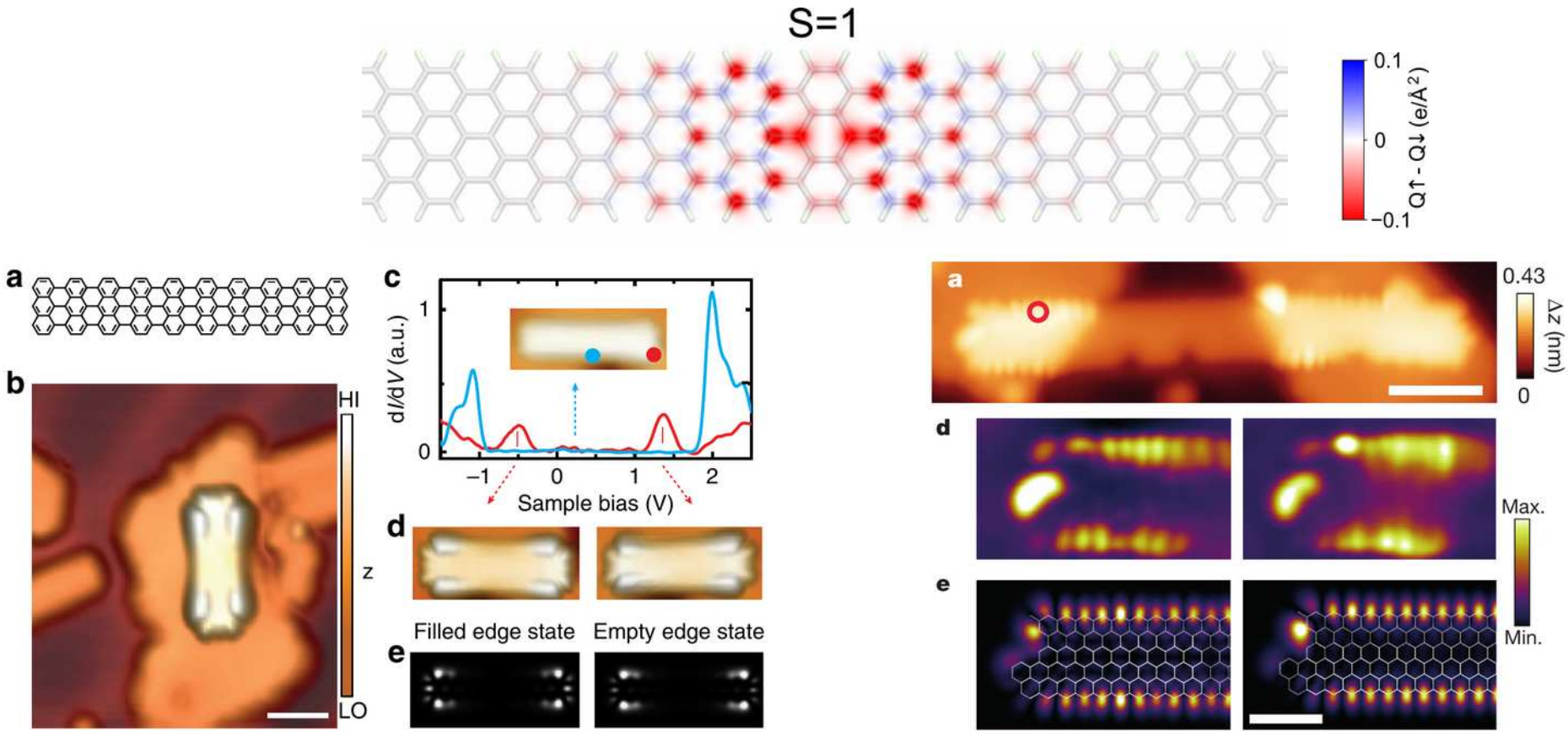
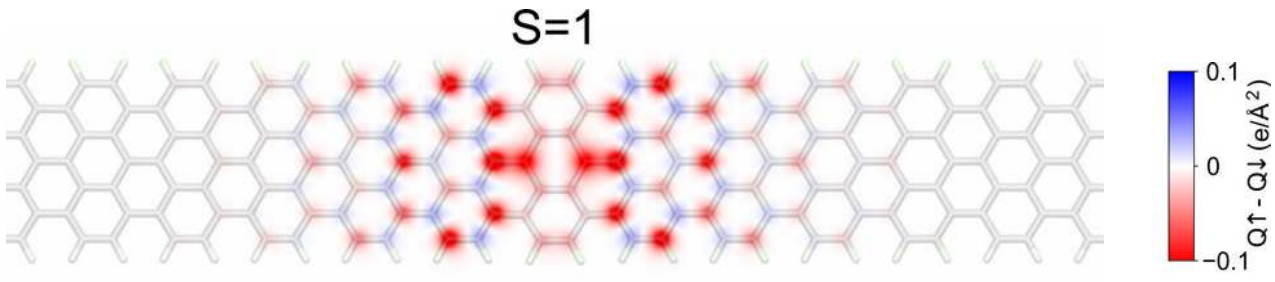
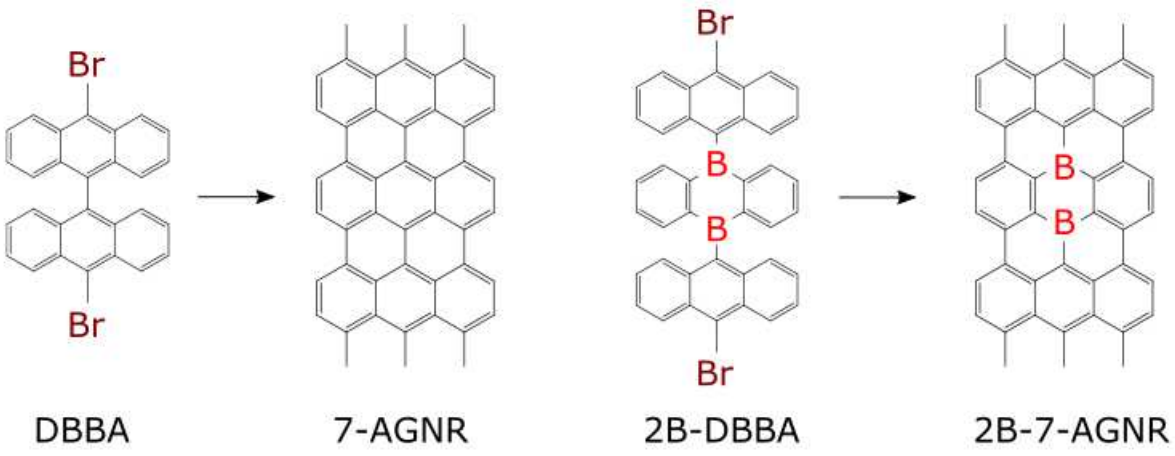


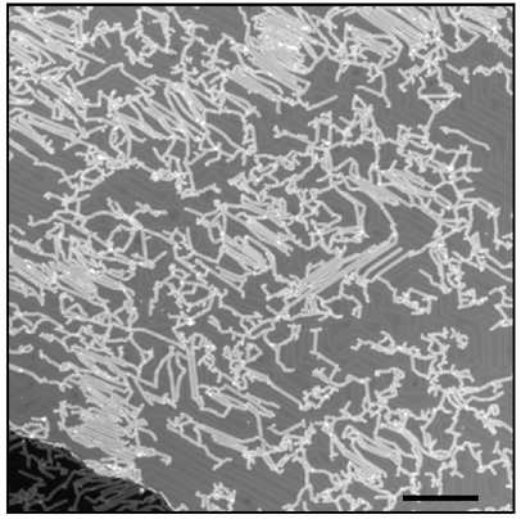
S. Wang *et al*. *Nat. Commun.* **7**, 11507 (2016).

P. Ruffieux *et al*. *Nature* **531**, 489 (2016).

Boron-doped GNR



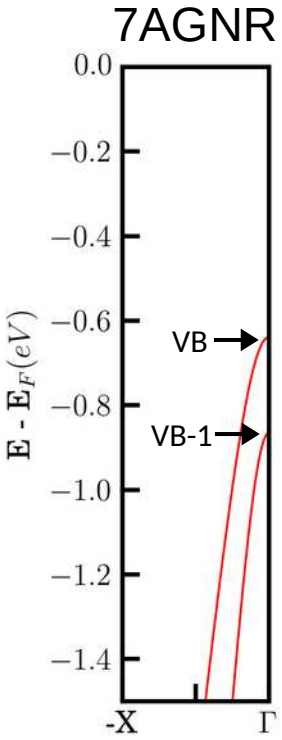




S. Kawai *et al*. *Nature Comm.* **6**, 8098 (2015).

R. R. Cloke et al. *J. A. Chem. Soc.* 137, 8872 (2015).

Boron-doped GNR – zero bias transmission



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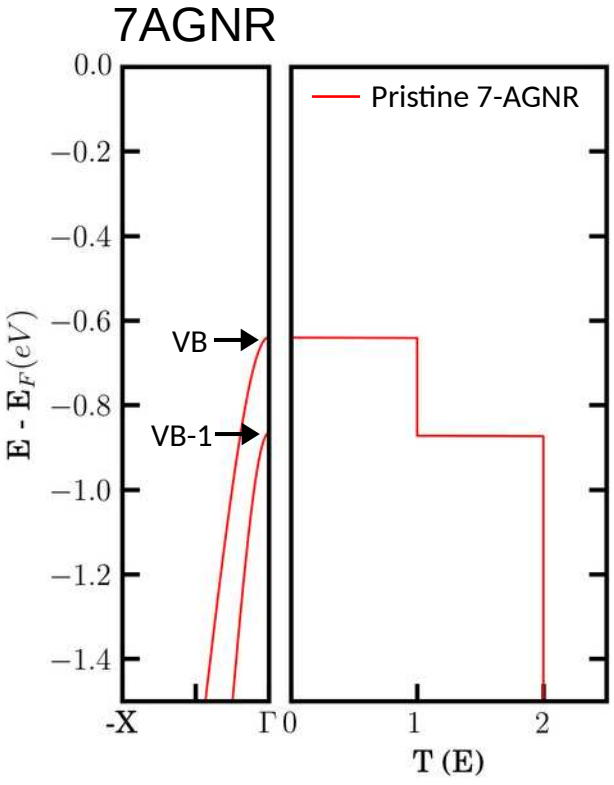

