



## PAMS Project meeting 28<sup>th</sup> November 2016, Brussels

Electronic properties of Cl doped 5-AGNR on  
Au(111) by first-principles calculations

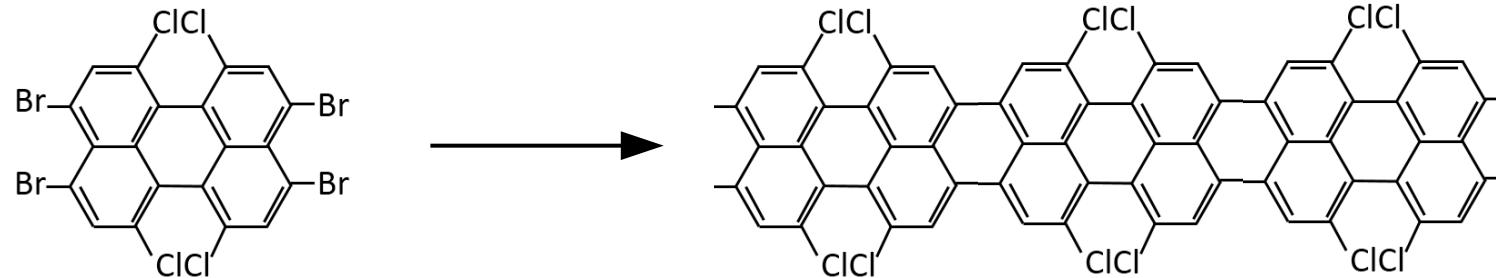
Pedro Brandimarte



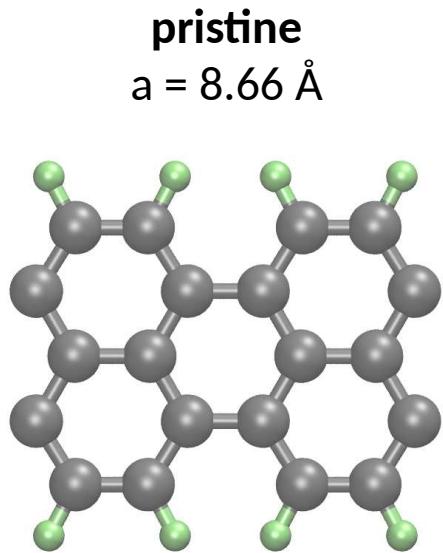
## 5-AGNR realised with one step reaction



UNIVERSITAS IAGELLONICA  
CRACOVIENSIS



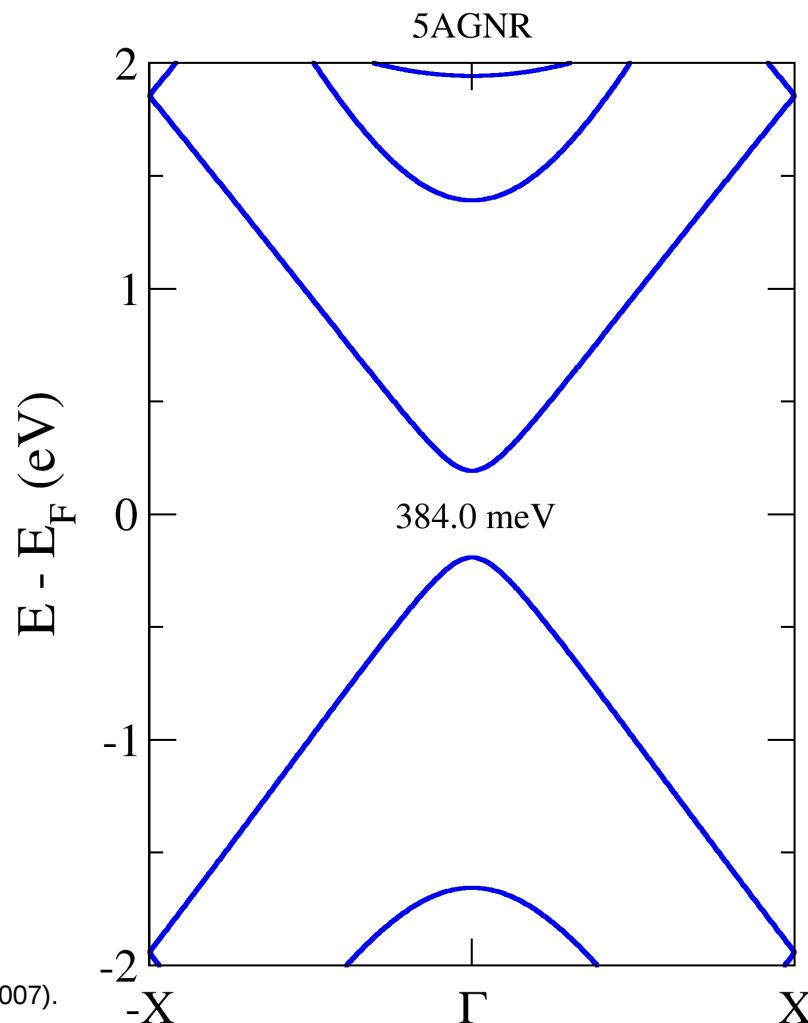
## The effect of Cl atoms on the electronic structure



LDA energy gap<sup>1</sup> ~ 0.4 eV

GW energy gap<sup>1</sup> ~ 1.7 eV  
GW energy gap<sup>1,2</sup> = 1.32 eV

STS gap<sup>2</sup> on Au =  $2.8 \pm 0.1$  eV



<sup>1</sup> L. Yang, C. H. Park, Y. W. Son, M. L. Cohen, and S. G. Louie. *PRL* **99**, 186801 (2007).

<sup>2</sup> H. Zhang et al. *JACS* **137**, 4022-4025 (2015).



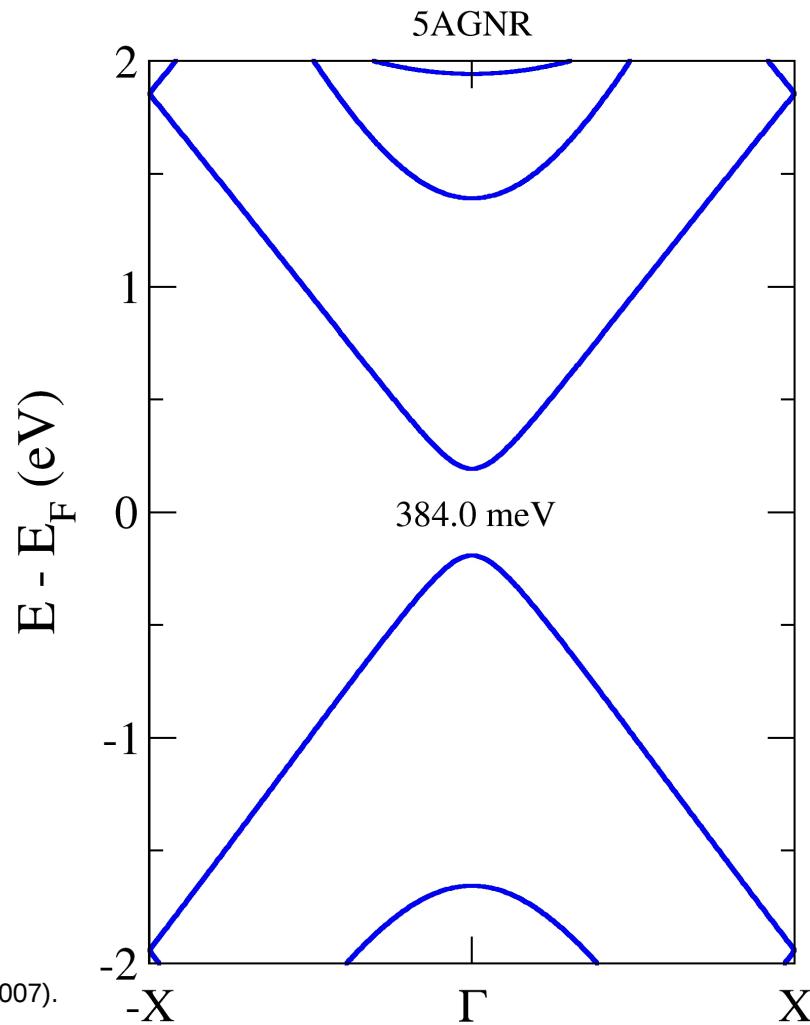
## The effect of Cl atoms on the electronic structure

vdW (optB88) energy gap  $\sim 0.38$  eV

LDA energy gap<sup>1</sup>  $\sim 0.4$  eV

GW energy gap<sup>1</sup>  $\sim 1.7$  eV  
GW energy gap<sup>1,2</sup> = 1.32 eV

STS gap<sup>2</sup> on Au =  $2.8 \pm 0.1$  eV



<sup>1</sup> L. Yang, C. H. Park, Y. W. Son, M. L. Cohen, and S. G. Louie. *PRL* **99**, 186801 (2007).

