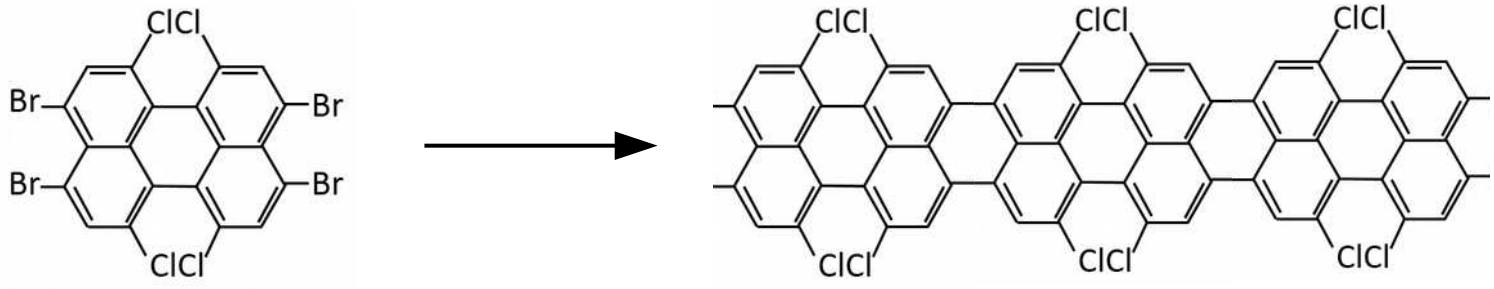
PAMS Project meeting
16th May 2017, Kraków

First principles study of Cl-doped 5-AGNR on Au(111) surface

Pedro Brandimarte

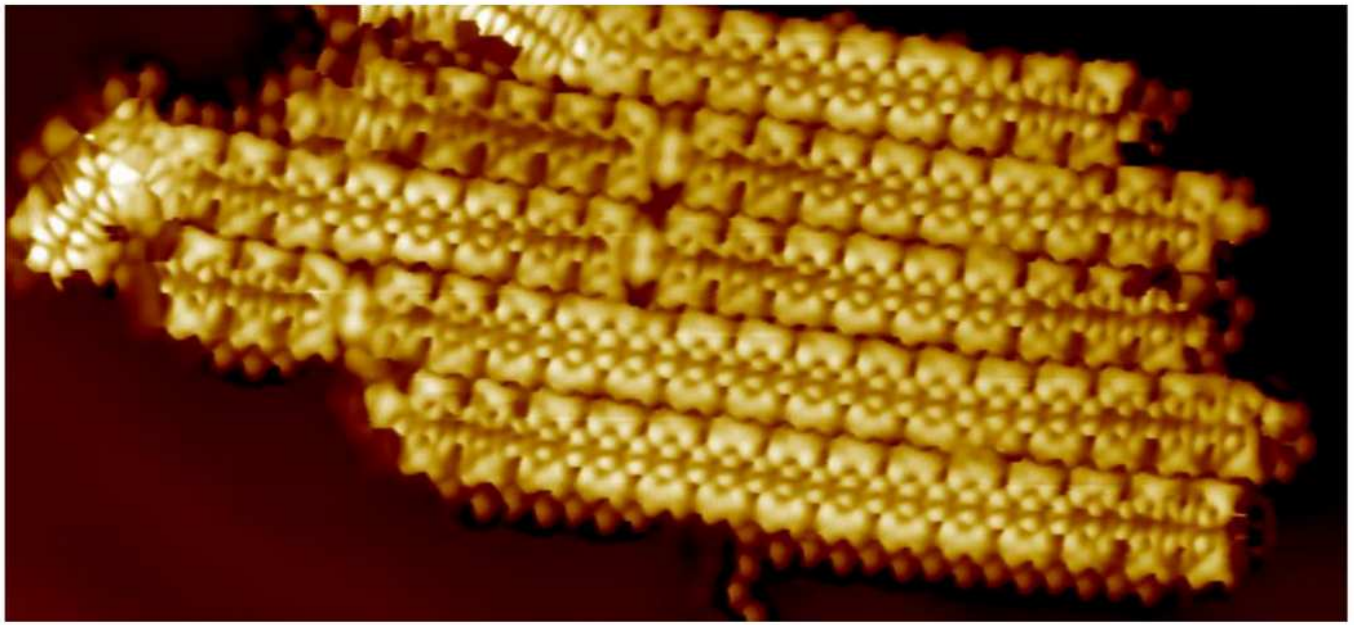
5-AGNR realized with one step reaction

UNIVERSITAS IAGELLONICA CRACOVIENSIS



5-AGNR realized with one step reaction

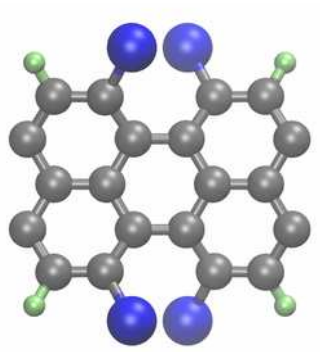
UNIVERSITAS IAGELLONICA
CRACOVIENSIS

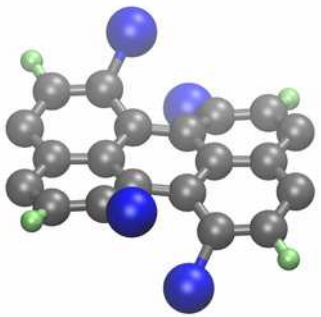


Free standing Cl-5-AGNR

symmetric

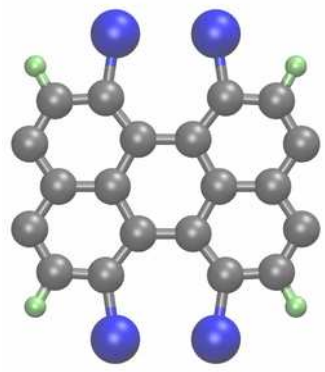
E_{tot} = -5178.84 eV

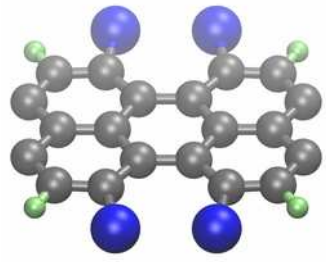




flat

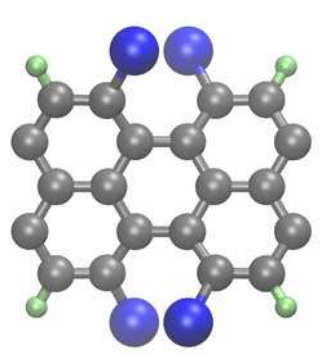
E_{tot} = -5175.93 eV

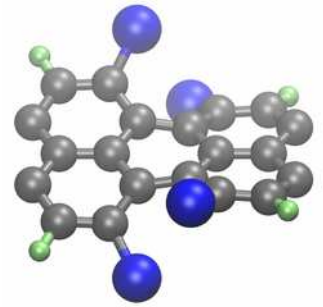




asymmetric

E_{tot} = -5179.04 eV





Population analysis: Mulliken

Partitioning in Hilbert space

$$N = \int d\boldsymbol{r} \sum_i n_i |\psi_i(\boldsymbol{r})|^2 = \sum_A \sum_{\mu \in A} (DS)_{\mu\mu}$$

Population analysis: Mulliken

Partitioning in Hilbert space

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Population analysis: Mulliken

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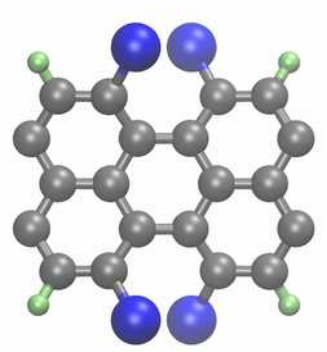
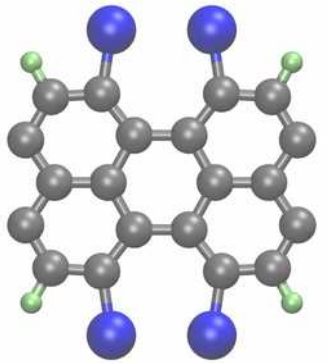
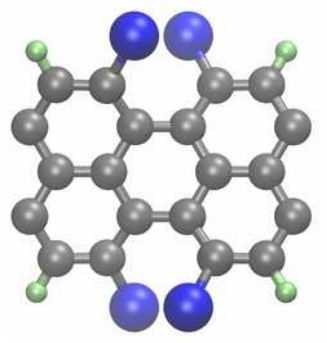
$$Q_A^{Mulliken} = eZ_A - eN_A$$