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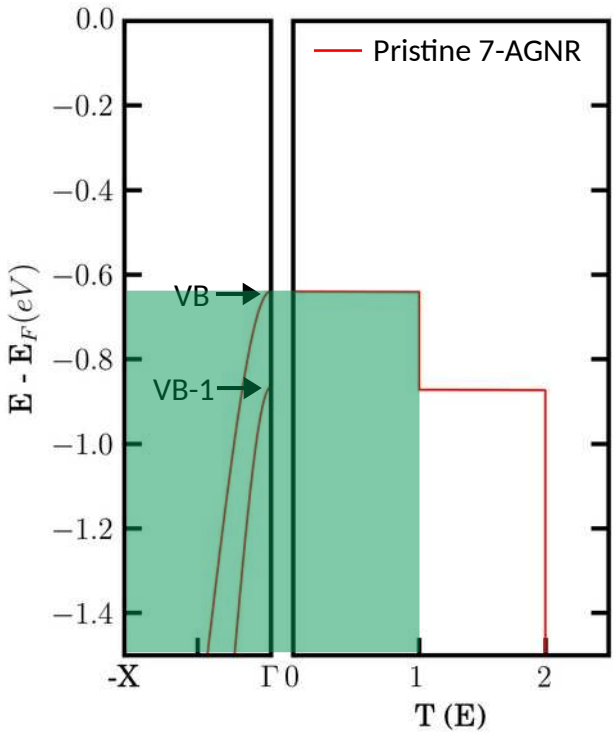

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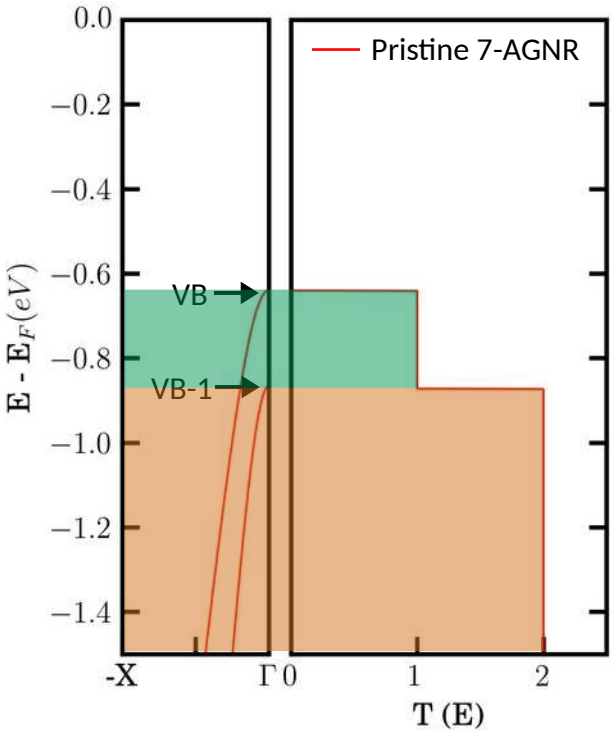

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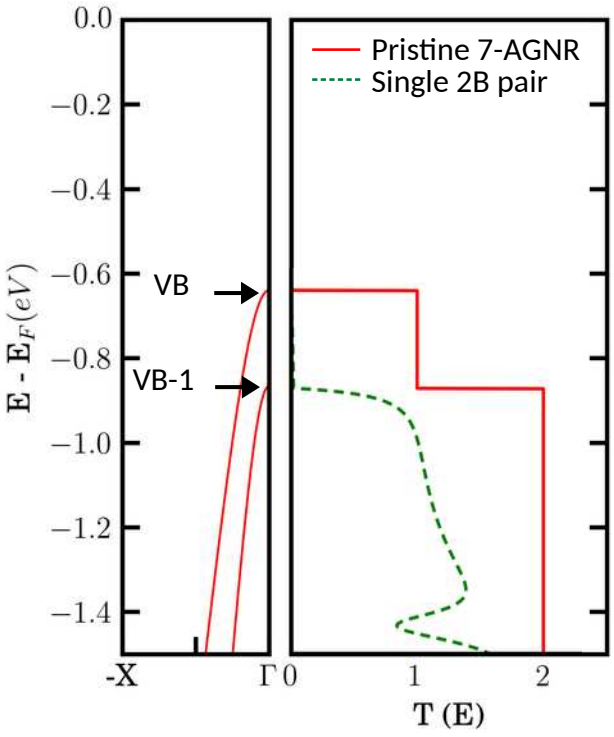

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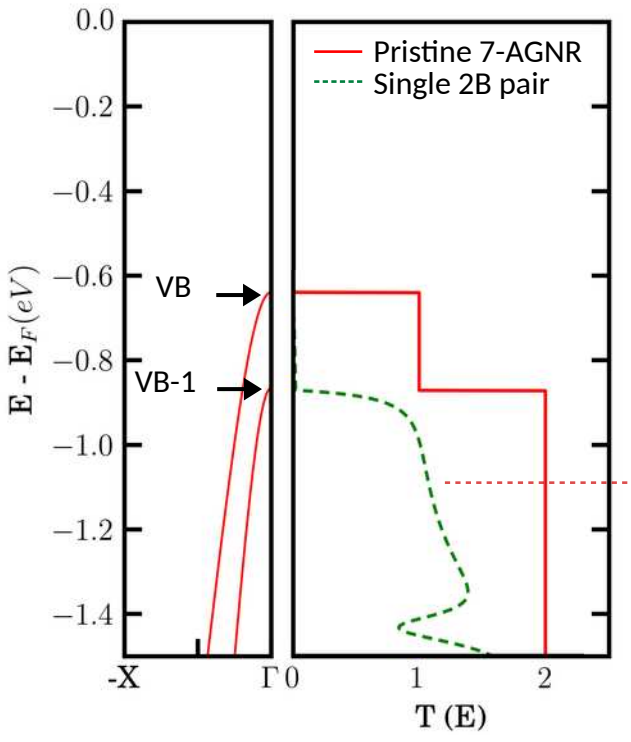

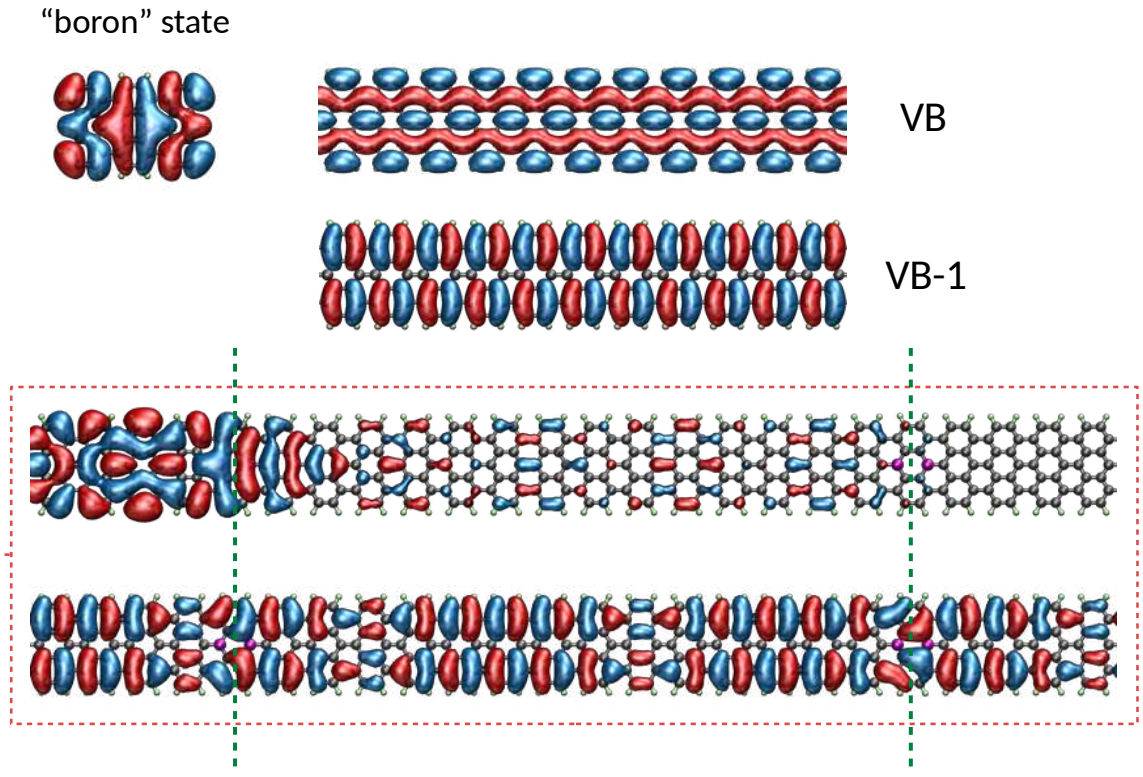

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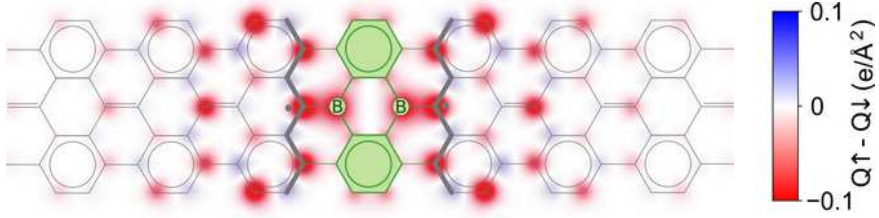