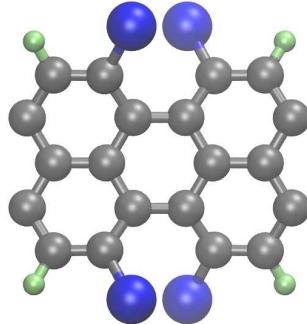
<sup>2</sup> H. Zhang et al. *JACS* **137**, 4022-4025 (2015).



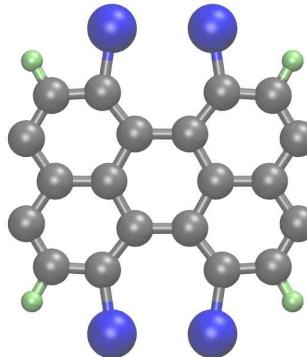
# Electronic properties of Cl doped 5-AGNR on Au(111) by first-principles calculations

## Free standing Cl-5-AGNR

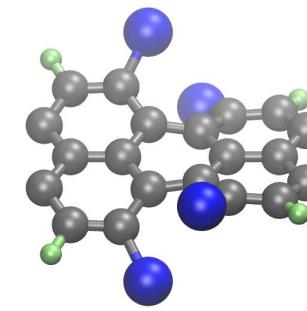
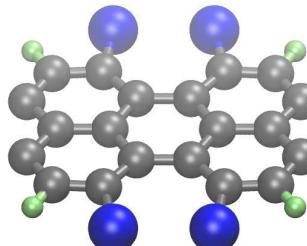
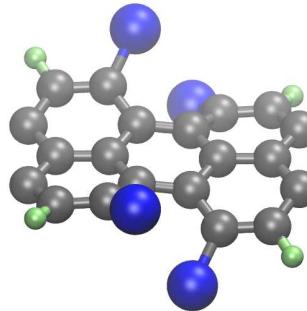
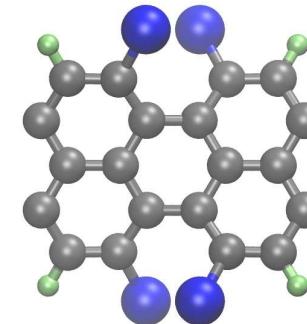
**symmetric**  
 $a = 8.64 \text{ \AA}$   
 $E_{\text{tot}} = -5178.84 \text{ eV}$



**flat**  
 $a = 8.93 \text{ \AA}$   
 $E_{\text{tot}} = -5175.93 \text{ eV}$



**asymmetric**  
 $a = 8.64 \text{ \AA}$   
 $E_{\text{tot}} = -5179.04 \text{ eV}$



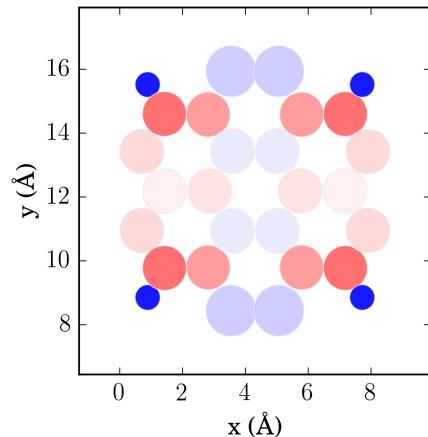
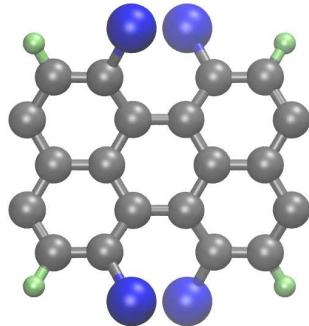
PS: no changes were observed in spin polarized calculations.



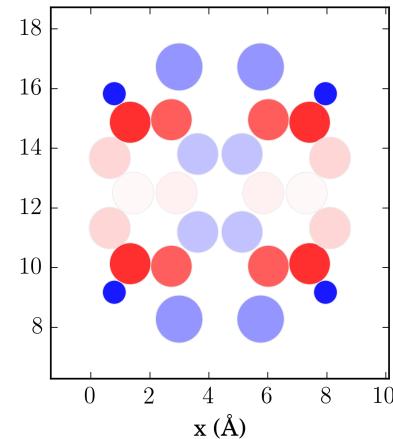
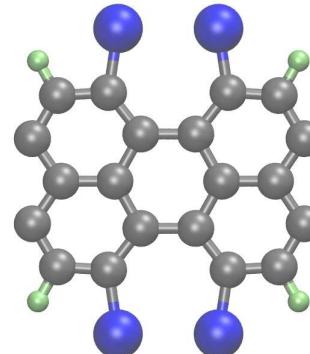
# Electronic properties of Cl doped 5-AGNR on Au(111) by first-principles calculations

## Free standing Cl-5-AGNR

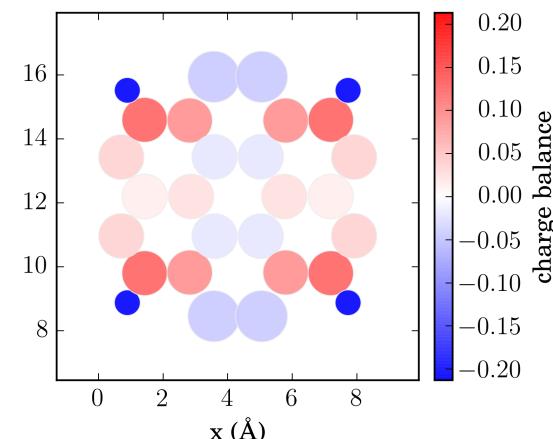
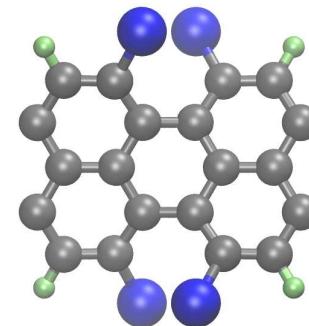
**symmetric**  
 $a = 8.64 \text{ \AA}$   
 $E_{\text{tot}} = -5178.84 \text{ eV}$



**flat**  
 $a = 8.93 \text{ \AA}$   
 $E_{\text{tot}} = -5175.93 \text{ eV}$



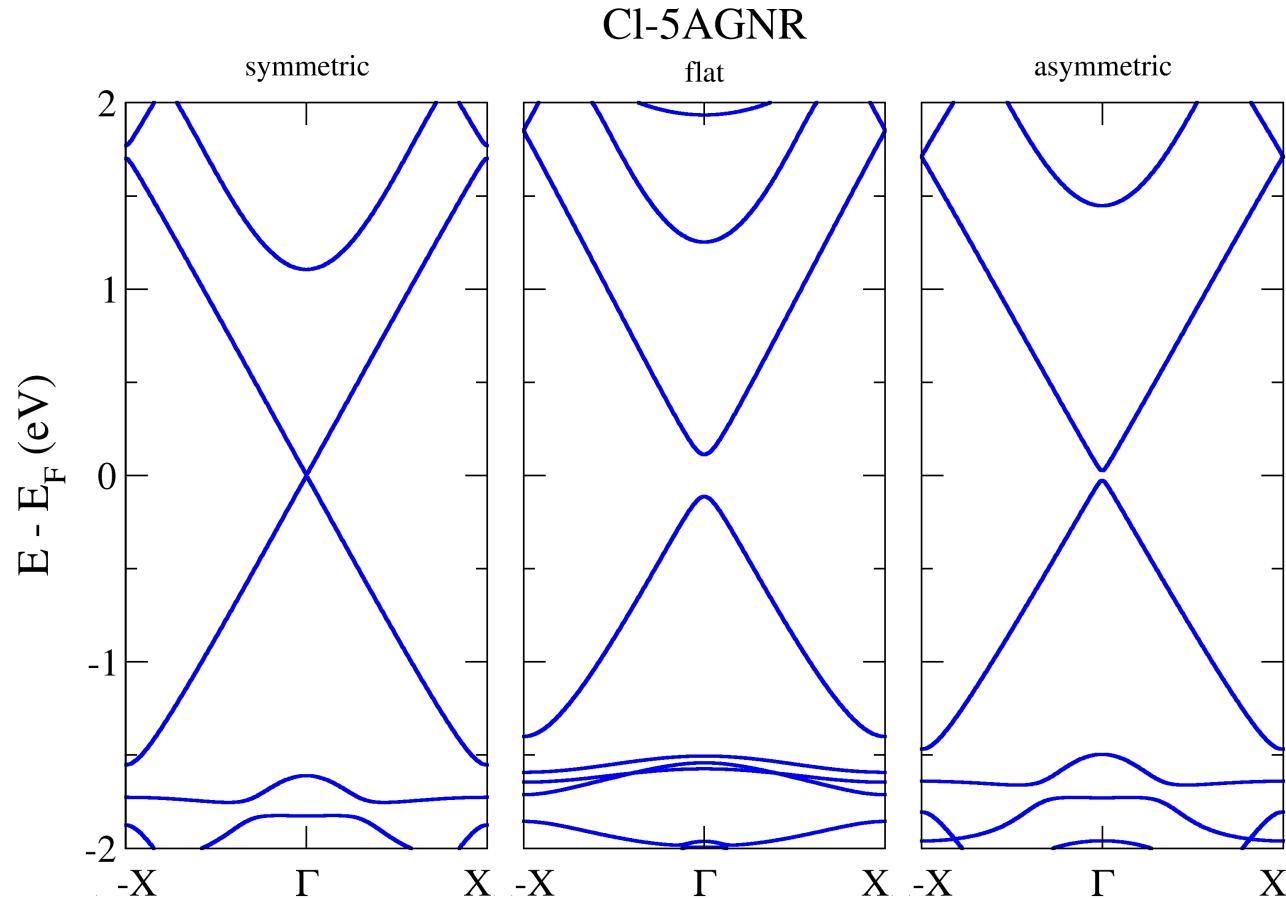
**asymmetric**  
 $a = 8.64 \text{ \AA}$   
 $E_{\text{tot}} = -5179.04 \text{ eV}$