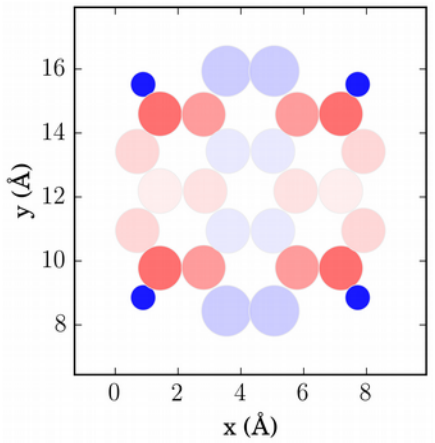
Population analysis: Mulliken

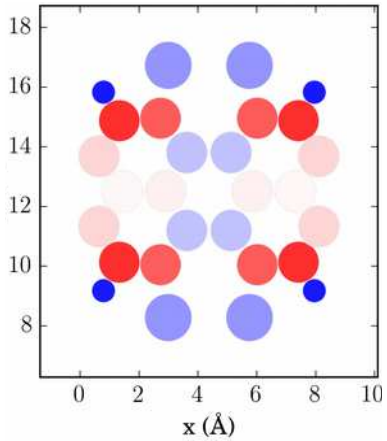
symmetric | **flat** | **asymmetric**

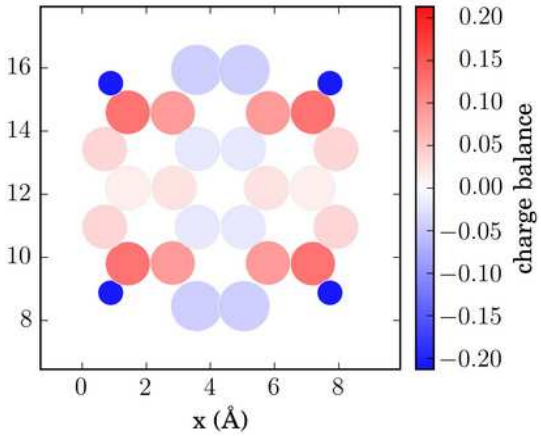












Population analysis: Hirshfeld

Partitioning in real space

$$\rho^{pro}(\boldsymbol{r}) = \sum_A \rho_A^{free}(\boldsymbol{r})$$

Population analysis: Hirshfeld

Partitioning in real space

$$\rho^{pro}(\boldsymbol{r}) = \sum_A \rho_A^{free}(\boldsymbol{r})$$

$$\rho_A^{eff}(\boldsymbol{r}) = \frac{\rho_A^{free}(\boldsymbol{r})}{\rho_A^{pro}(\boldsymbol{r})} \rho^{mol}(\boldsymbol{r})$$

Population analysis: Hirshfeld

Partitioning in real space

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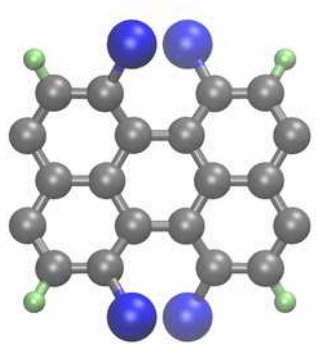
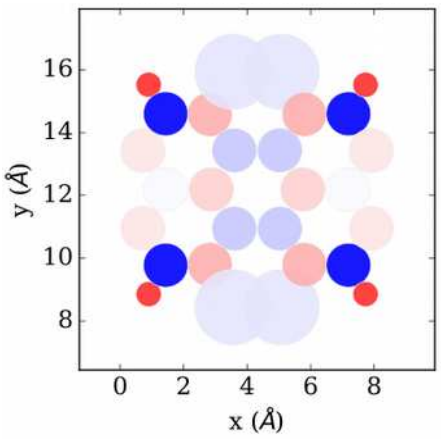
$$\rho_A^{eff}(\boldsymbol{r}) = \frac{\rho_A^{free}(\boldsymbol{r})}{\rho_A^{pro}(\boldsymbol{r})} \rho^{mol}(\boldsymbol{r})$$

$$Q_A^{Hirshfeld} = eZ_A - e \int d\boldsymbol{r} \rho_A^{eff}(\boldsymbol{r})$$

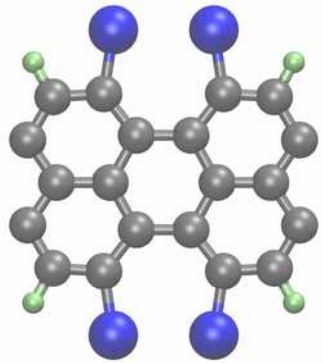
Population analysis: Hirshfeld

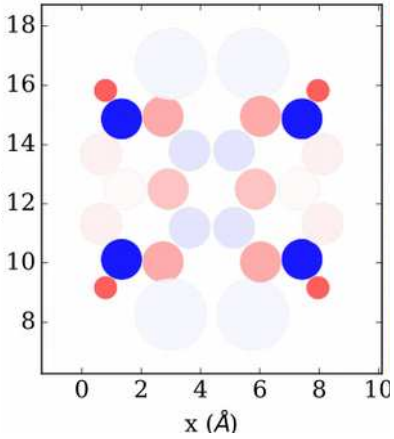
symmetric



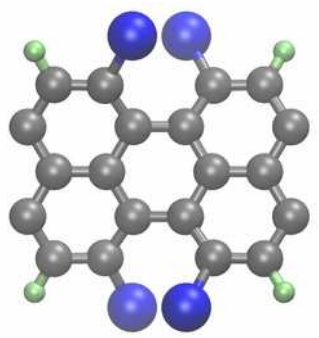


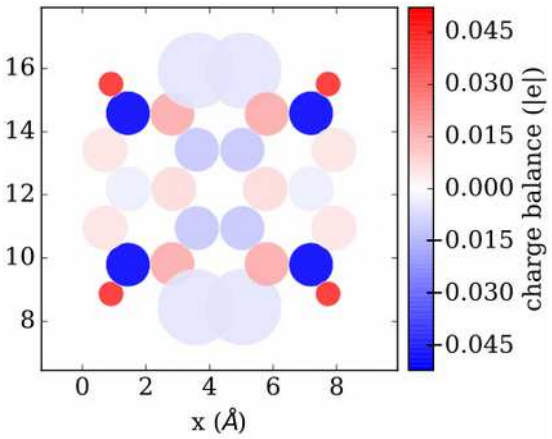
flat



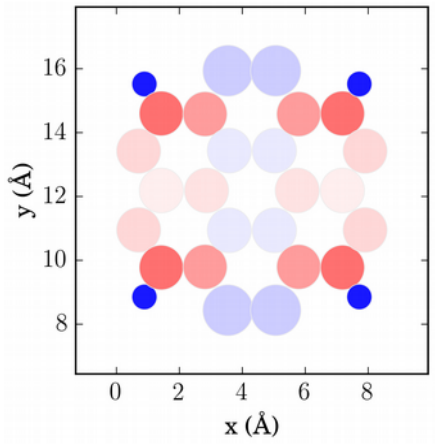
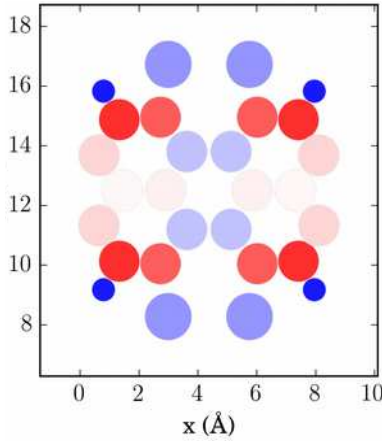
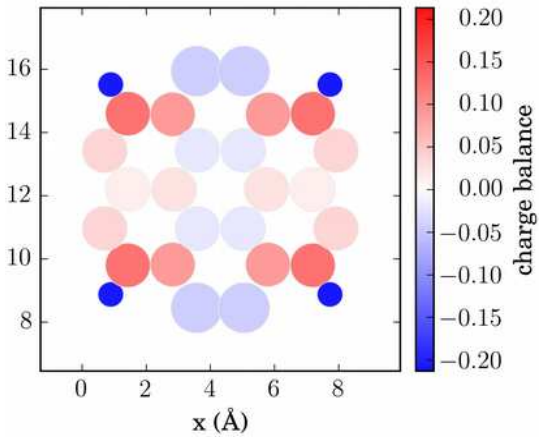
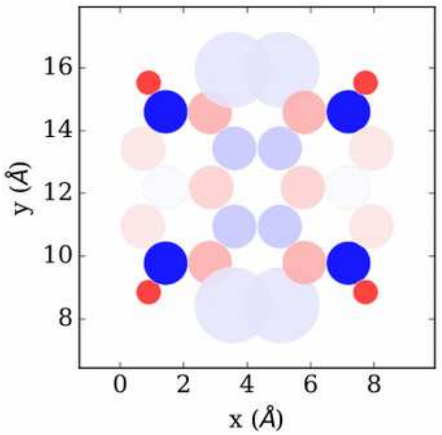
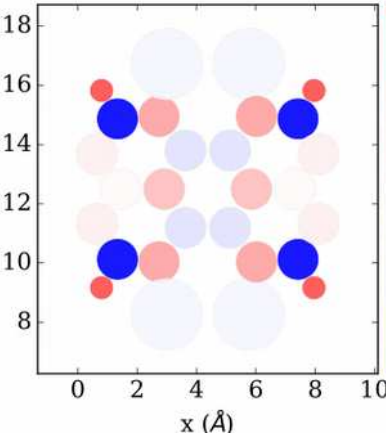
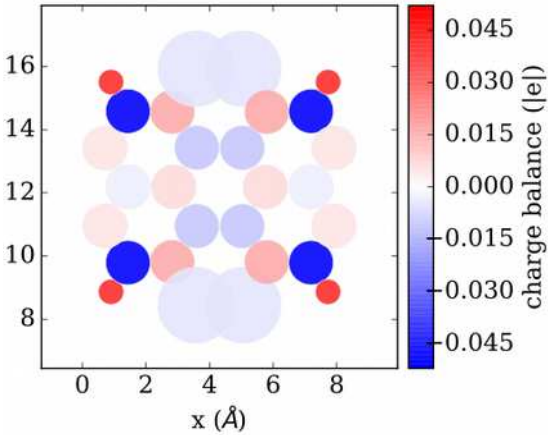