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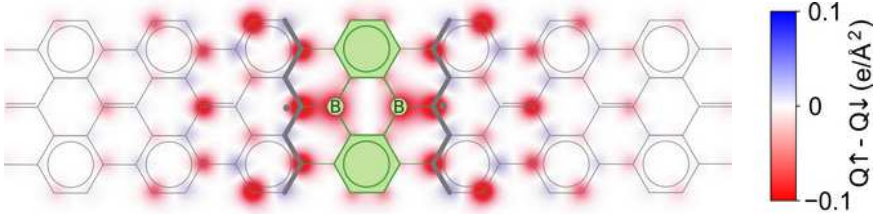

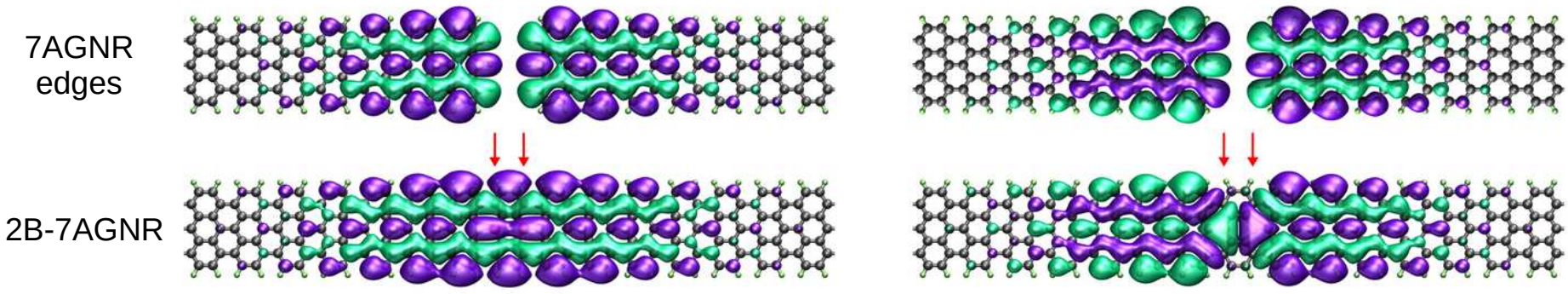

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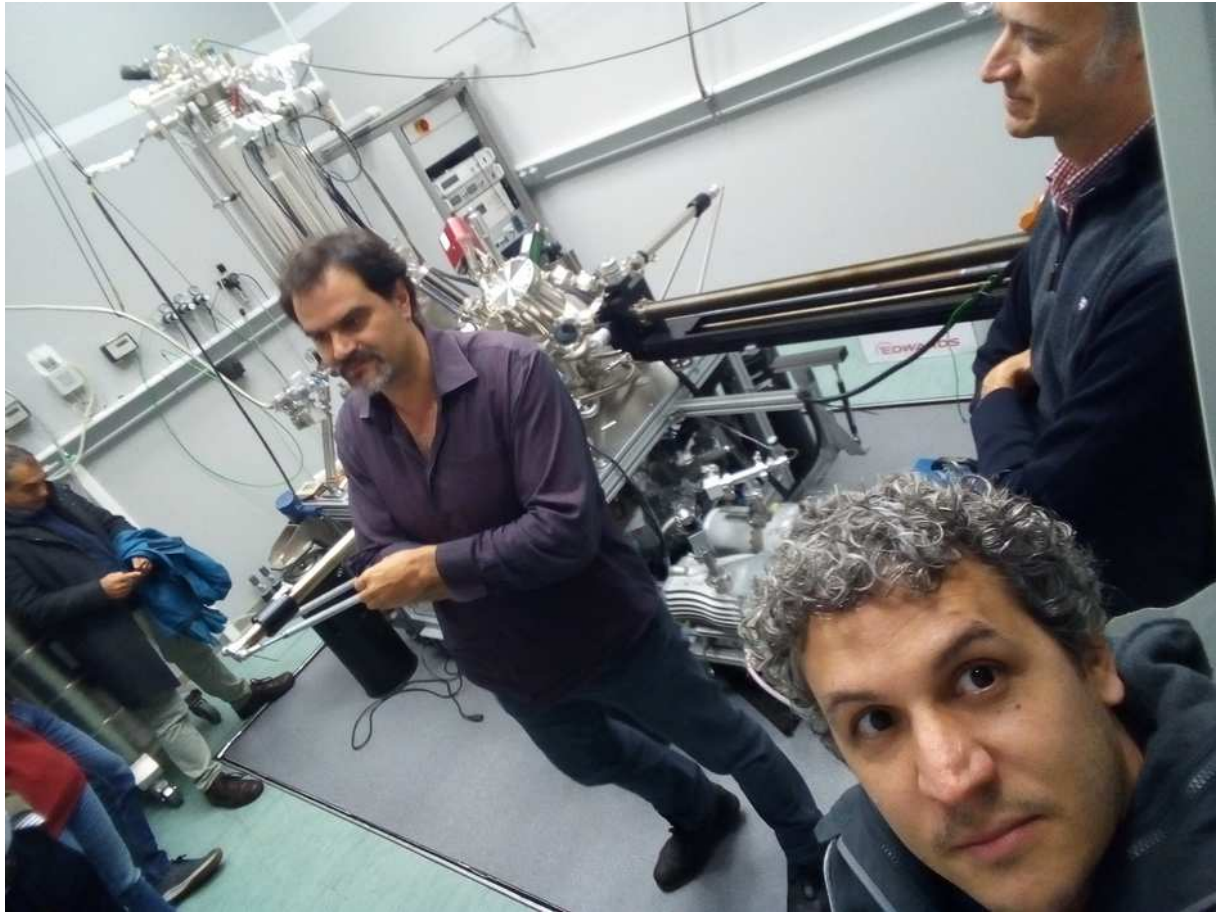
STM/STS analysis of 2B-7AGNRs



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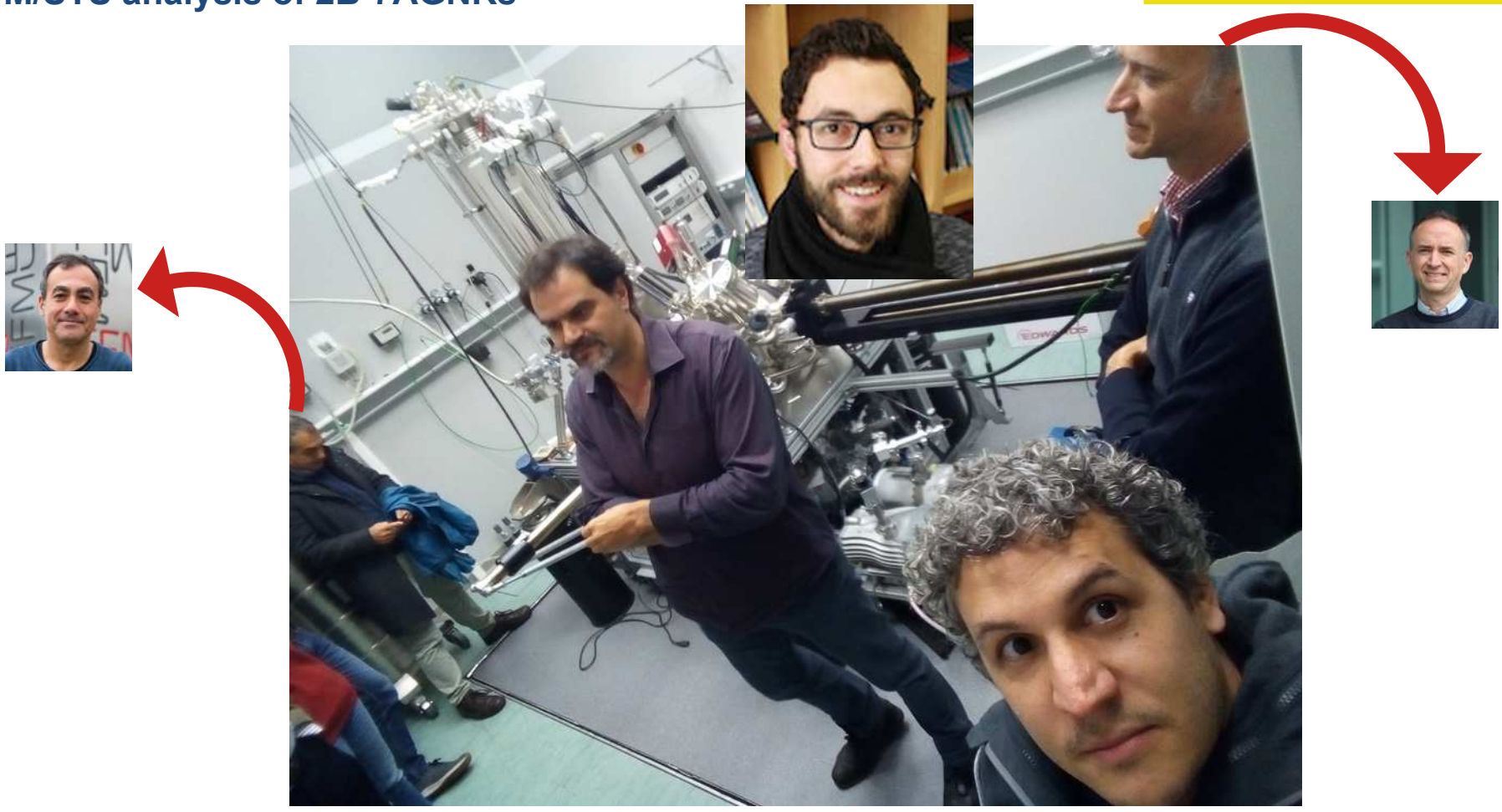