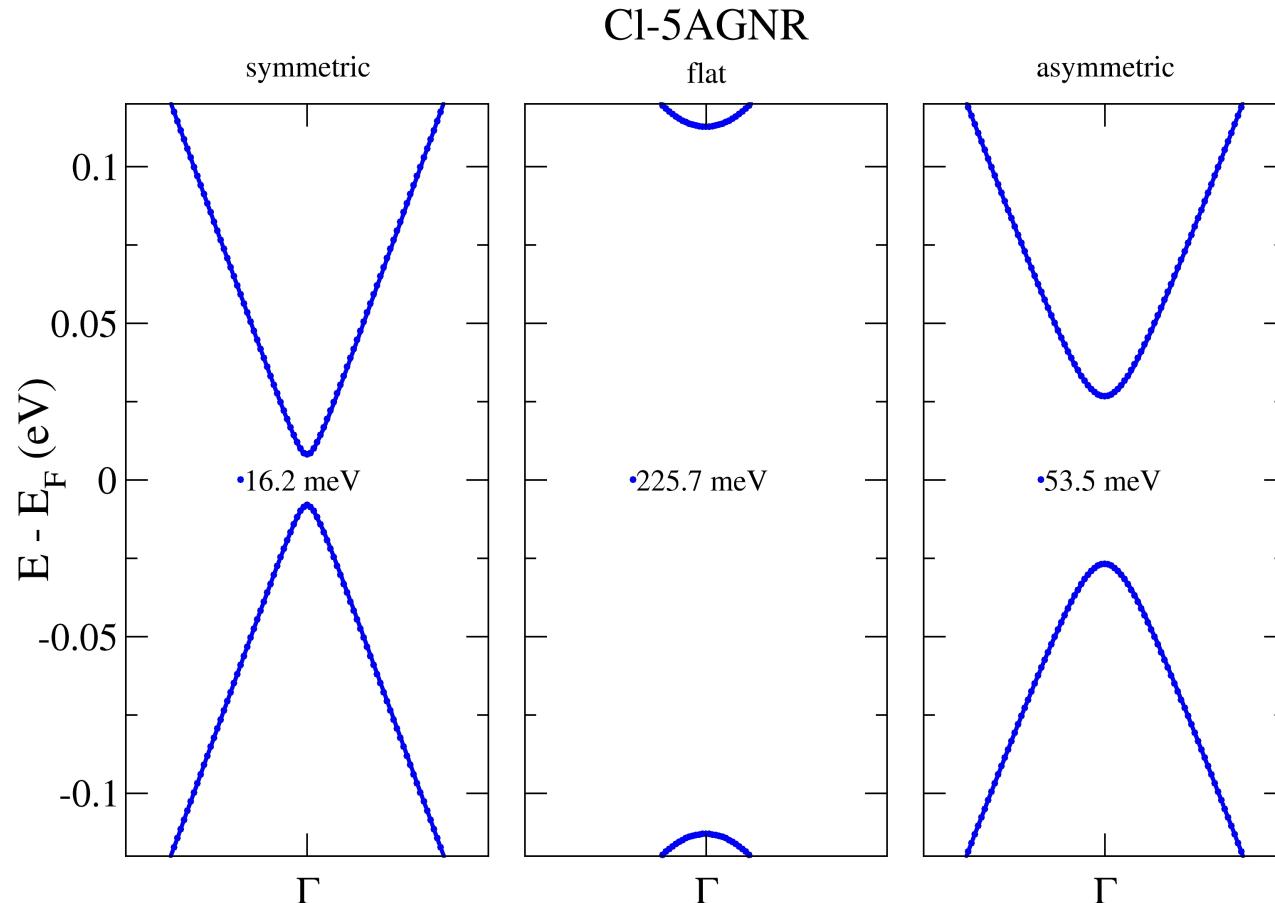
PS: no changes were observed in spin polarized calculations.