asymmetric





Population analysis: Hirshfeld

	symmetric	flat	asymmetric
Mulliken			
Hirshfeld			

Population analysis: Bader

Partitioning in real space

$$\nabla\rho(\boldsymbol{r}) \cdot \boldsymbol{n}(\boldsymbol{r}) = 0\,, \quad \forall \boldsymbol{r} \in \partial\Omega$$

Population analysis: Bader

Partitioning in real space

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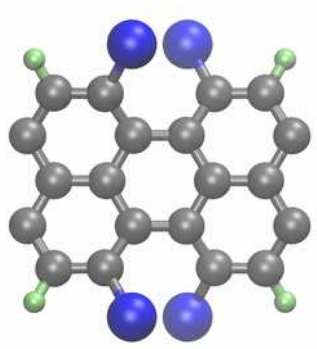
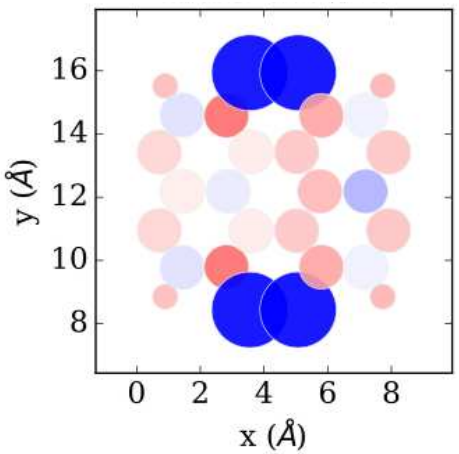
$$Q_A^{Bader} = eZ_A - e\int_{\Omega_A} d\boldsymbol{r}\rho(\boldsymbol{r})$$