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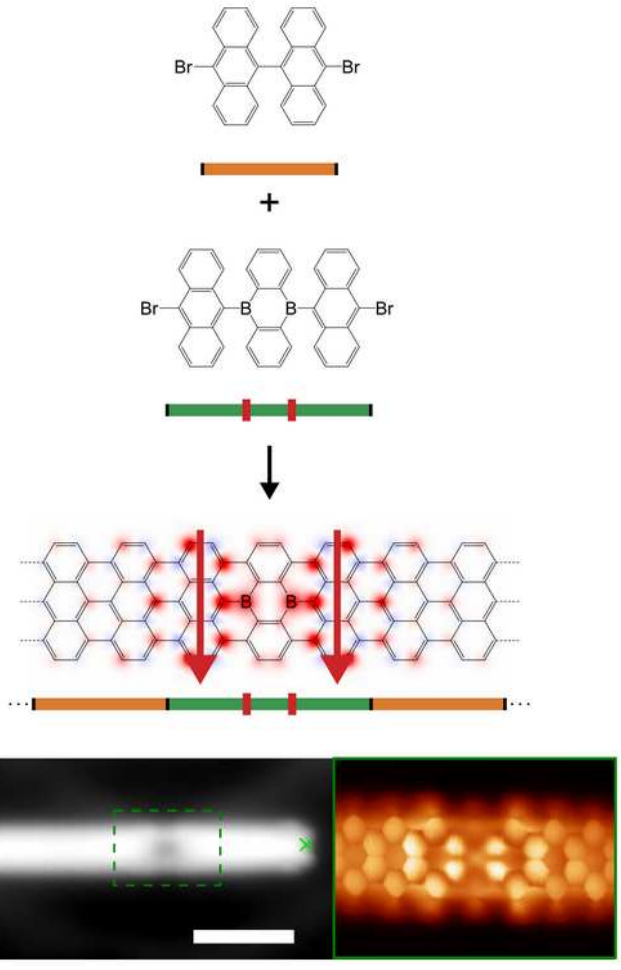
Single 2B-7AGNR



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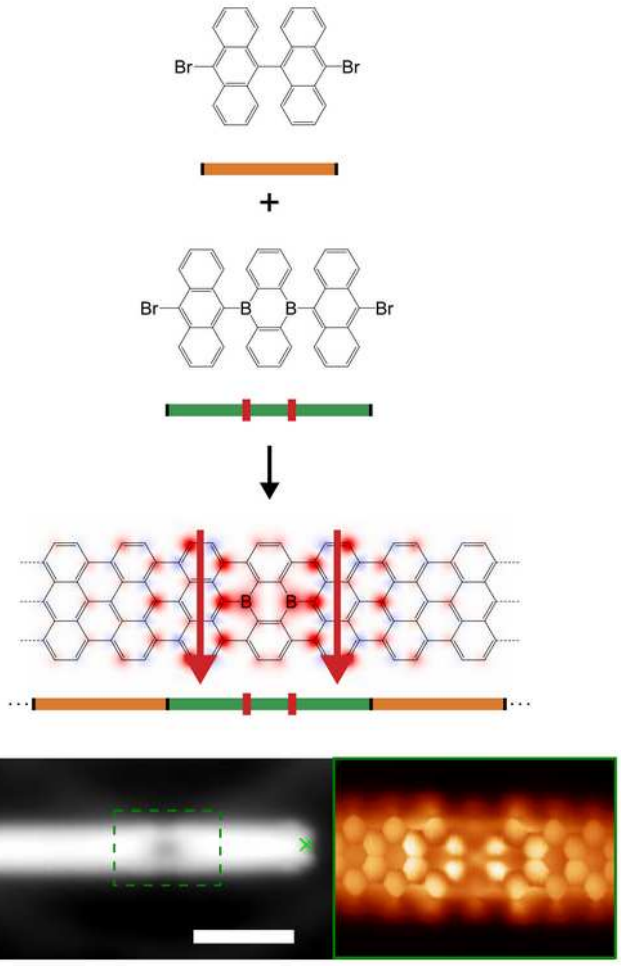

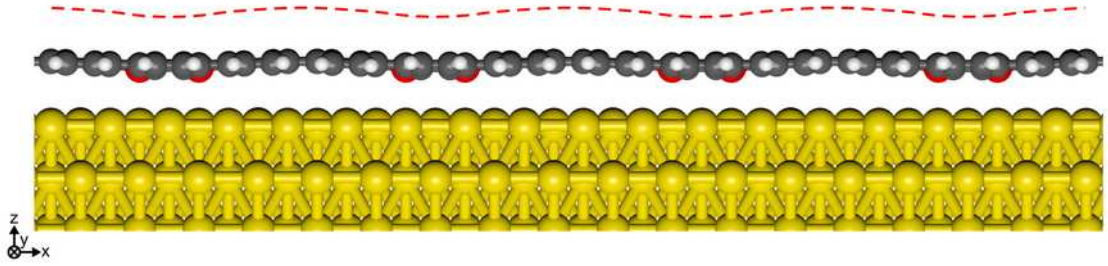

E. Carbonell-Sanromà *et al*. *J. Phys. Chem. C* **122**, 16092 (2018).

N. Friedrich*, P. Brandimarte* *et al*. (2020). Submitted!

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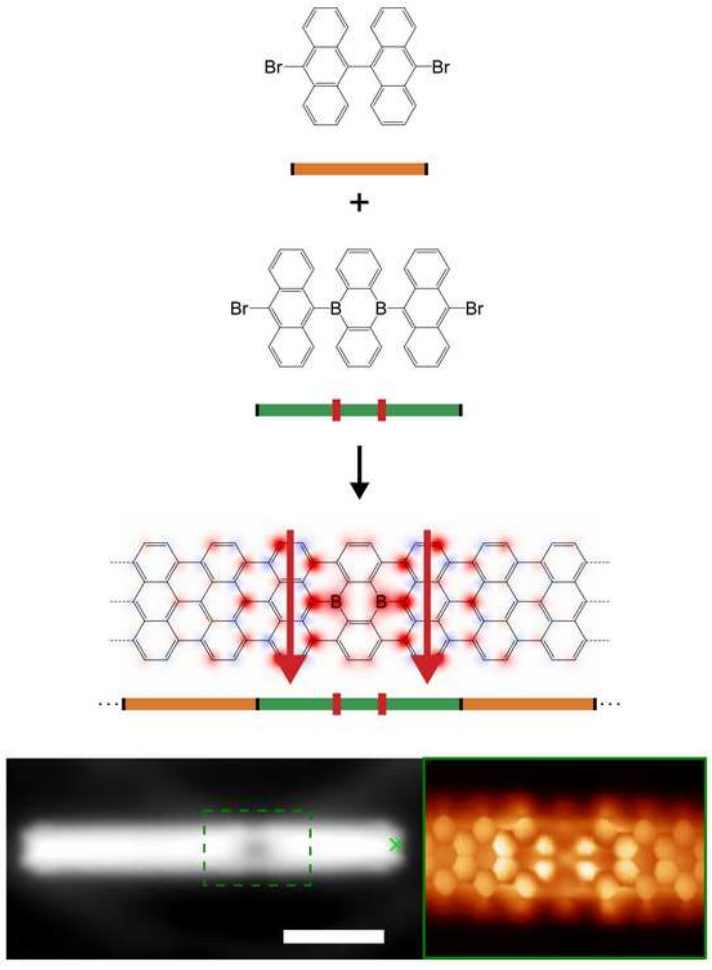