## Free standing Cl-5-AGNR

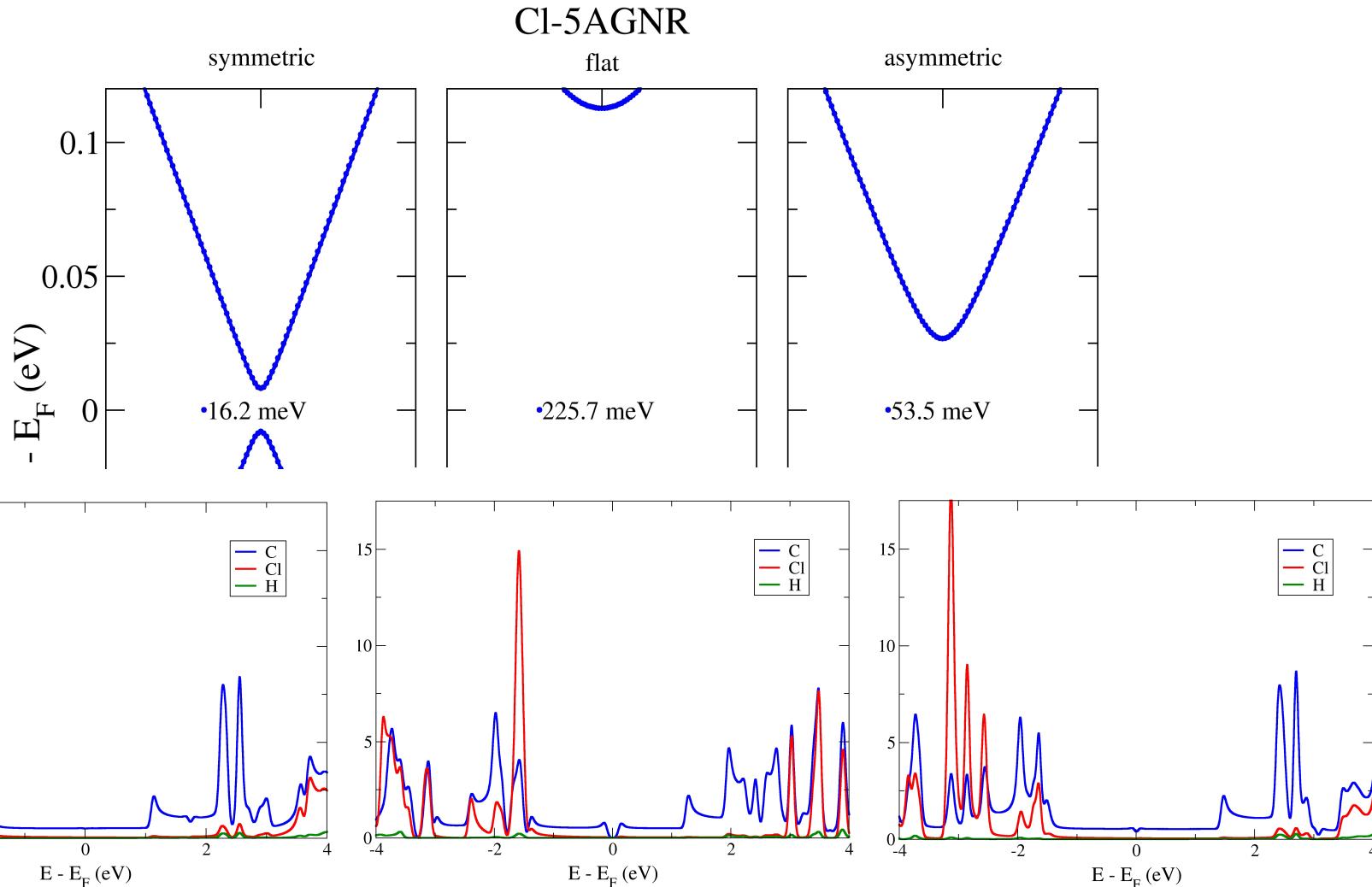


## Free standing Cl-5-AGNR

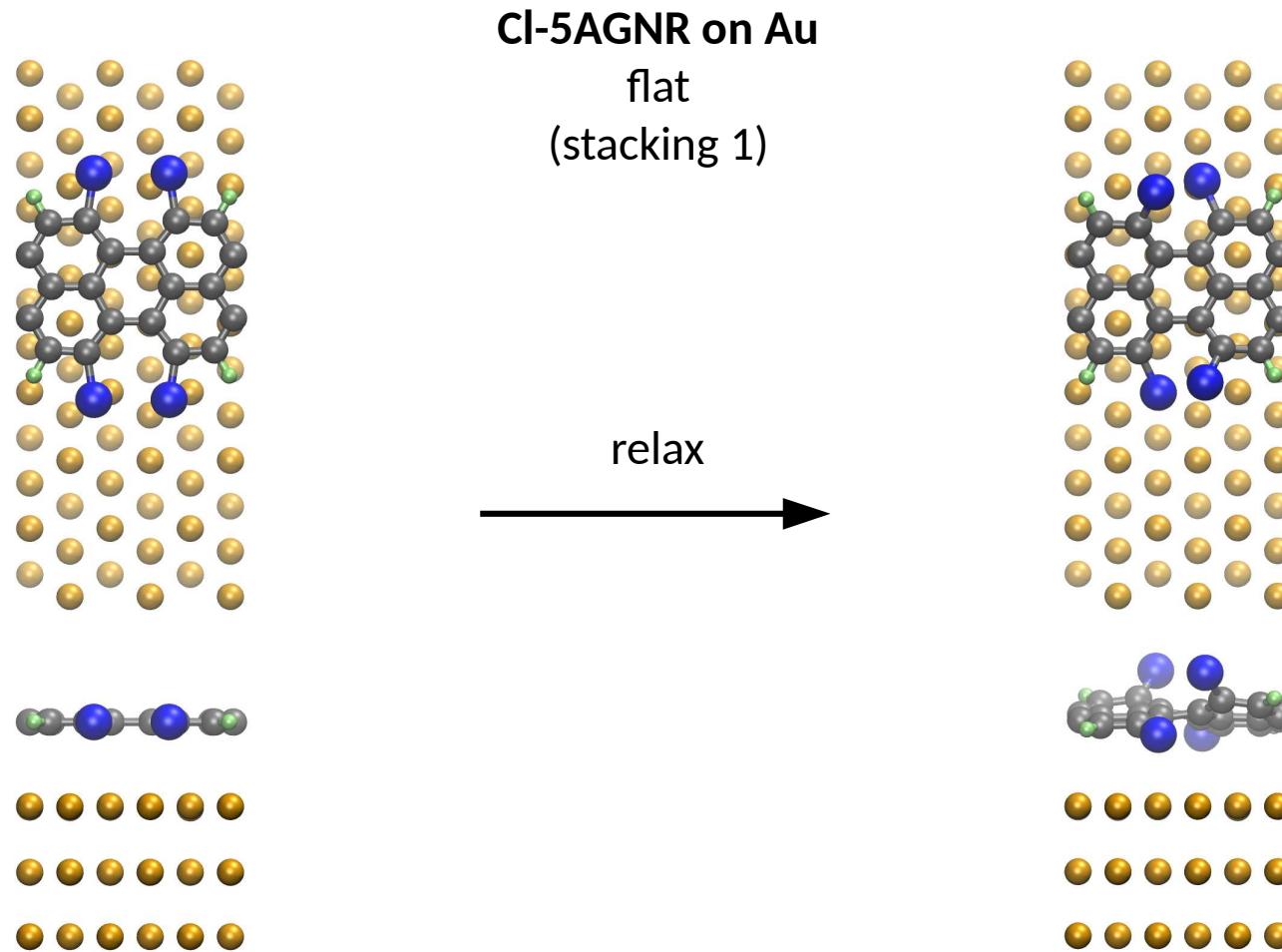


# Electronic properties of Cl doped 5-AGNR on Au(111) by first-principles calculations

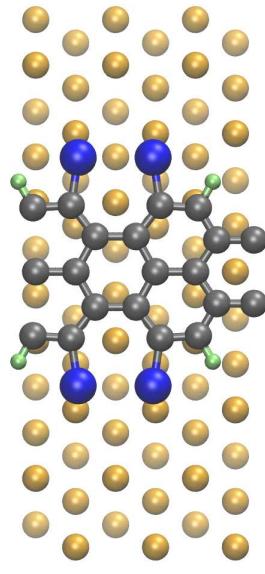
## Free standing Cl-5-AGNR



## Cl-5-AGNR on Au(111)

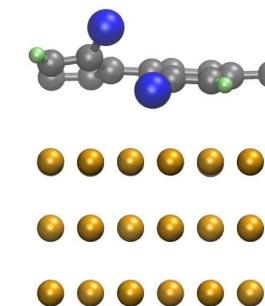
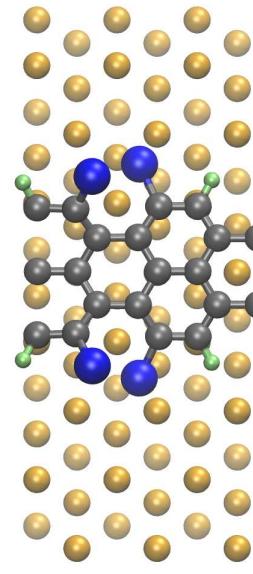
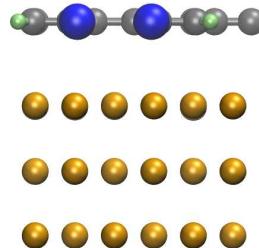


## Cl-5-AGNR on Au(111)



Cl-5AGNR on Au  
flat  
(stacking 2)

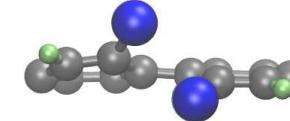
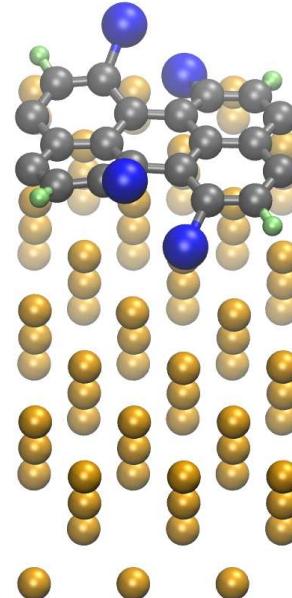
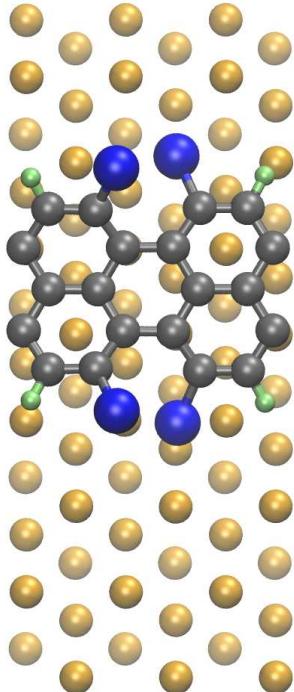
relax



## Cl-5-AGNR on Au(111)

Cl-5AGNR on Au - symmetric

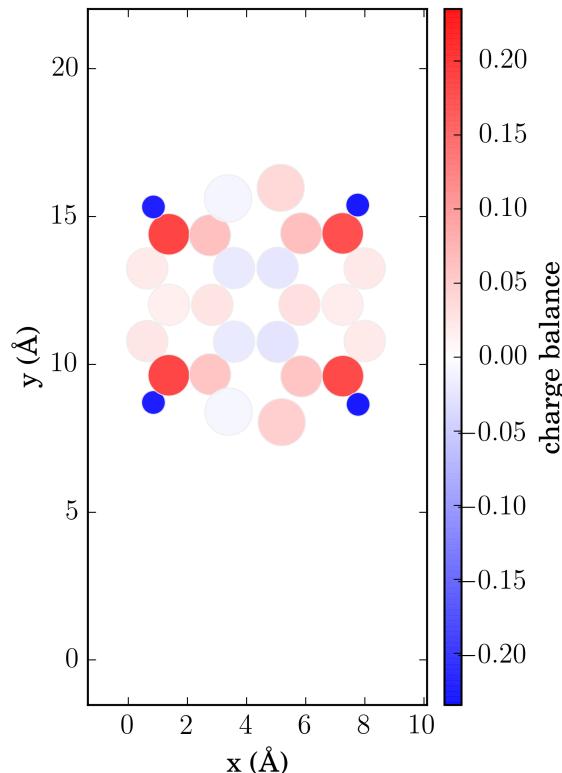
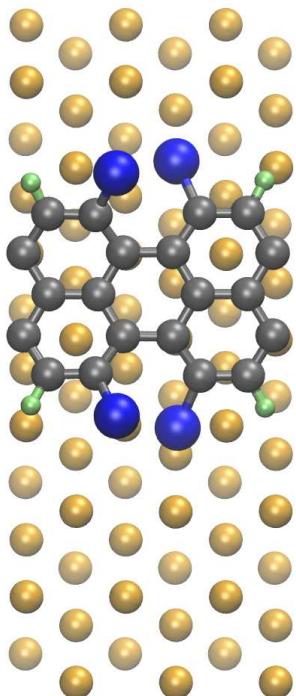
$$E_{\text{tot}} = -78965.51 \text{ eV}$$