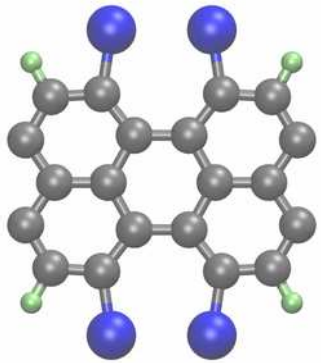
Population analysis: Bader

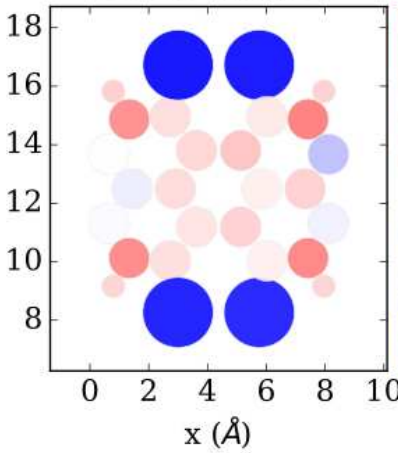
symmetric



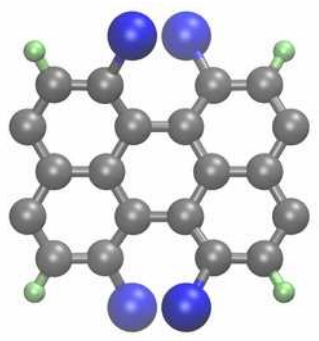


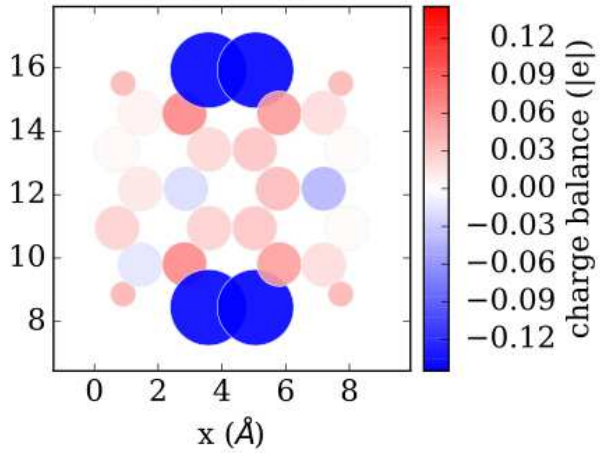
flat





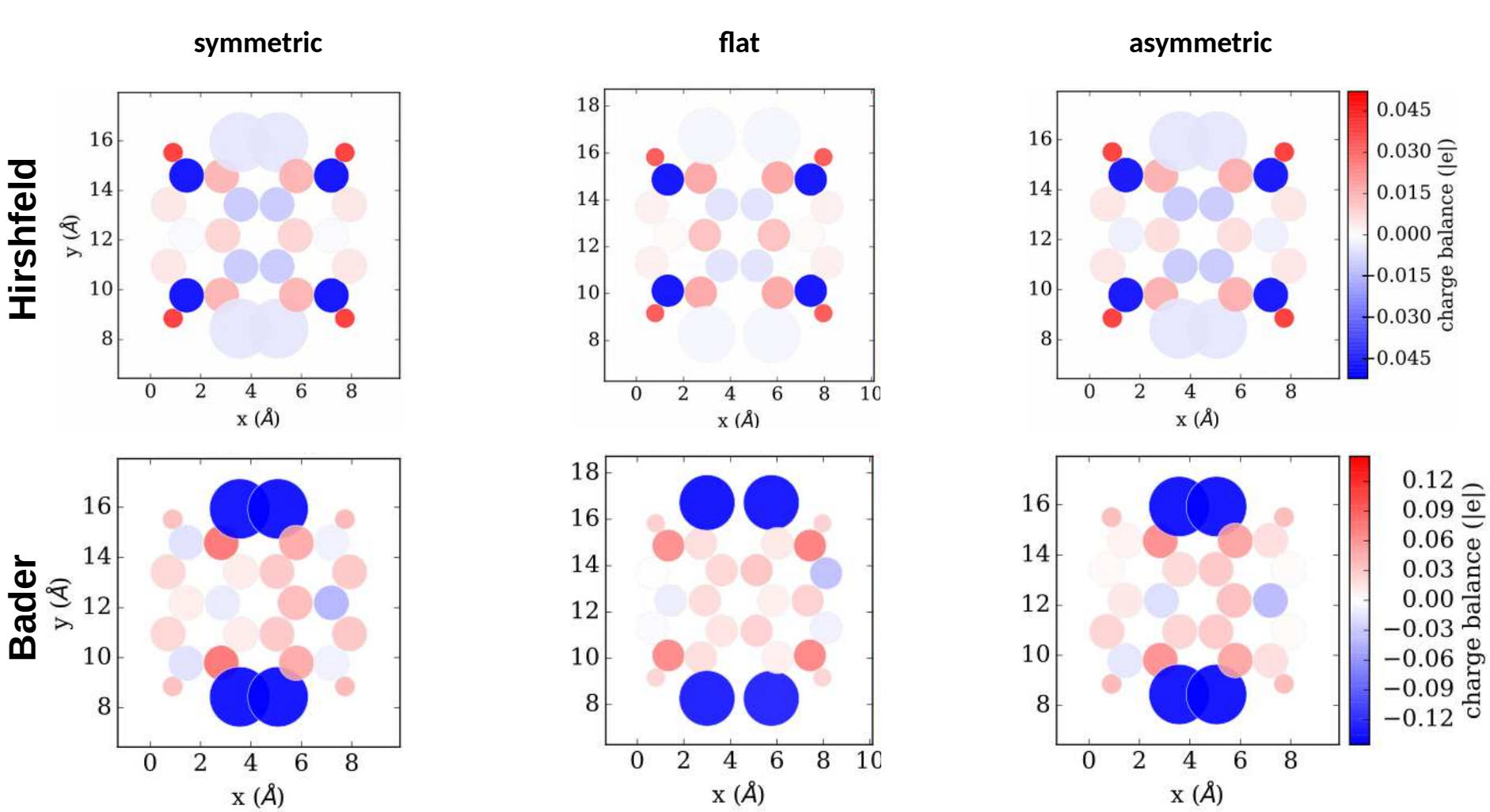
asymmetric





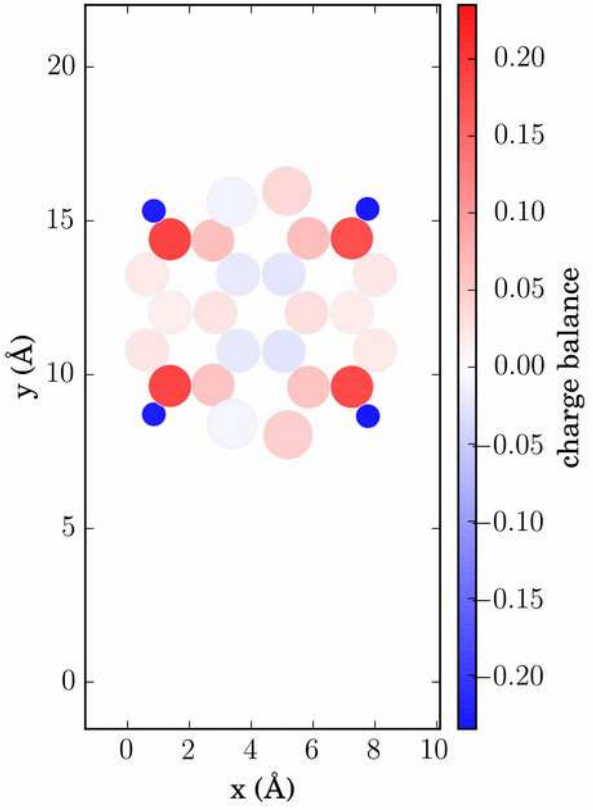
First principles study of Cl-doped 5-AGNR on Au(111) surface

Population analysis: Bader



Population analysis: symmetric Cl-5-AGNR on Au(111)

Mulliken



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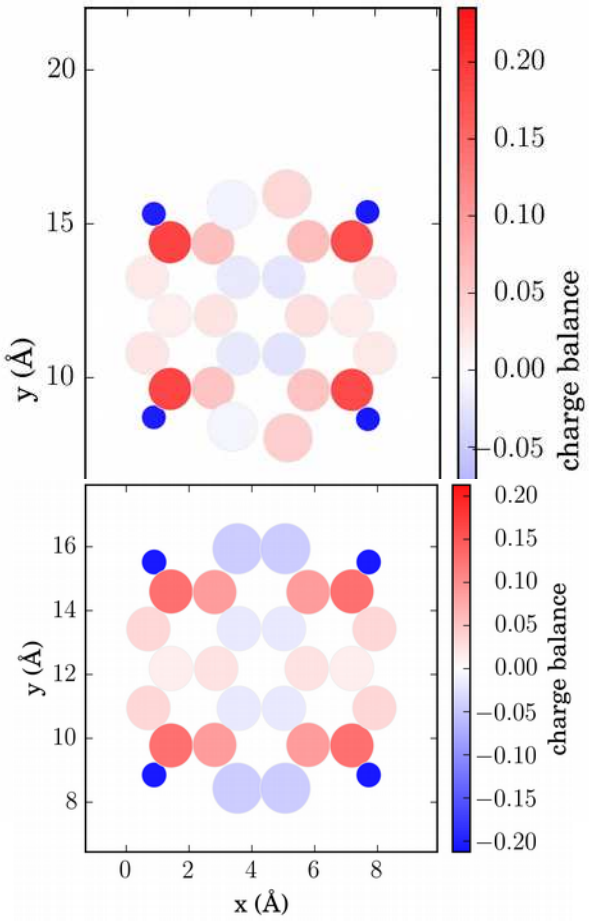

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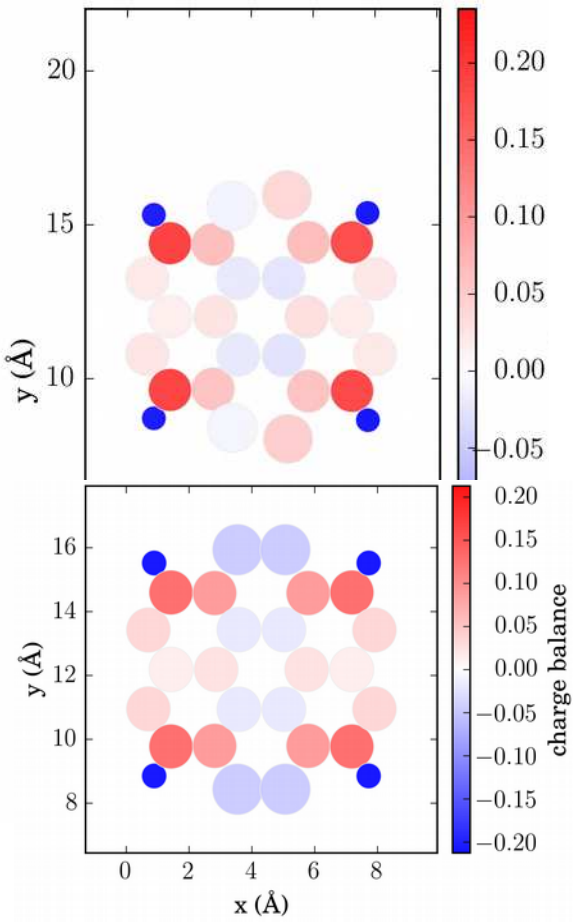
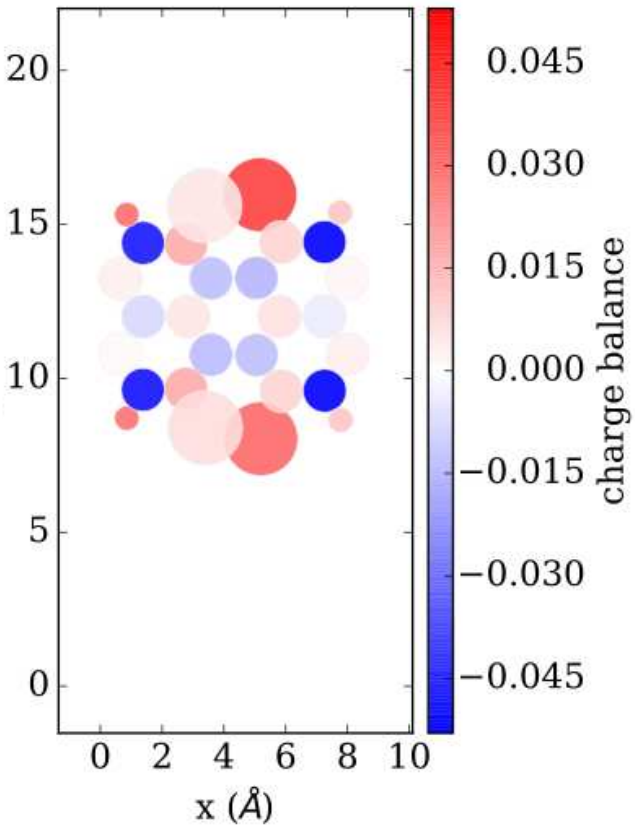