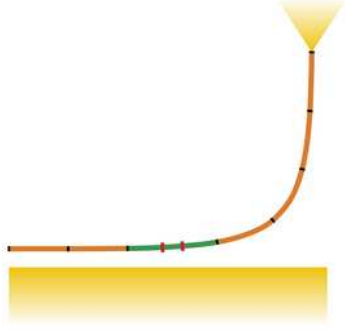

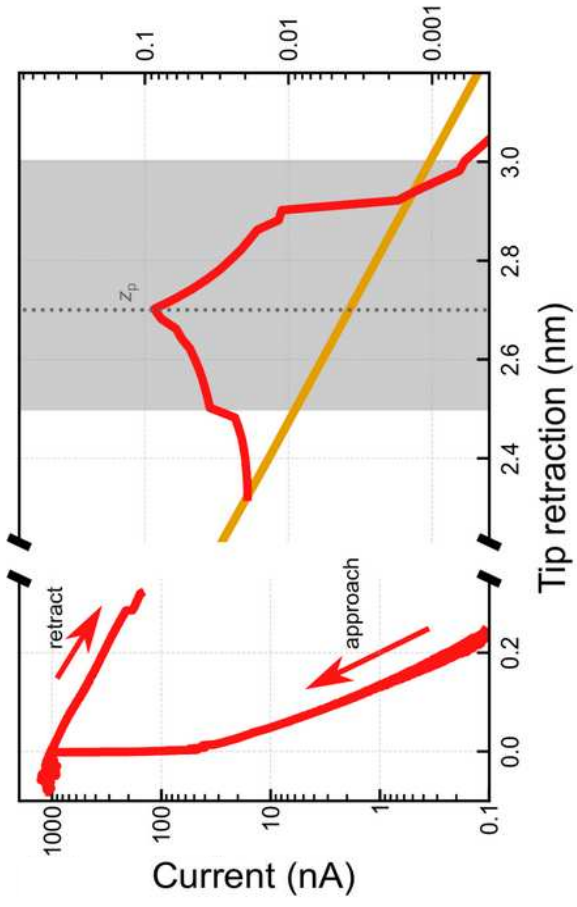

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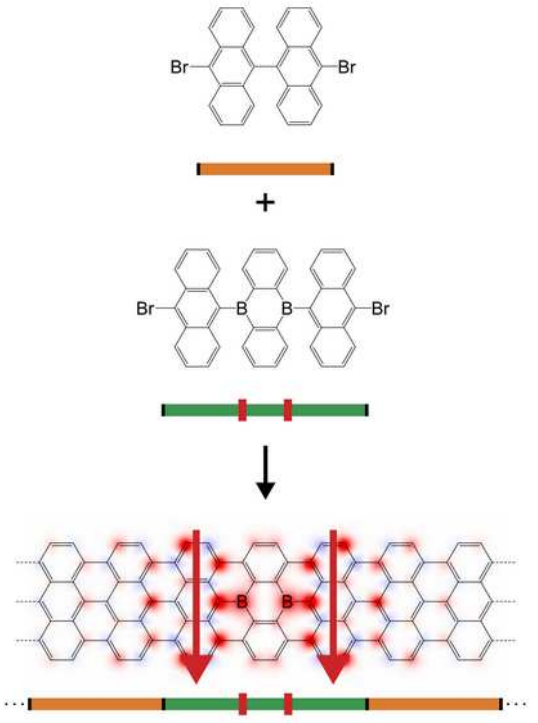