## Cl-5-AGNR on Au(111)

Cl-5AGNR on Au - symmetric

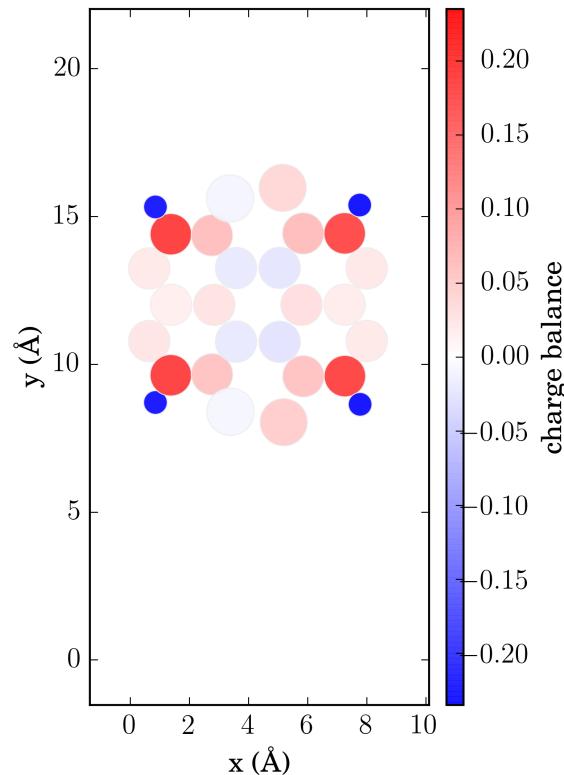
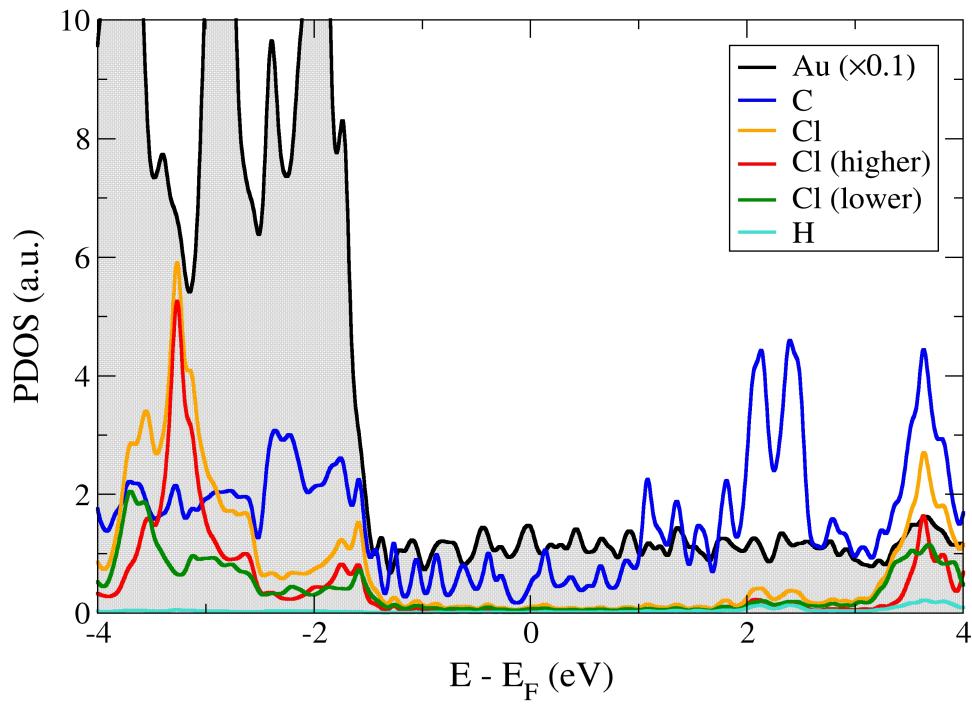
$$E_{\text{tot}} = -78965.51 \text{ eV}$$



## Cl-5-AGNR on Au(111)

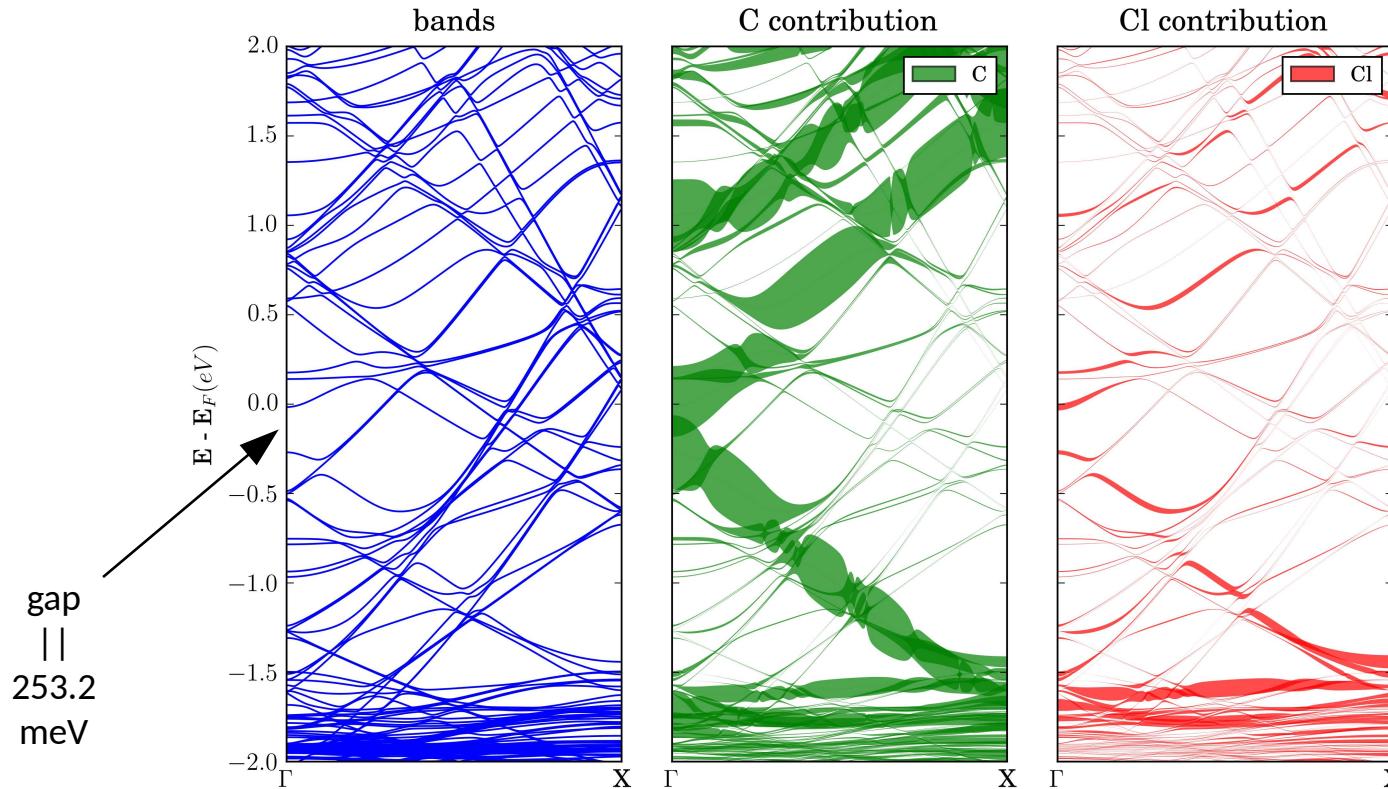
Cl-5AGNR on Au - symmetric

$$E_{\text{tot}} = -78965.51 \text{ eV}$$



## Cl-5-AGNR on Au(111)

Cl-5AGNR on Au - symmetric



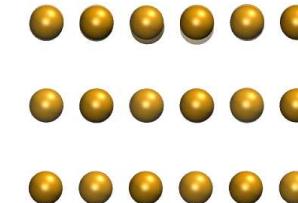
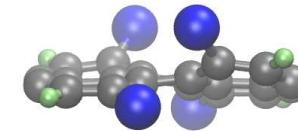
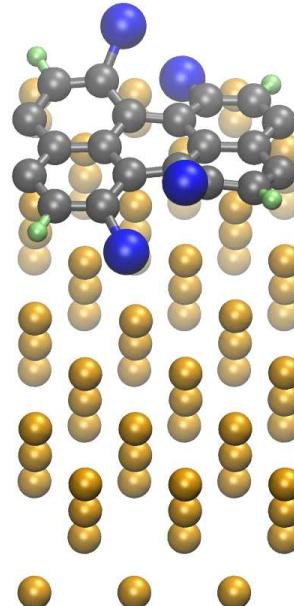
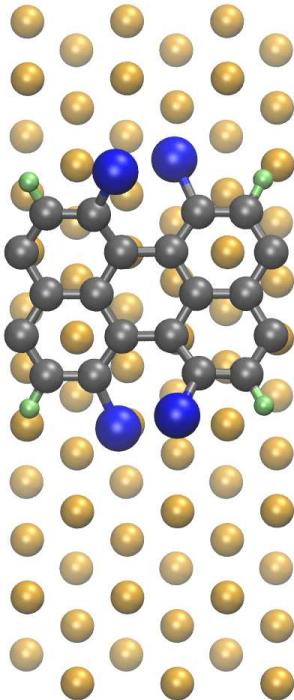
PS: equivalent results were obtained for different stacking.