Hirshfeld



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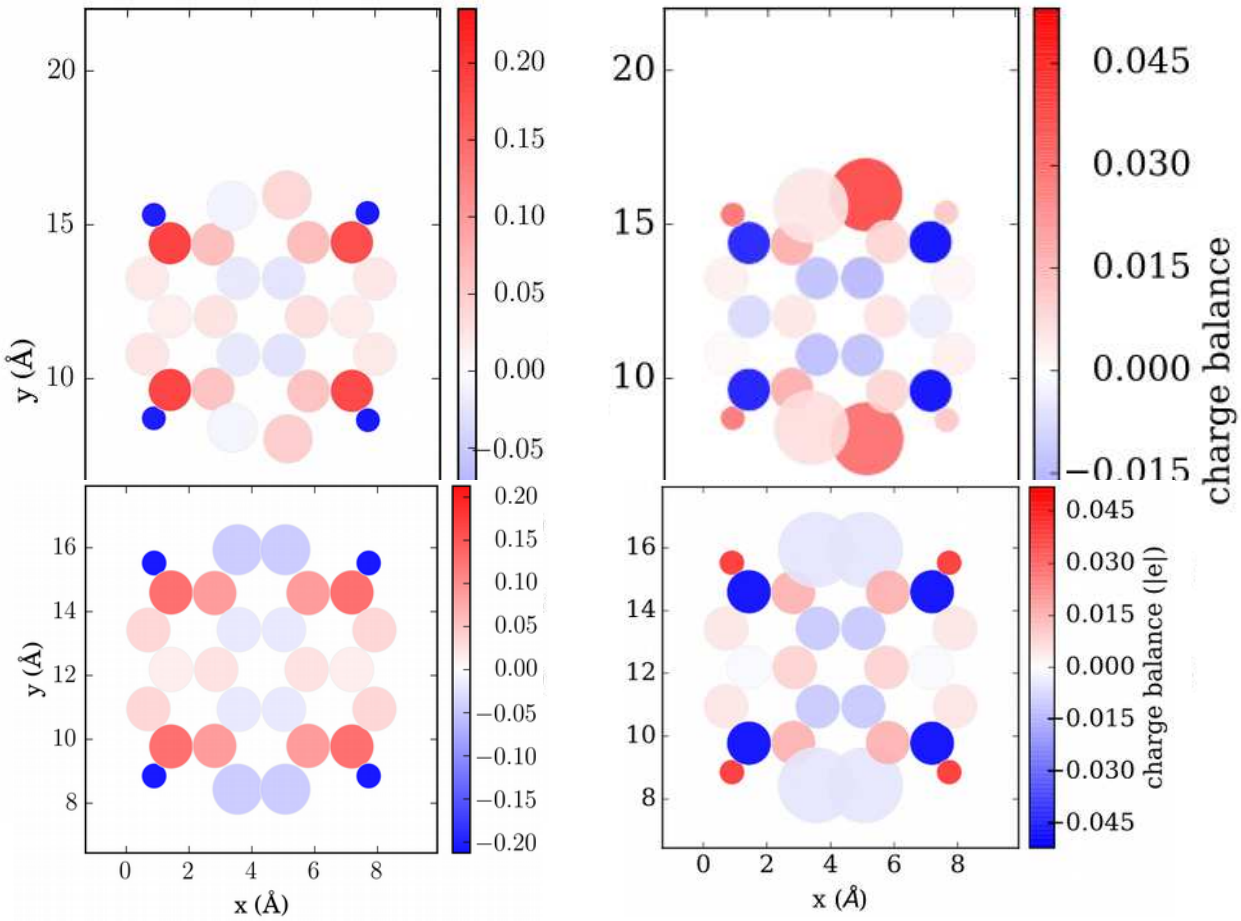
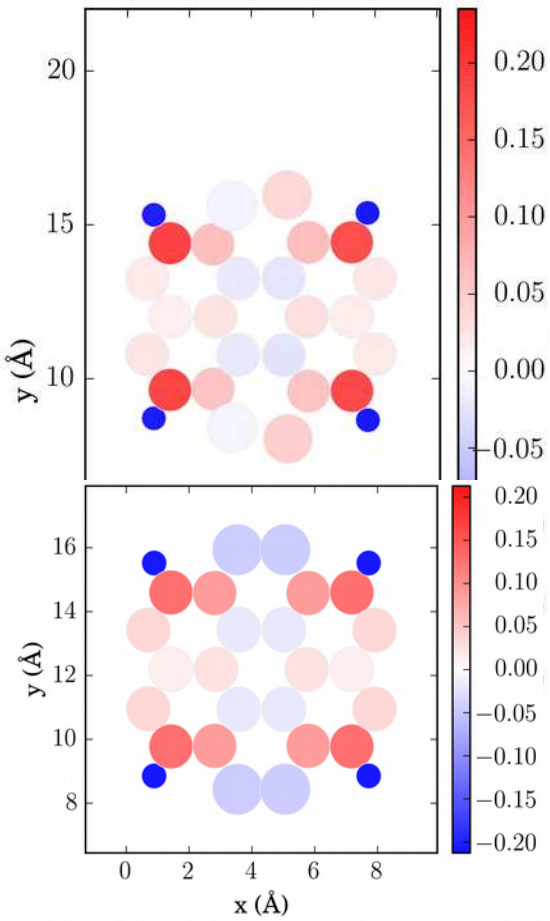
Mulliken

Hirshfeld

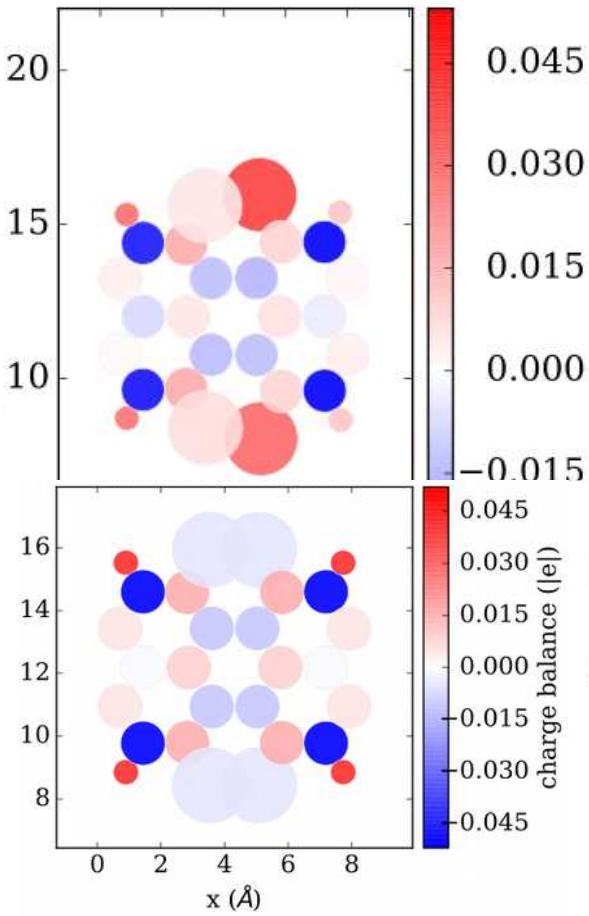


Population analysis: symmetric Cl-5-AGNR on Au(111)