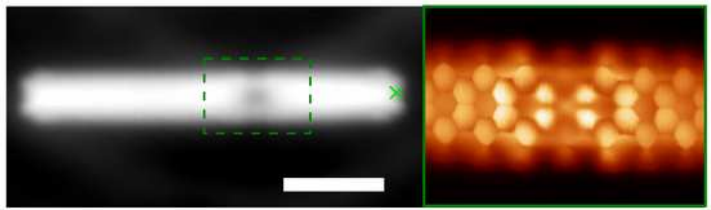

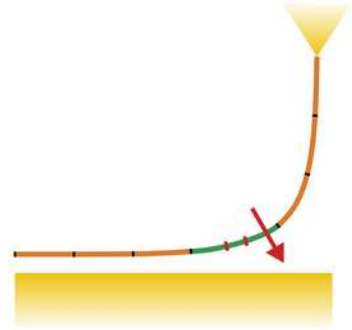

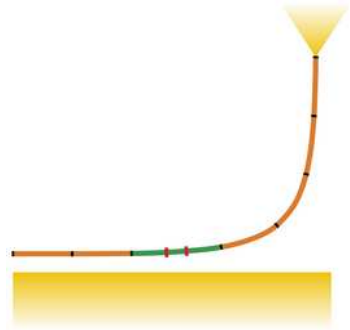

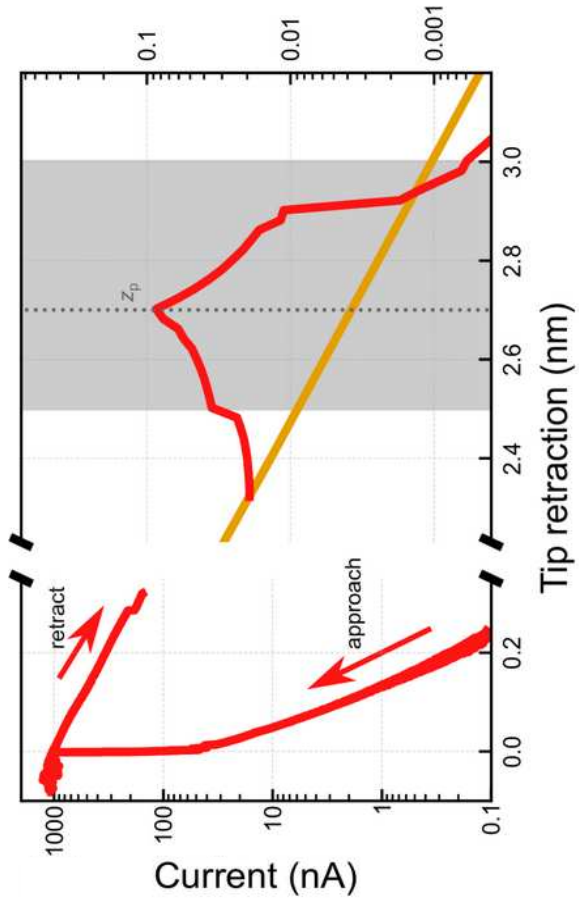

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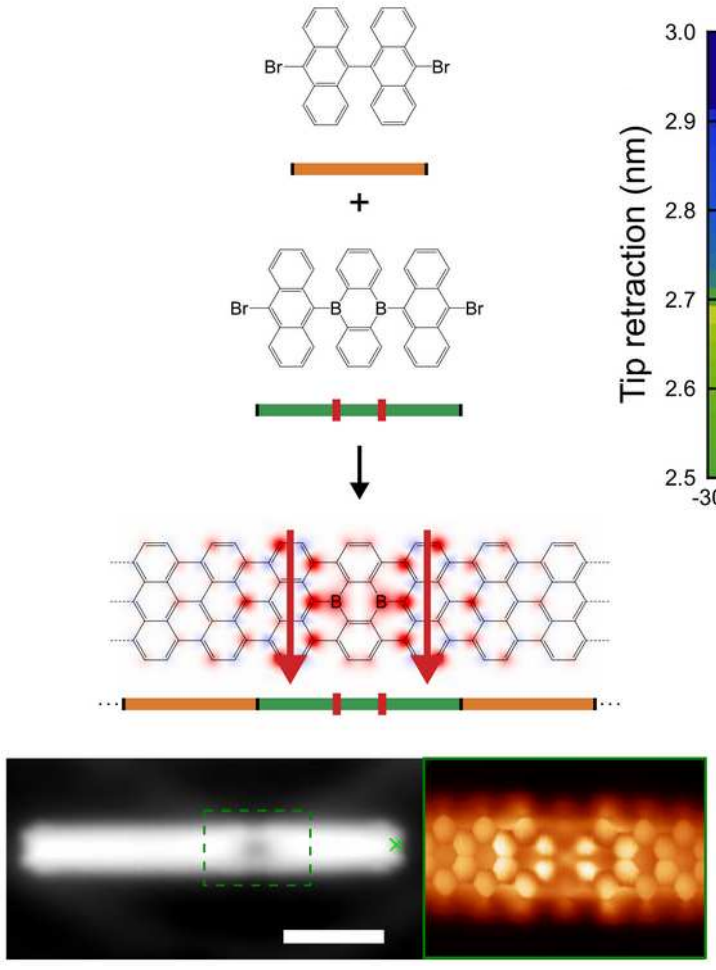
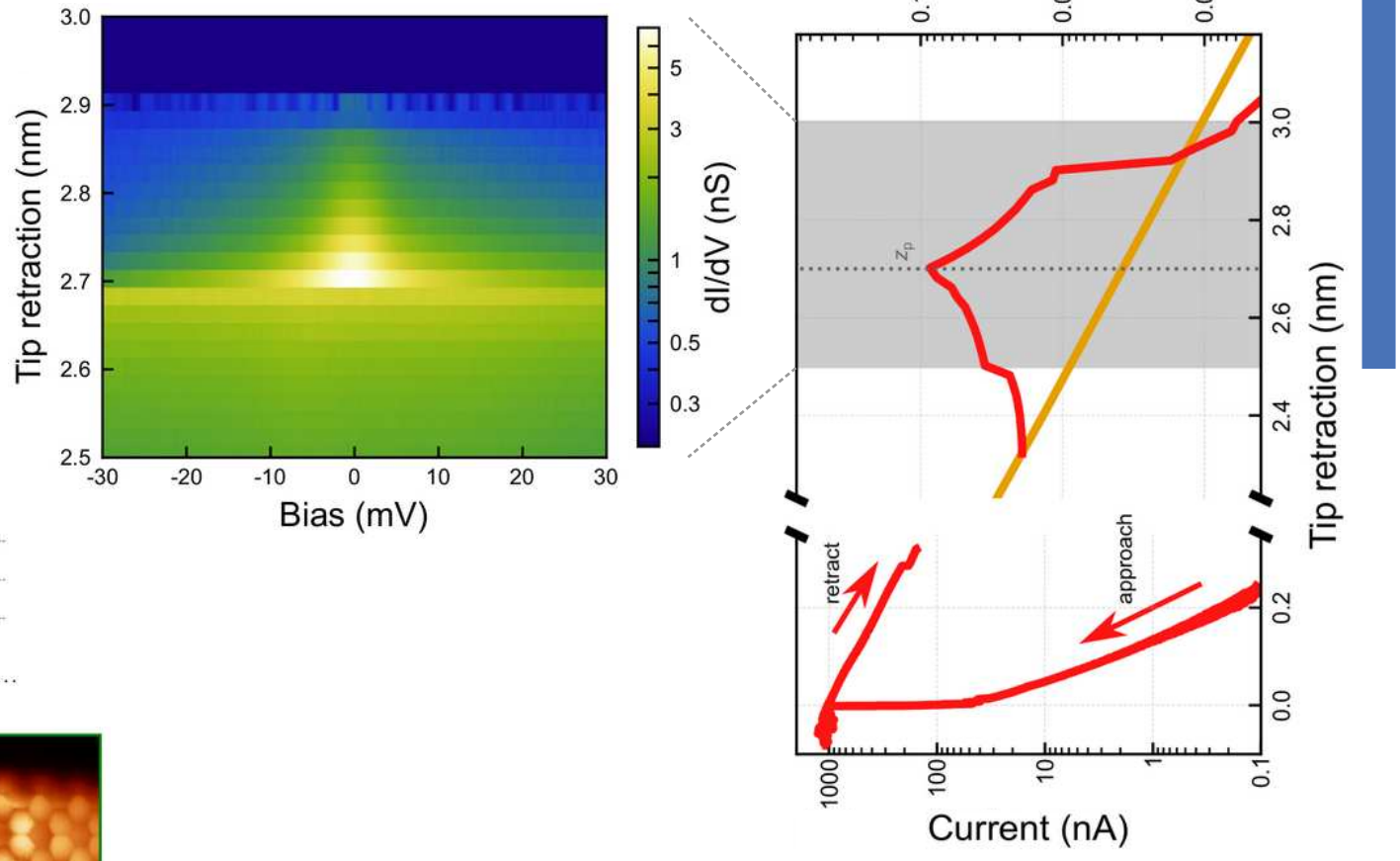
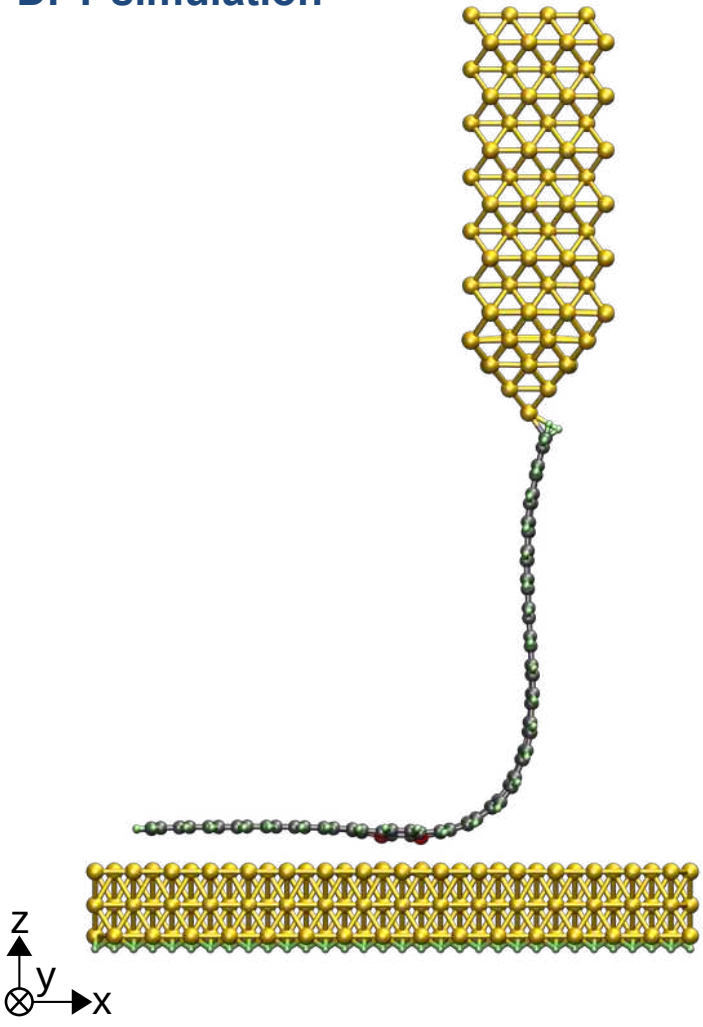
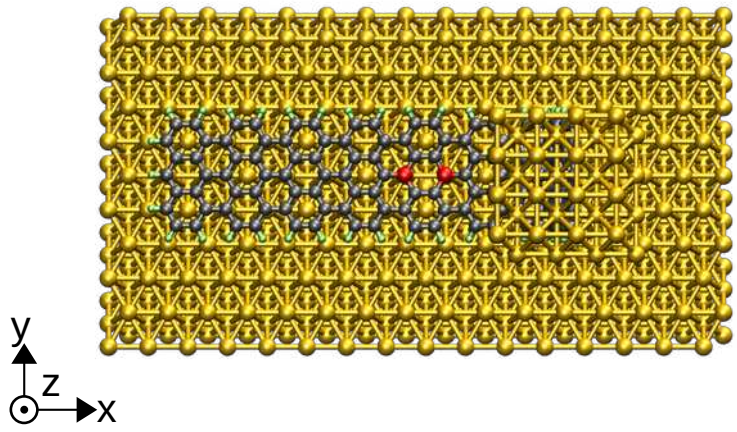




N. Friedrich*, P. Brandimarte* *et al*. (2020). Submitted!

DFT simulation

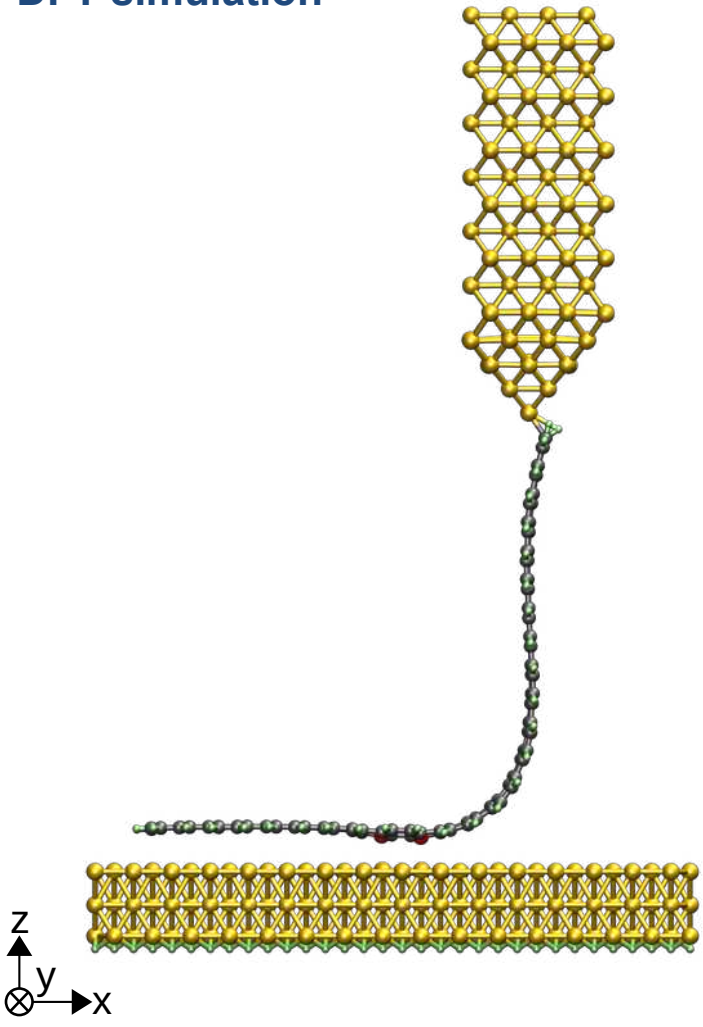


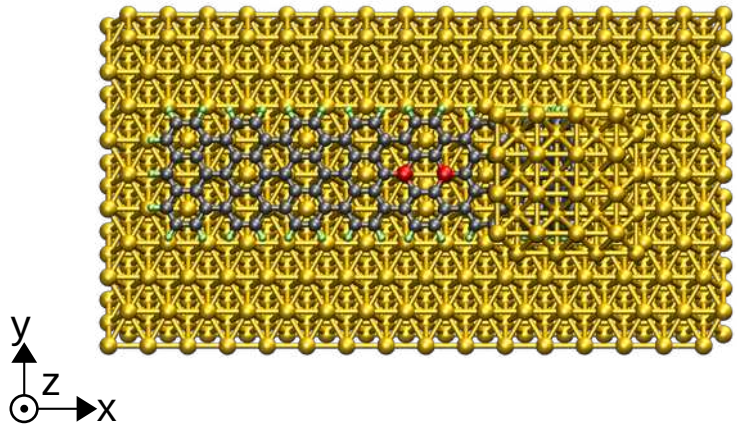


SIESTA

E. Artacho *et al*. *Phys. Stat. Sol.* (b) **215**, 809 (1999).
J. M. Soler *et al*. *J. Phys. Condens. Matter.* **14**, 2745 (2002).
A. Garcia *et al*. "The Siesta method: recent developments and applications", (2020). Submitted!