## Cl-5-AGNR on Au(111)

Cl-5AGNR on Au - asymmetric

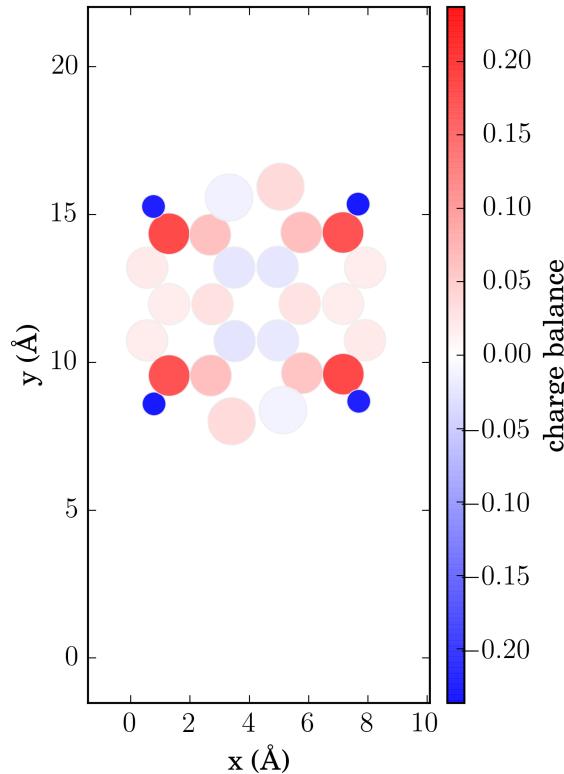
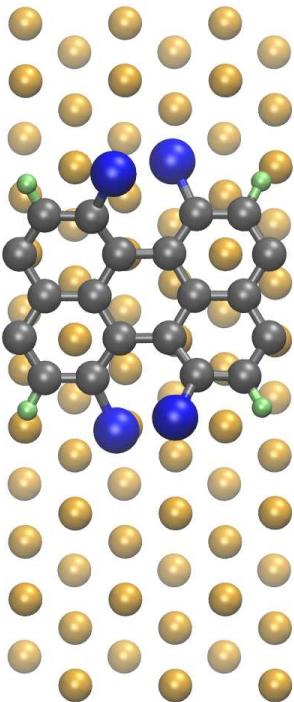
$$E_{\text{tot}} = -78965.59 \text{ eV}$$



## Cl-5-AGNR on Au(111)

Cl-5AGNR on Au - asymmetric

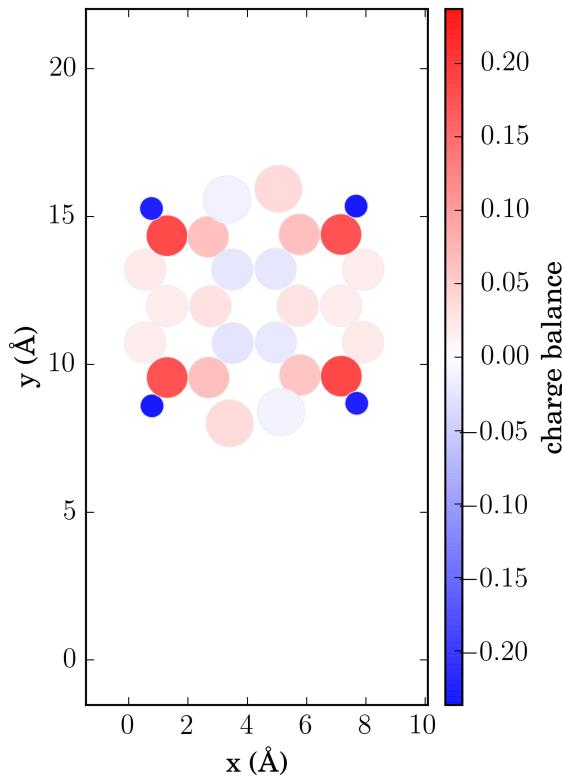
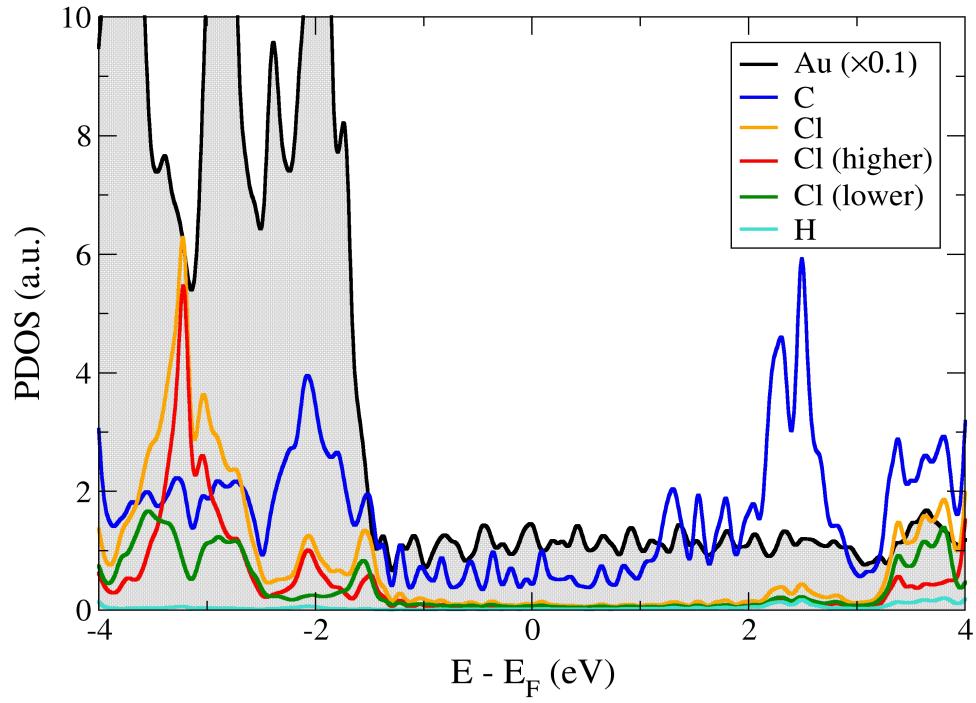
$$E_{\text{tot}} = -78965.59 \text{ eV}$$