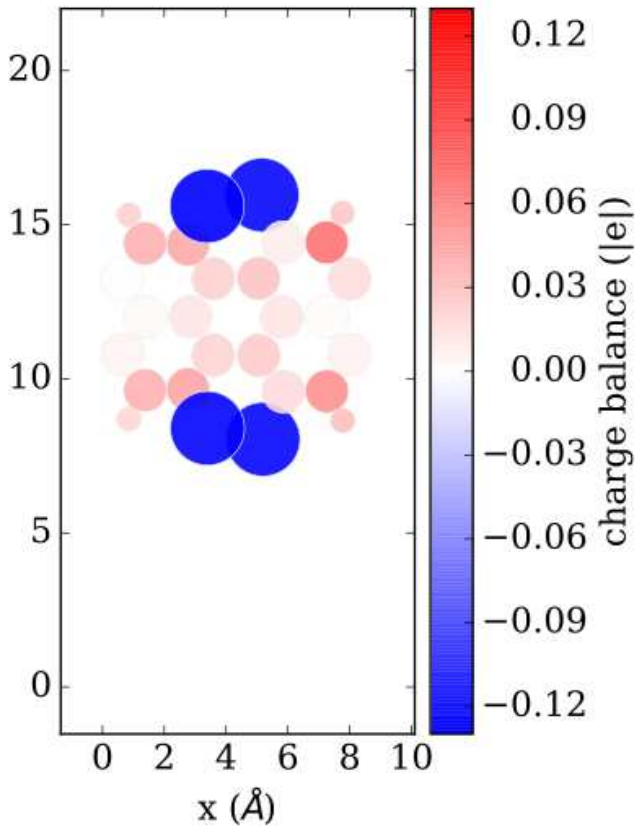
Mulliken



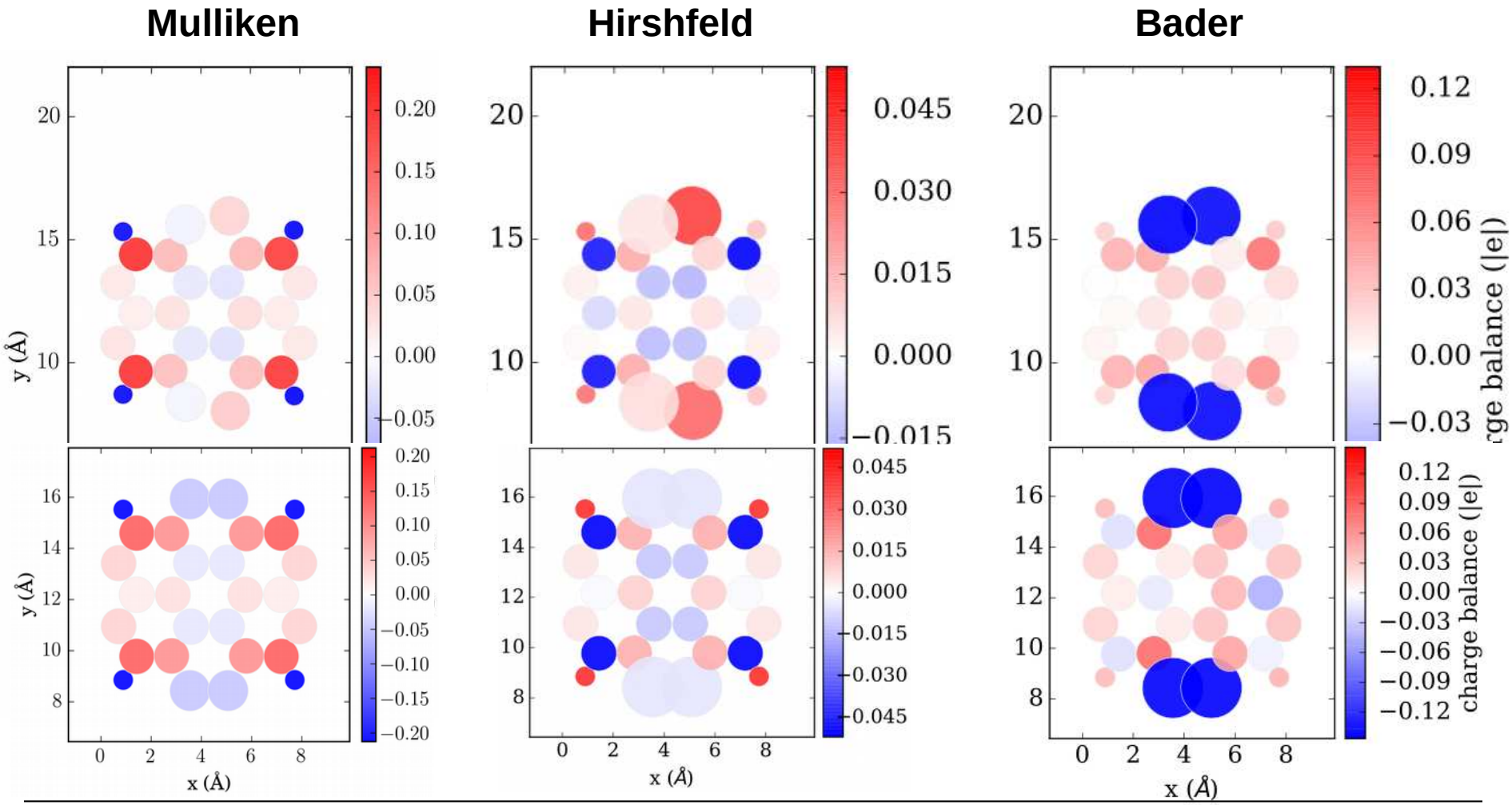
Hirshfeld



Bader

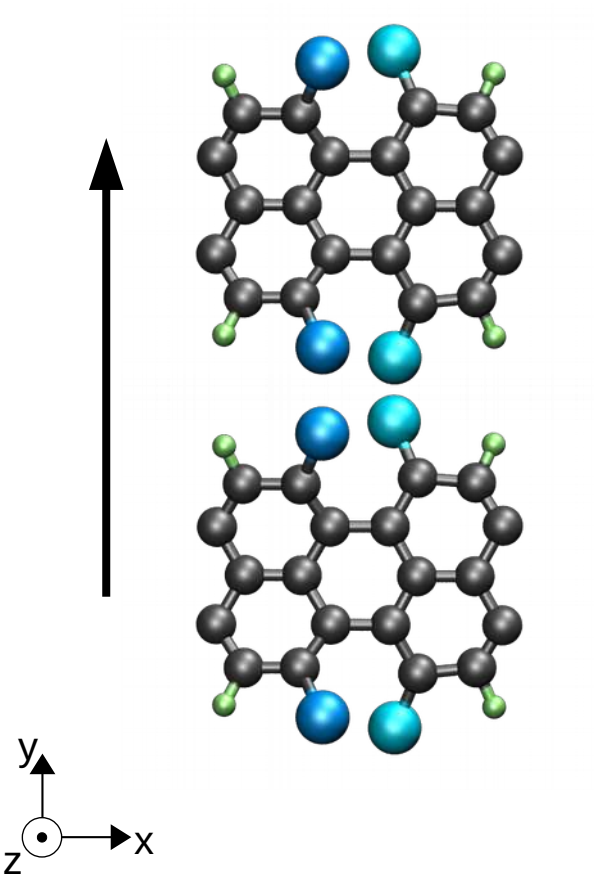


Population analysis: symmetric Cl-5-AGNR on Au(111)