DFT simulation

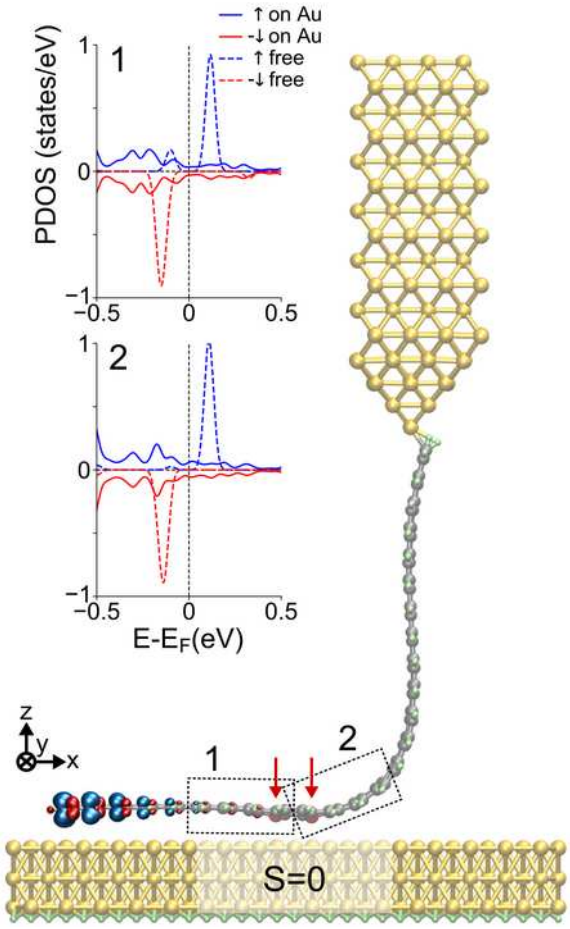




SIESTA

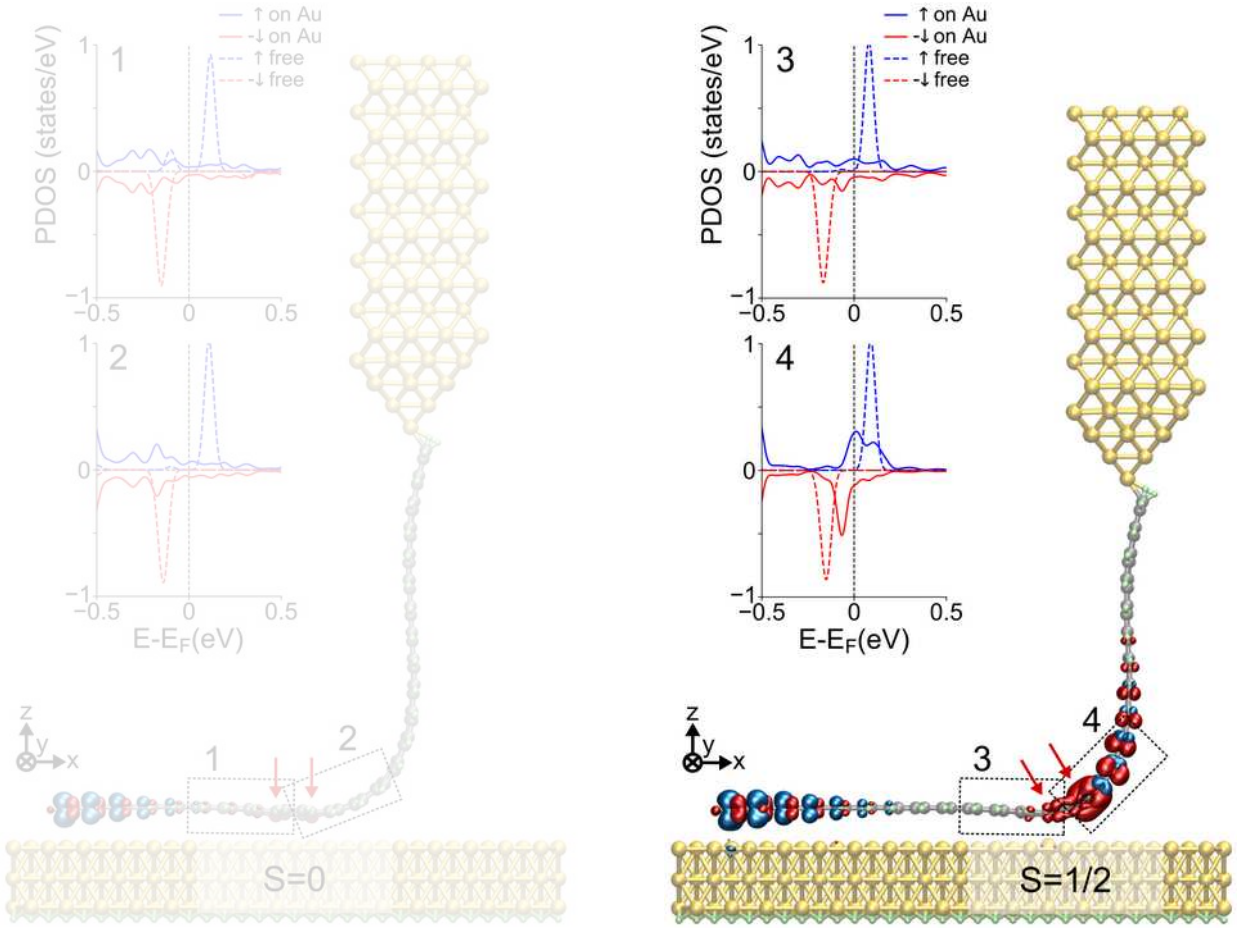
E. Artacho *et al*. *Phys. Stat. Sol.* (b) **215**, 809 (1999).
J. M. Soler *et al*. *J. Phys. Condens. Matter.* **14**, 2745 (2002).
A. Garcia *et al*. "The Siesta method: recent developments and applications", (2020). Submitted!

2B close to the Au(100)



N. Friedrich*, P. Brandimarte* *et al*. (2020). Submitted!

2B decoupling from Au(100)

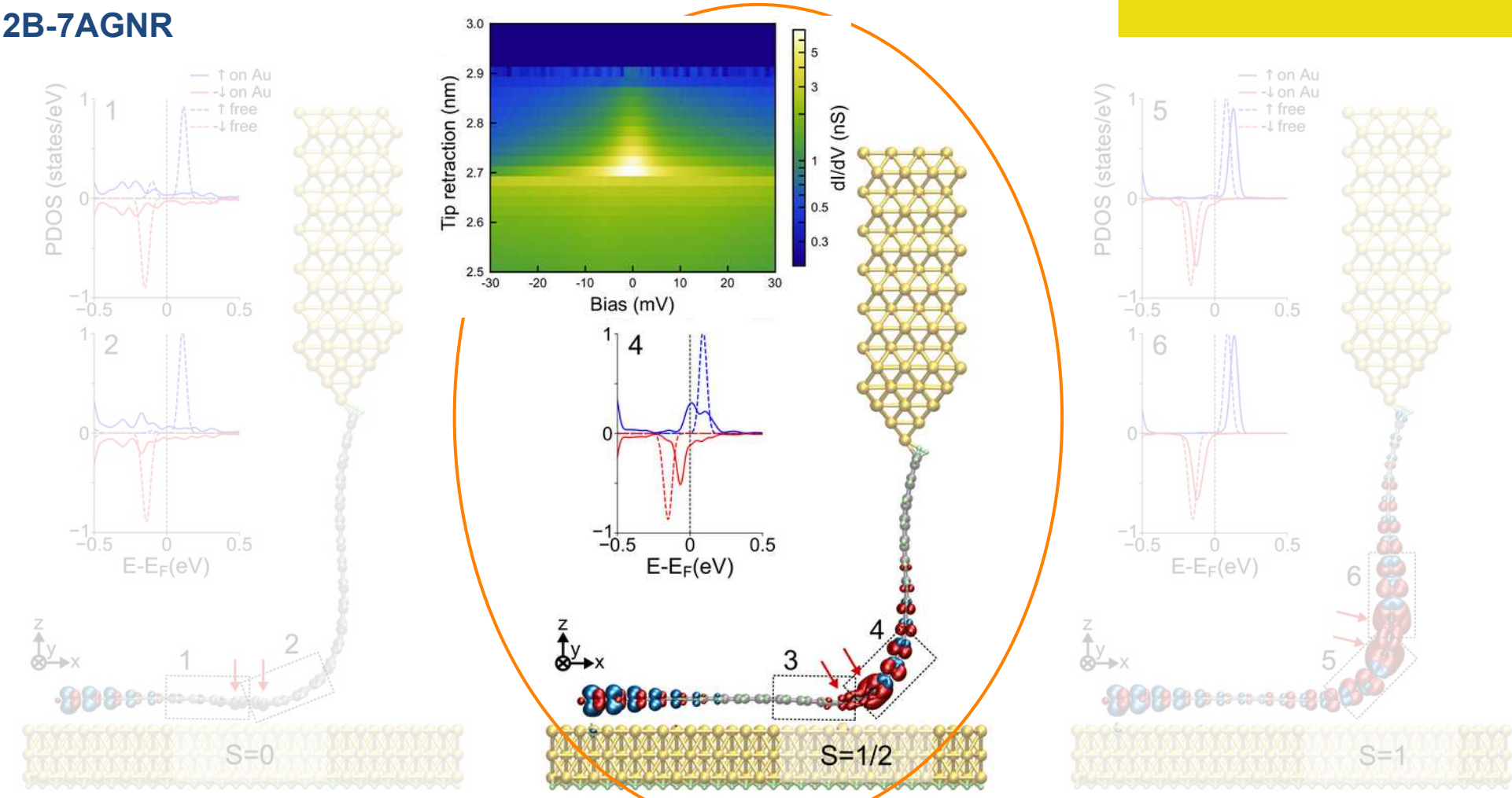


N. Friedrich*, P. Brandimarte* *et al*. (2020). Submitted!

2B far from Au(100)

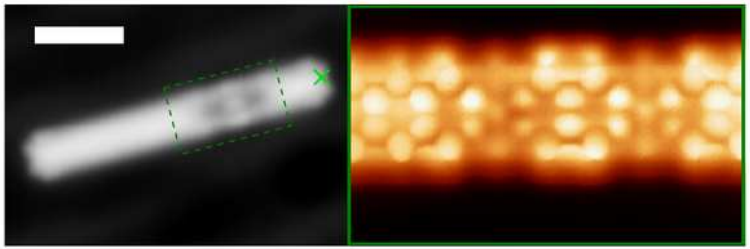
N. Friedrich*, P. Brandimarte* *et al.* (2020). Submitted!