## Cl-5-AGNR on Au(111)

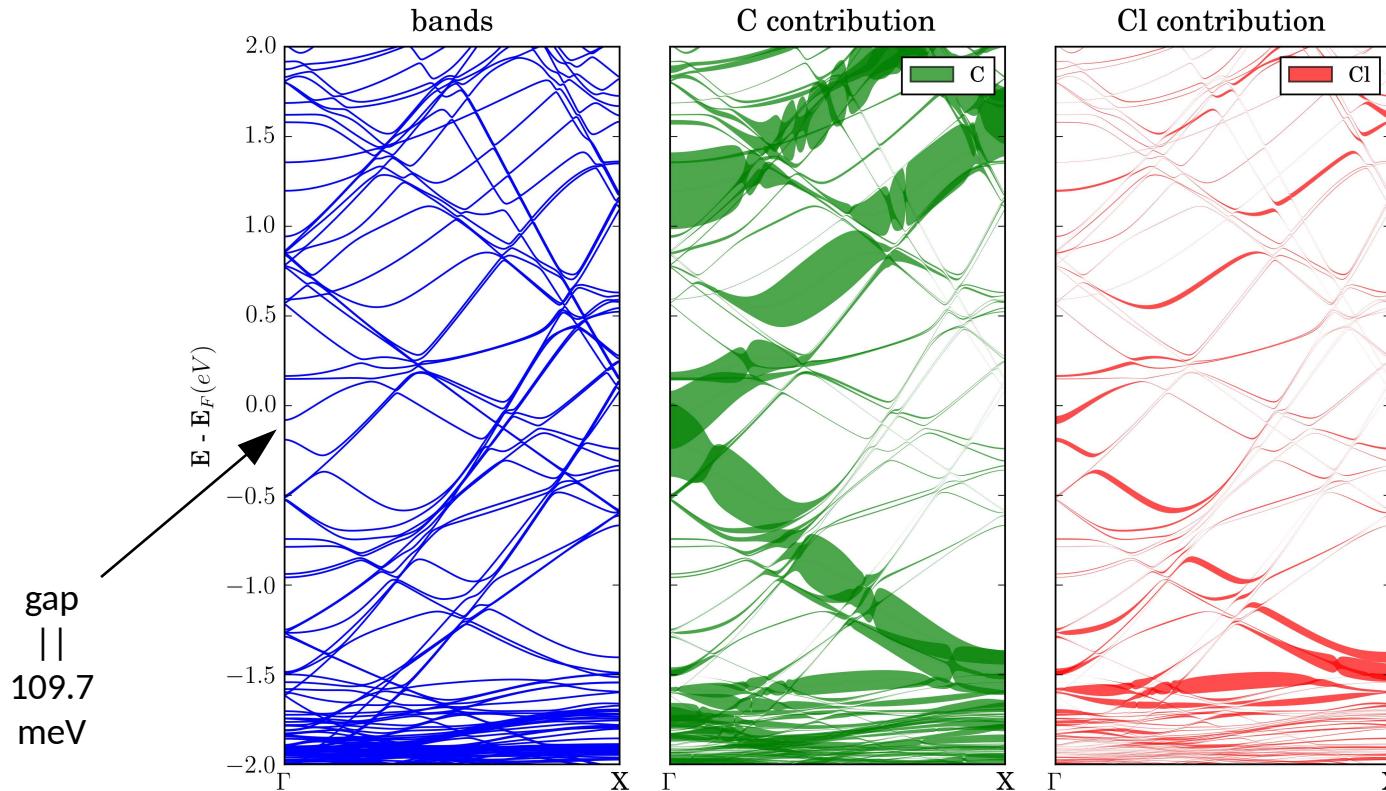
Cl-5AGNR on Au - asymmetric

$$E_{\text{tot}} = -78965.59 \text{ eV}$$



## Cl-5-AGNR on Au(111)

Cl-5AGNR on Au - asymmetric



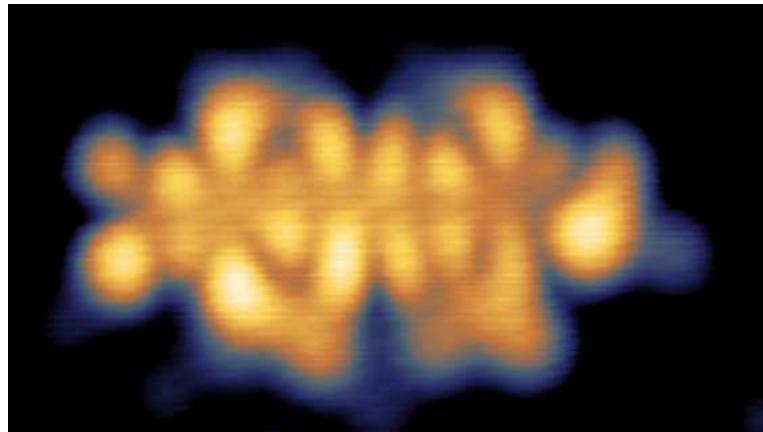
PS: equivalent results were obtained for different stacking but with larger energy gap of 183.5 meV.



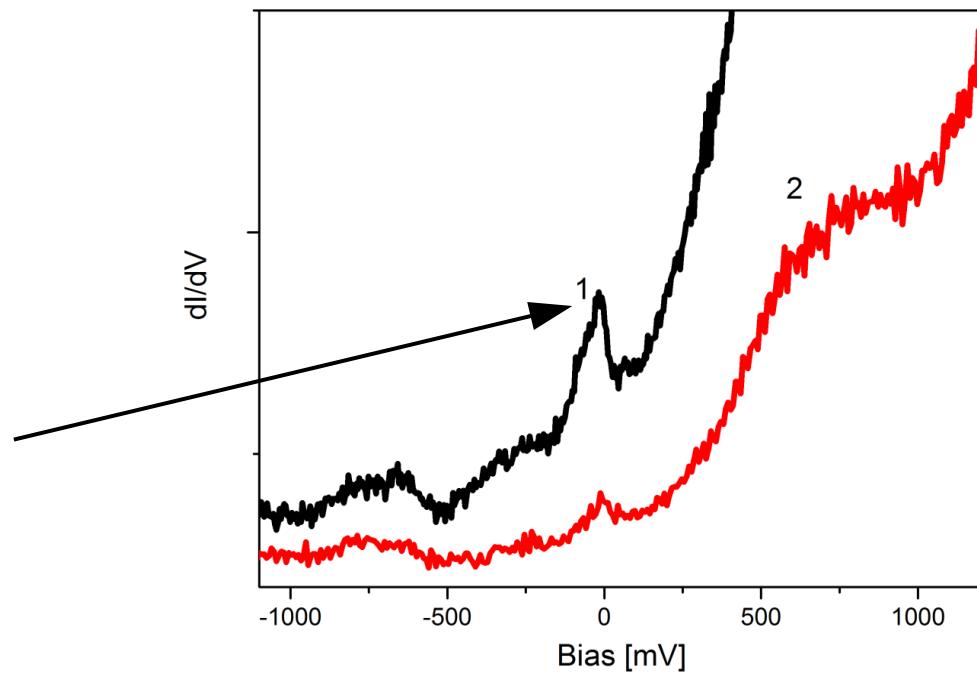
## Cl-5-AGNR dimer



UNIVERSITAS IAGELLONICA  
CRACOVIENSIS



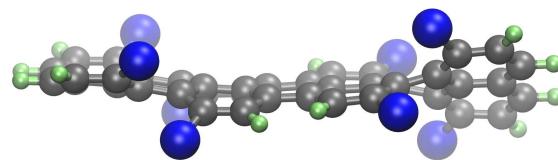
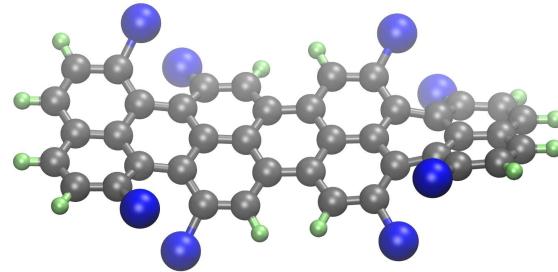
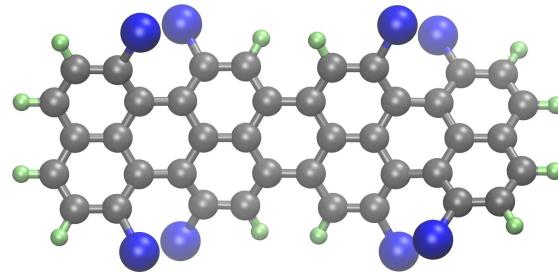
10 mV, 100 pA



## Free standing Cl-5-AGNR dimer

Cl-5AGNR dimer - sym-asym

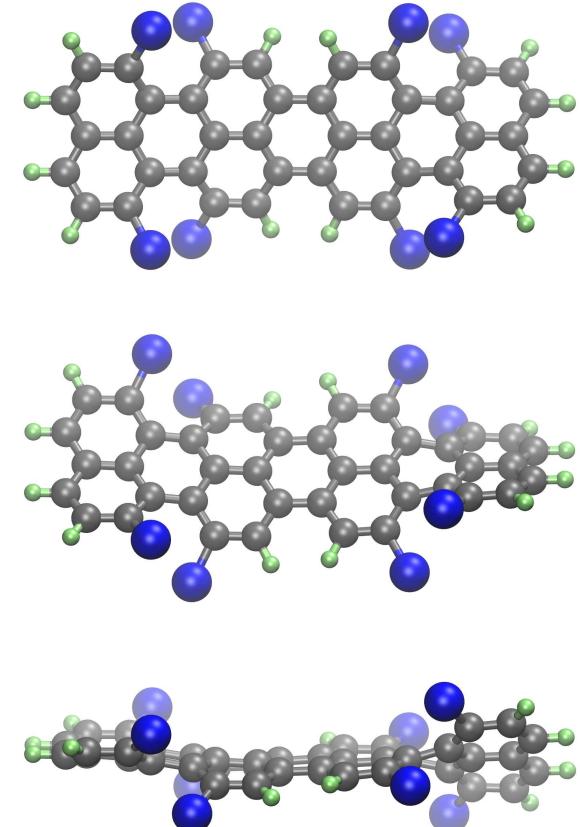
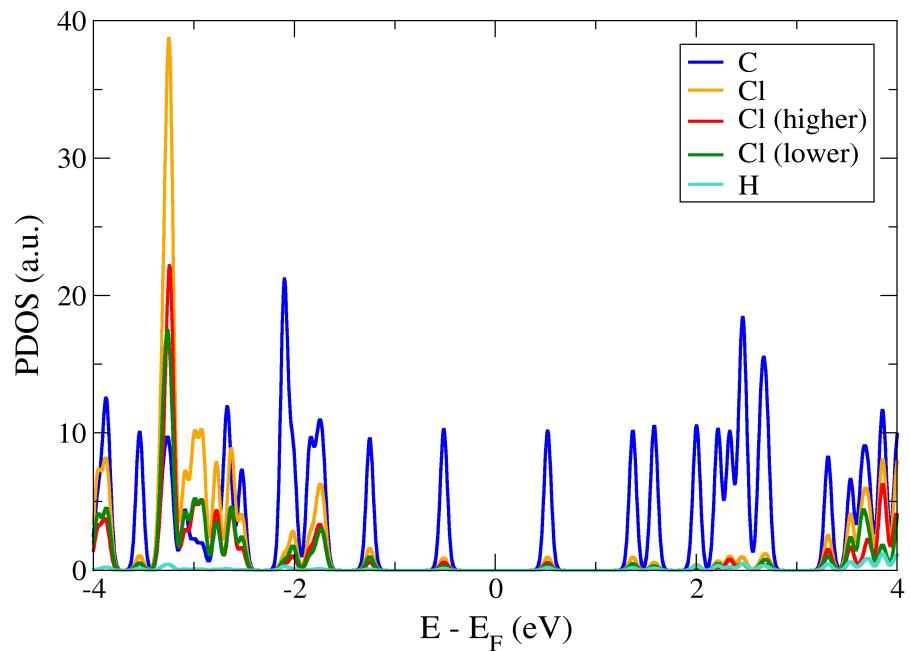
$$E_{\text{tot}} = -10422.23 \text{ eV}$$