Interaction between Cl-5AGNRs

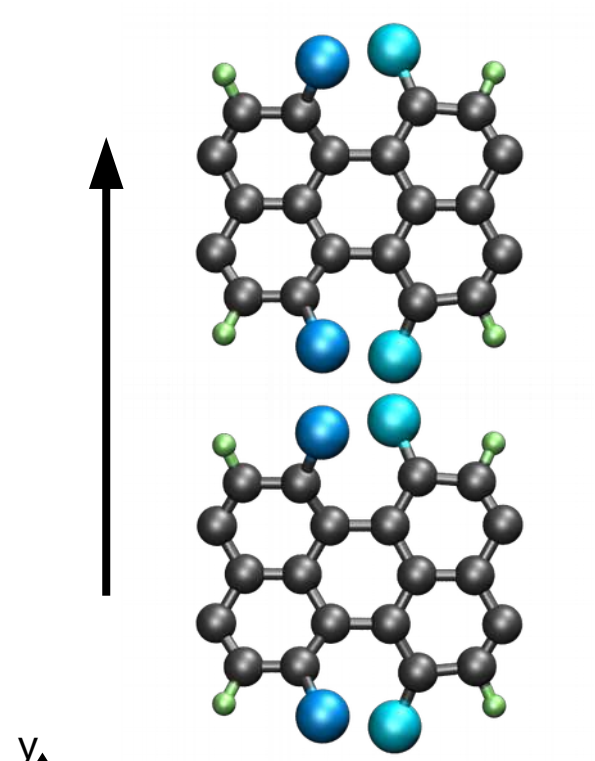
initial

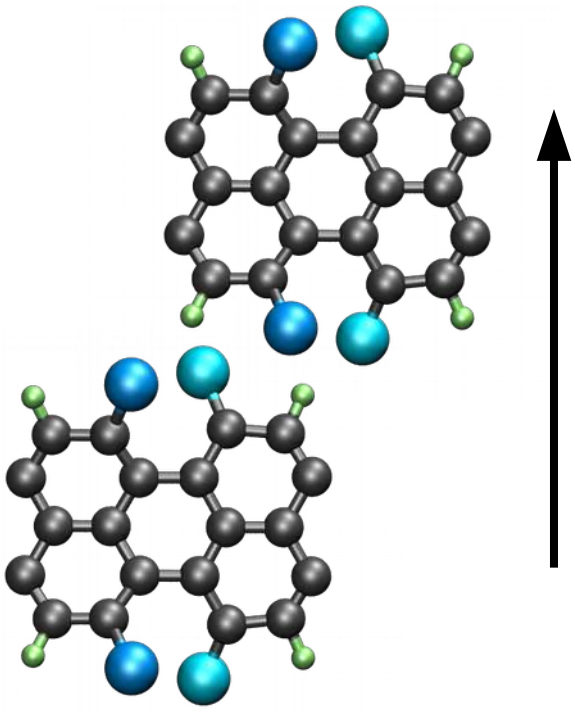


Interaction between Cl-5AGNRs

initial

final

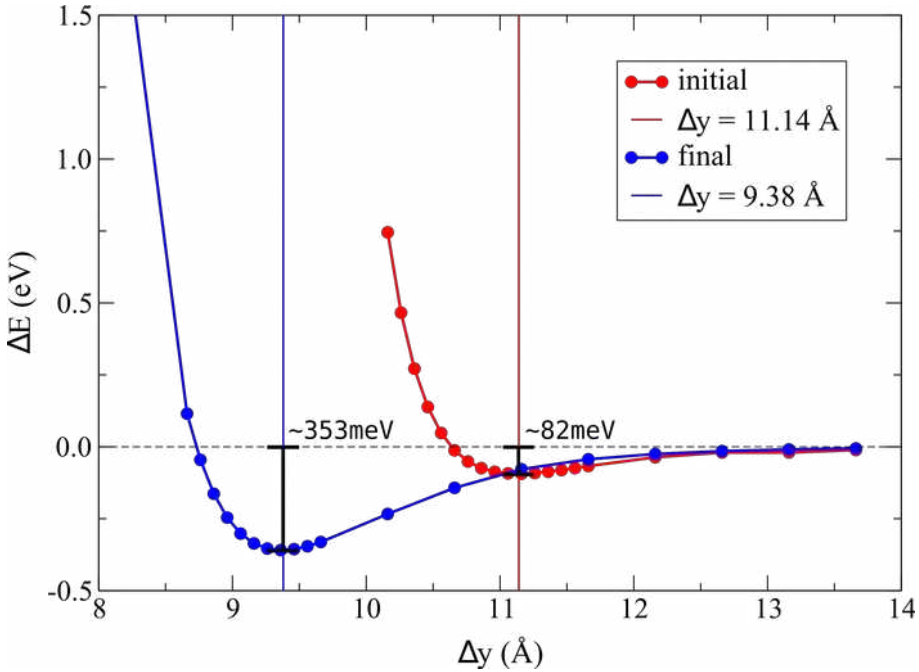




Interaction between Cl-5AGNRs

Interaction energy: $\Delta E = E_{tot} - E_{GNR1} - E_{GNR2}$

gas phase geometry



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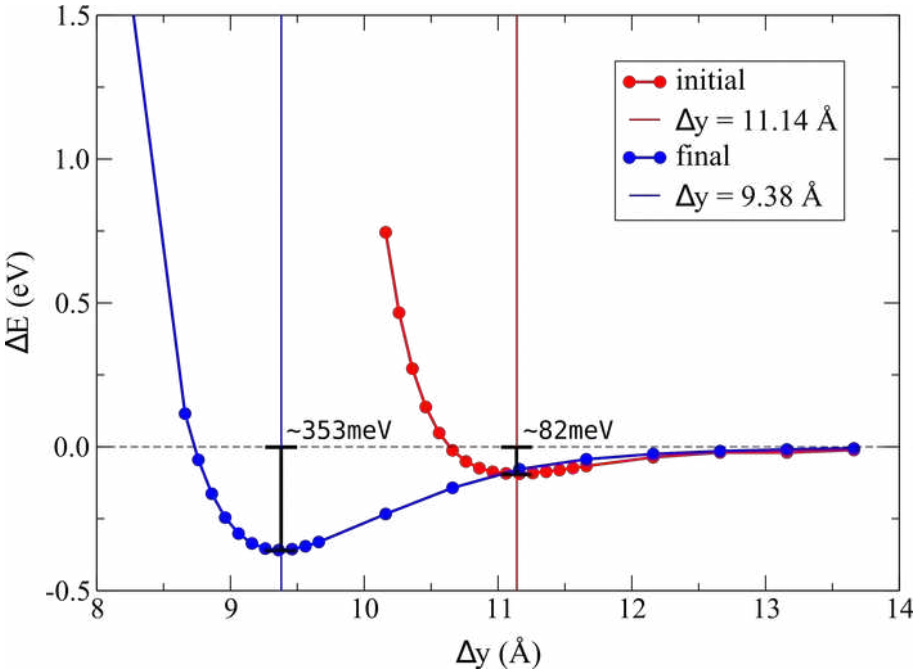
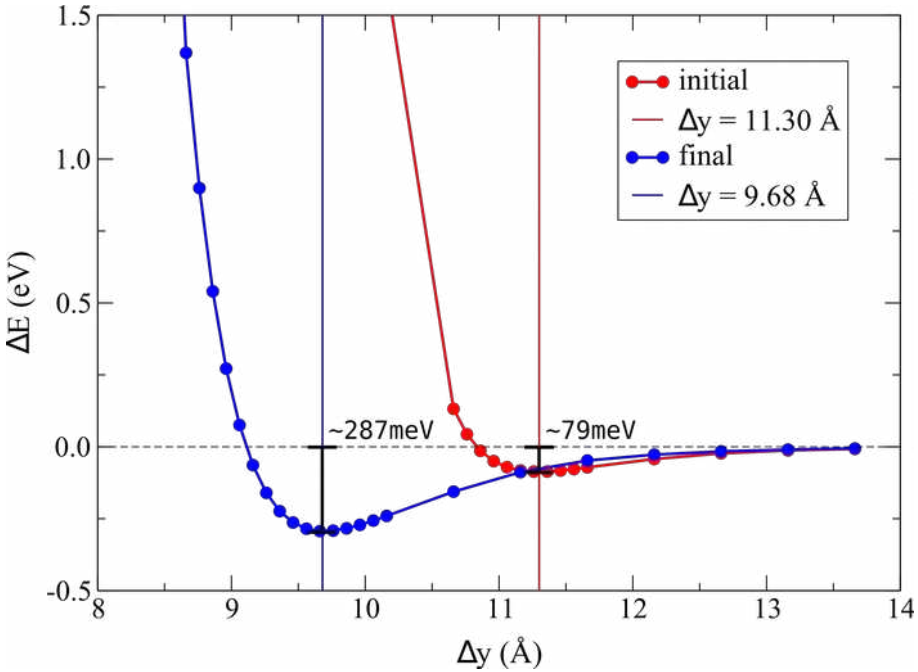
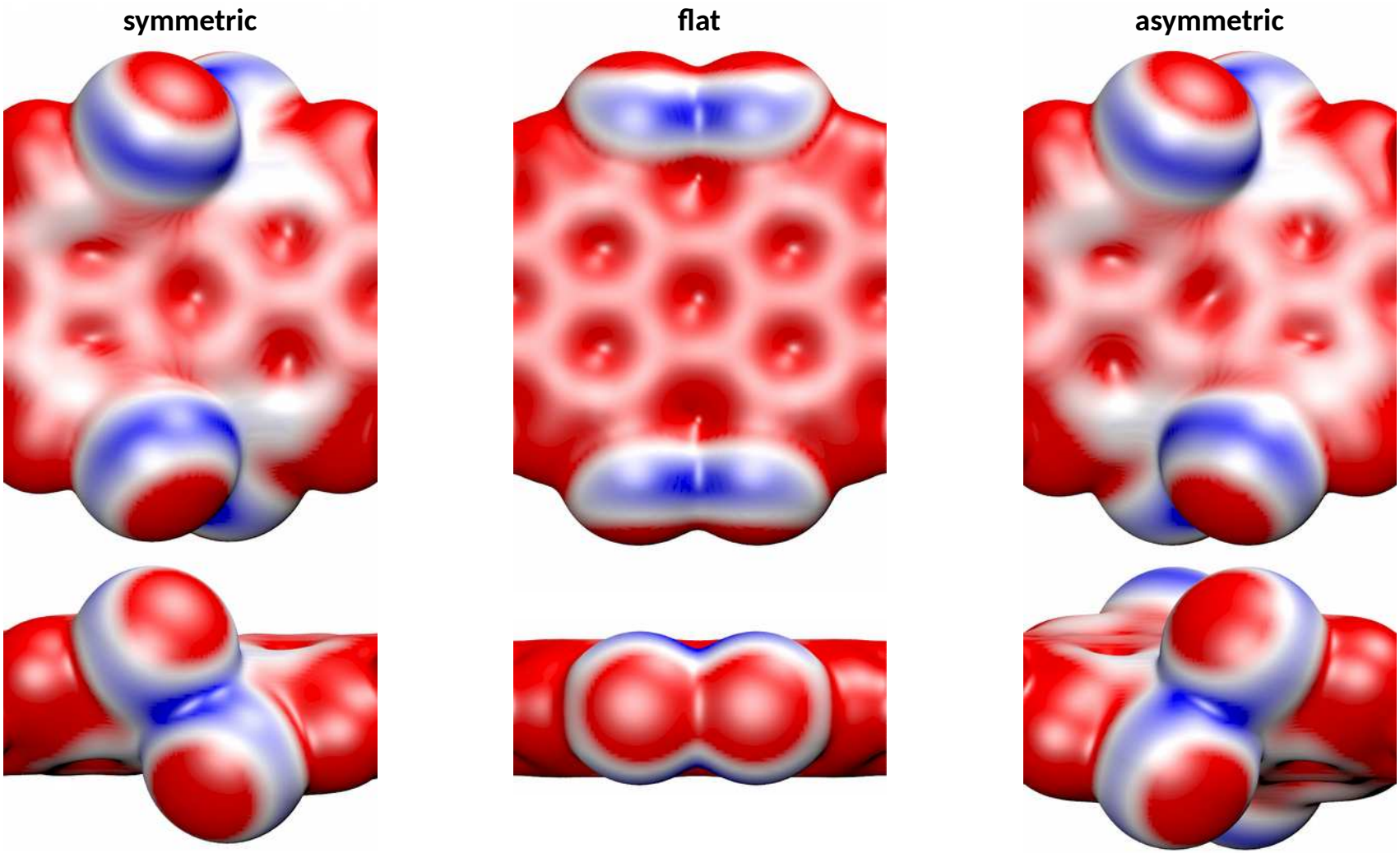