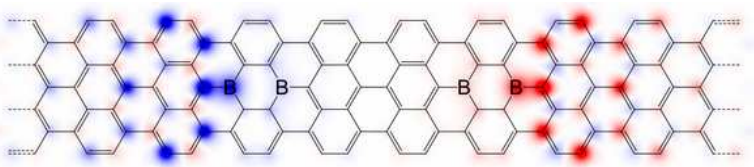
2B-7AGNR



N. Friedrich*, P. Brandimarte* *et al*. (2020). Submitted!

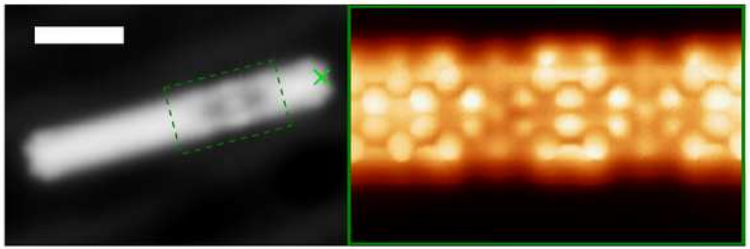
$(2B)_2$-7AGNR

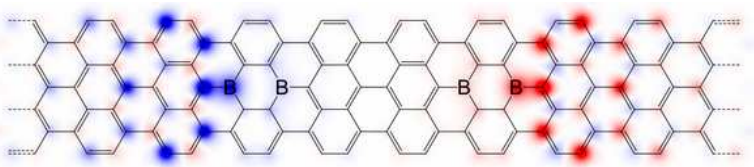


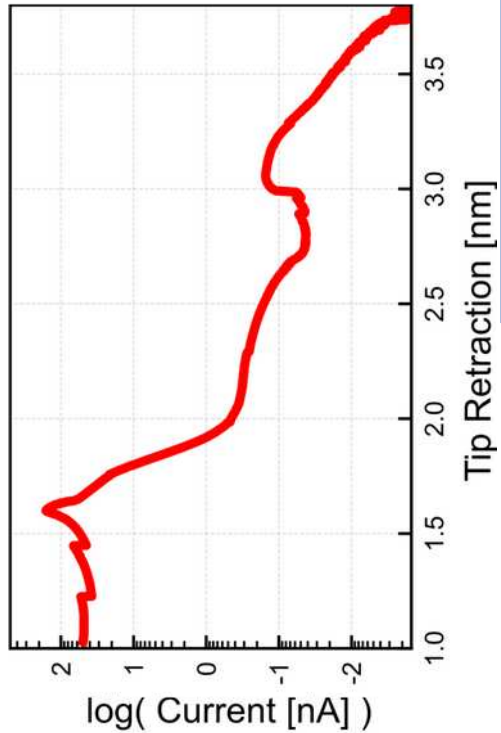


N. Friedrich*, P. Brandimarte* *et al*. (2020). Submitted!

$(2B)_2$-7AGNR

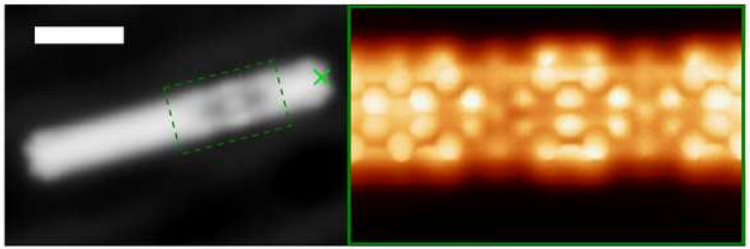


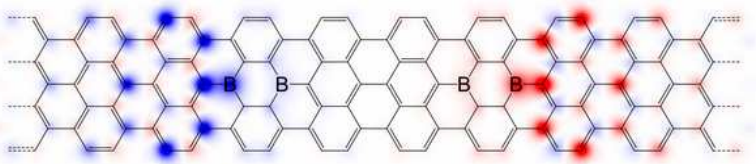


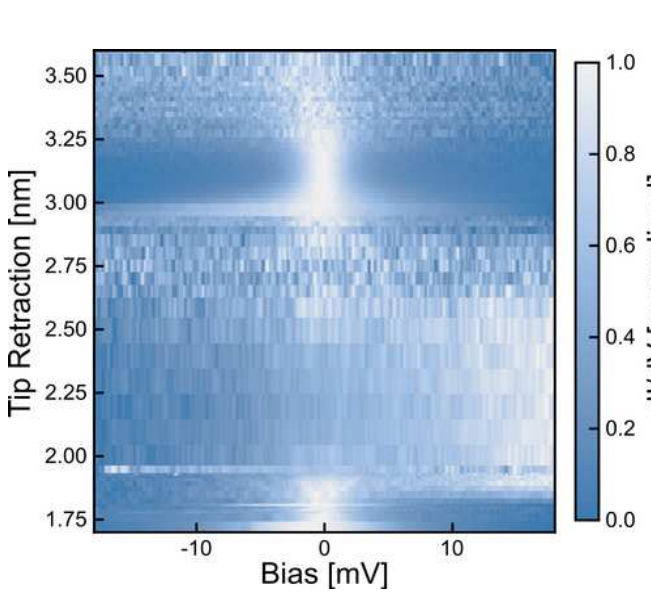


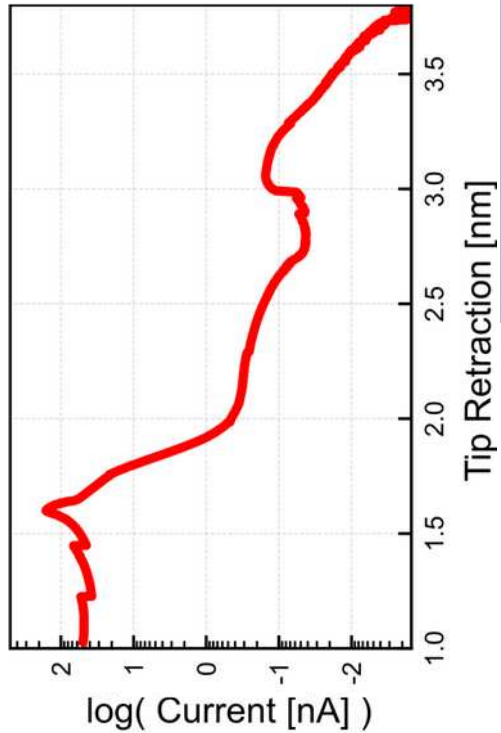
N. Friedrich*, P. Brandimarte* *et al*. (2020). Submitted!

$(2B)_2$-7AGNR









N. Friedrich*, P. Brandimarte* *et al*. (2020). Submitted!

Conclusions

Observation and characterization of boundary states upon substitutional B doping

Spin polarization of $(2B)_n$-7AGNR:

- low concentrations of 2B units ⟶ chain of S = 1 spins
- sufficiently dense doping ⟶ S = 1/2 spins at the boundary

Thanks

For your attention!

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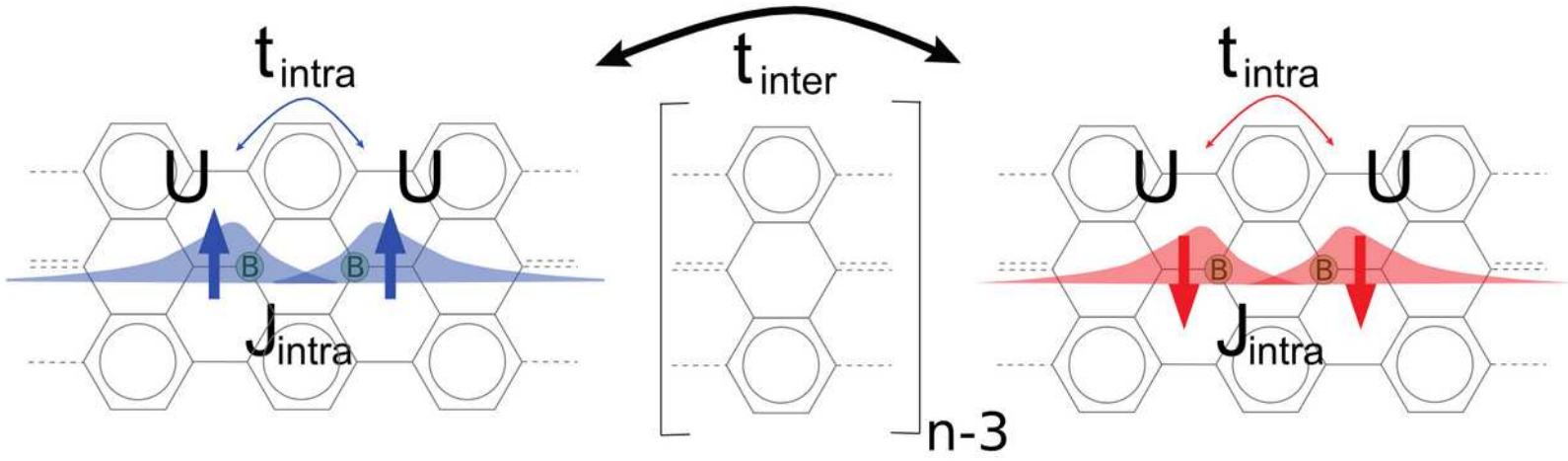
$(2B)_2$-7AGNR



N. Friedrich*, P. Brandimarte* *et al*. (2020). Submitted!