## Free standing Cl-5-AGNR dimer

Cl-5AGNR dimer - sym-asym

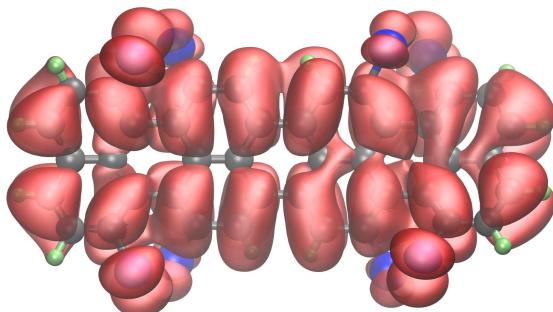
$$E_{\text{tot}} = -10422.23 \text{ eV}$$



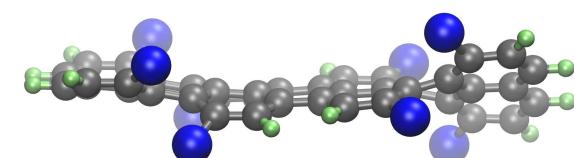
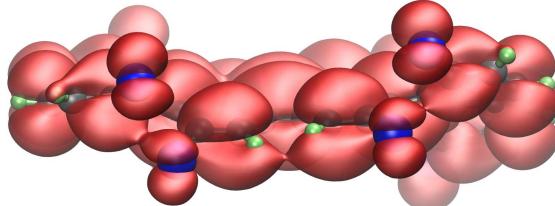
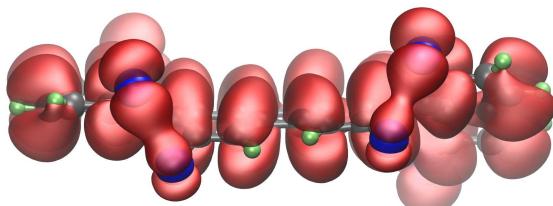
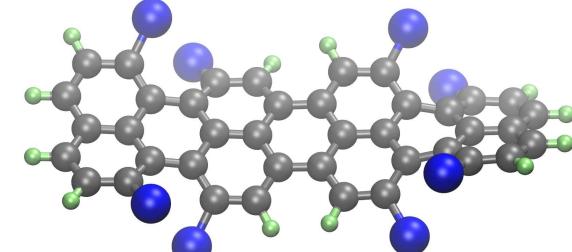
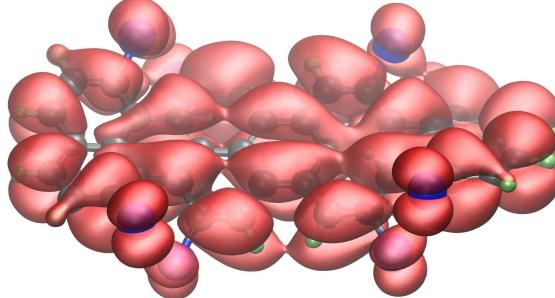
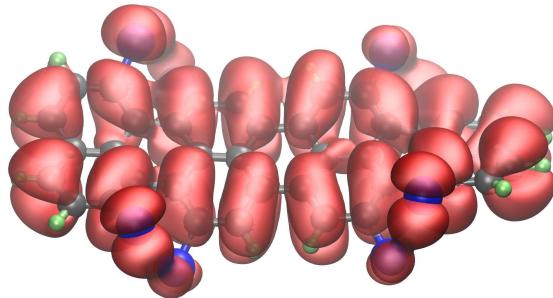
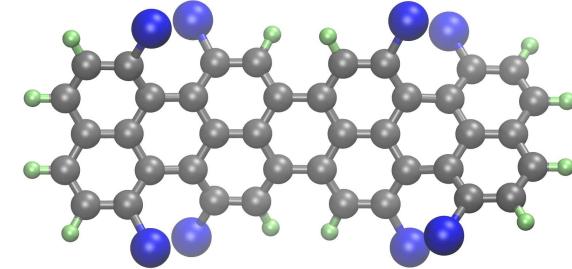
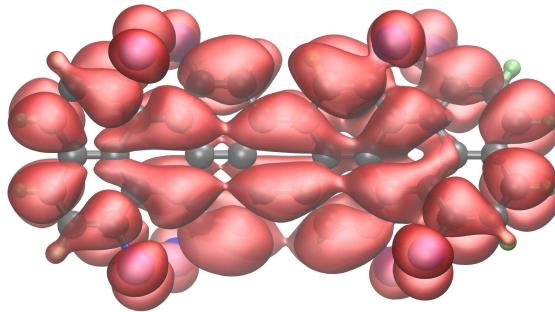
## Free standing Cl-5-AGNR dimer

Cl-5AGNR dimer - sym-asym

LDOS - HOMO



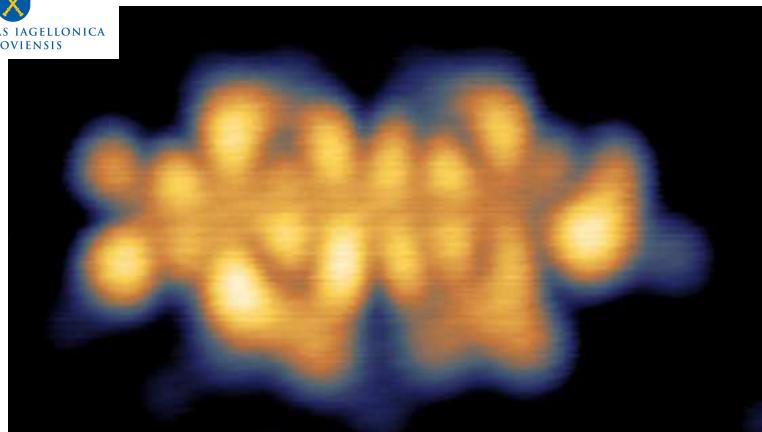
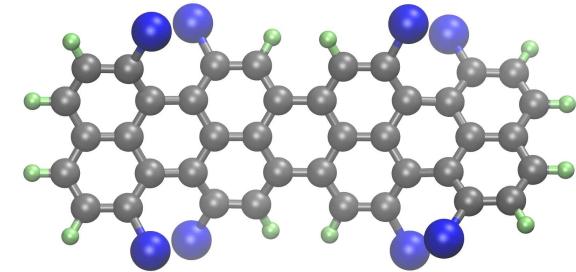
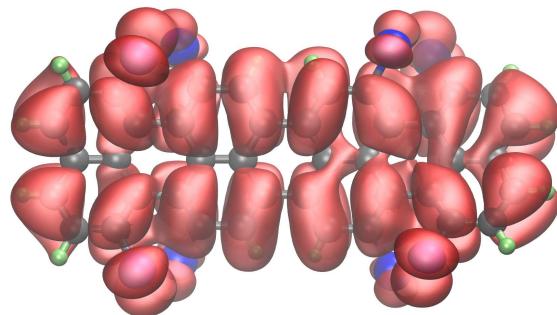
LDOS - LUMO



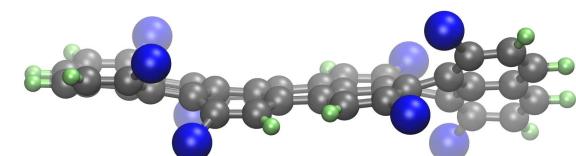
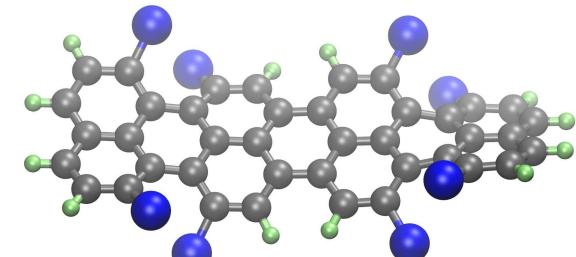
## Free standing Cl-5-AGNR dimer

Cl-5AGNR dimer – sym-asym

LDOS - HOMO



10 mV, 100 pA



# Thank you for your attention!



PAMS Project meeting, Brussels – 28 November 2016