geometry relaxed on Au surface



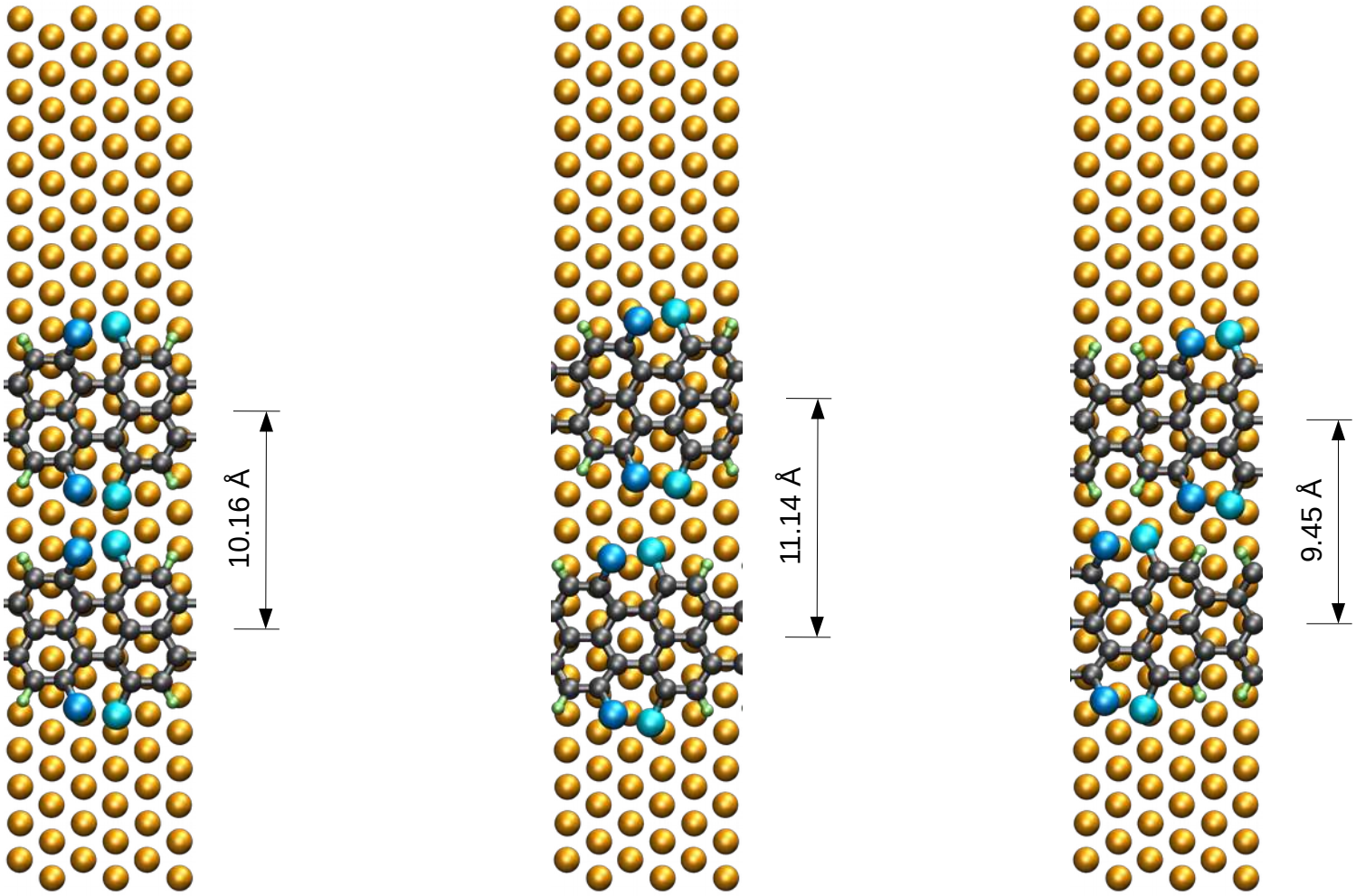
Electrostatic potential (mapped on charge density surface)



Interaction between Cl-5AGNRs on Au(111) surface

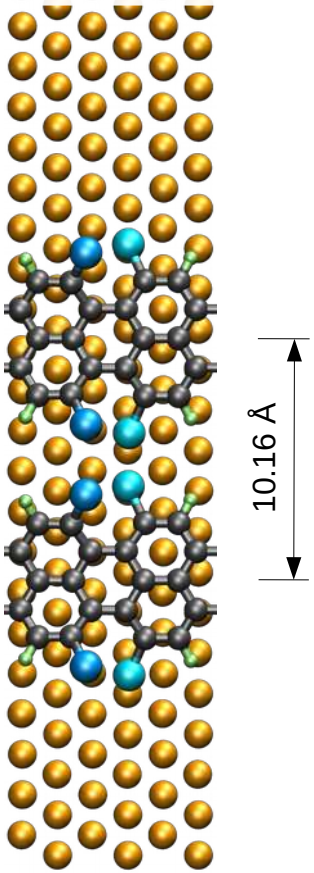
optimization

Interaction between Cl-5AGNRs on Au(111) surface

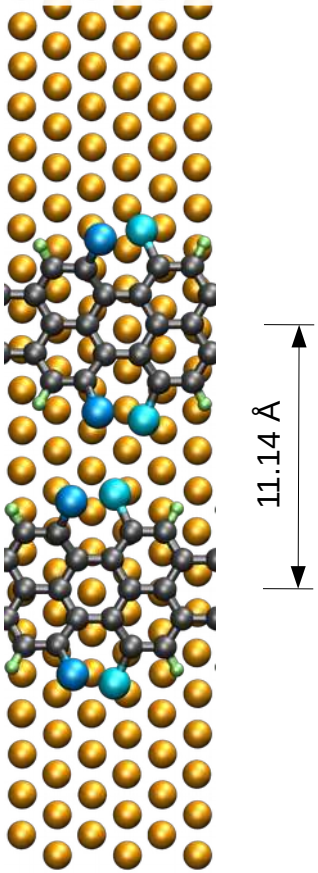


Interaction between Cl-5AGNRs on Au(111) surface

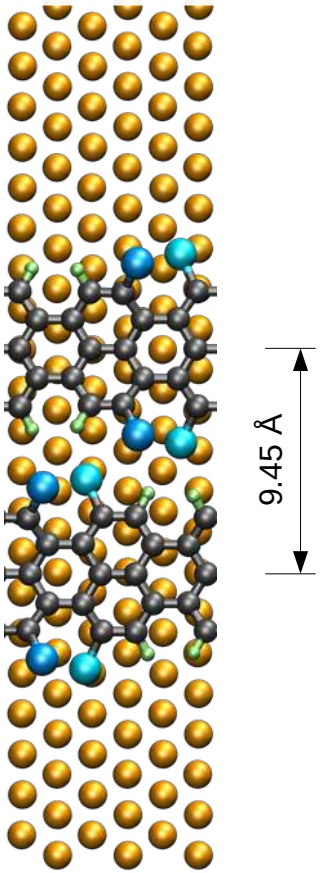
Initial
E_{tot} = -157929.59 eV
ΔE_I = -1.088 eV



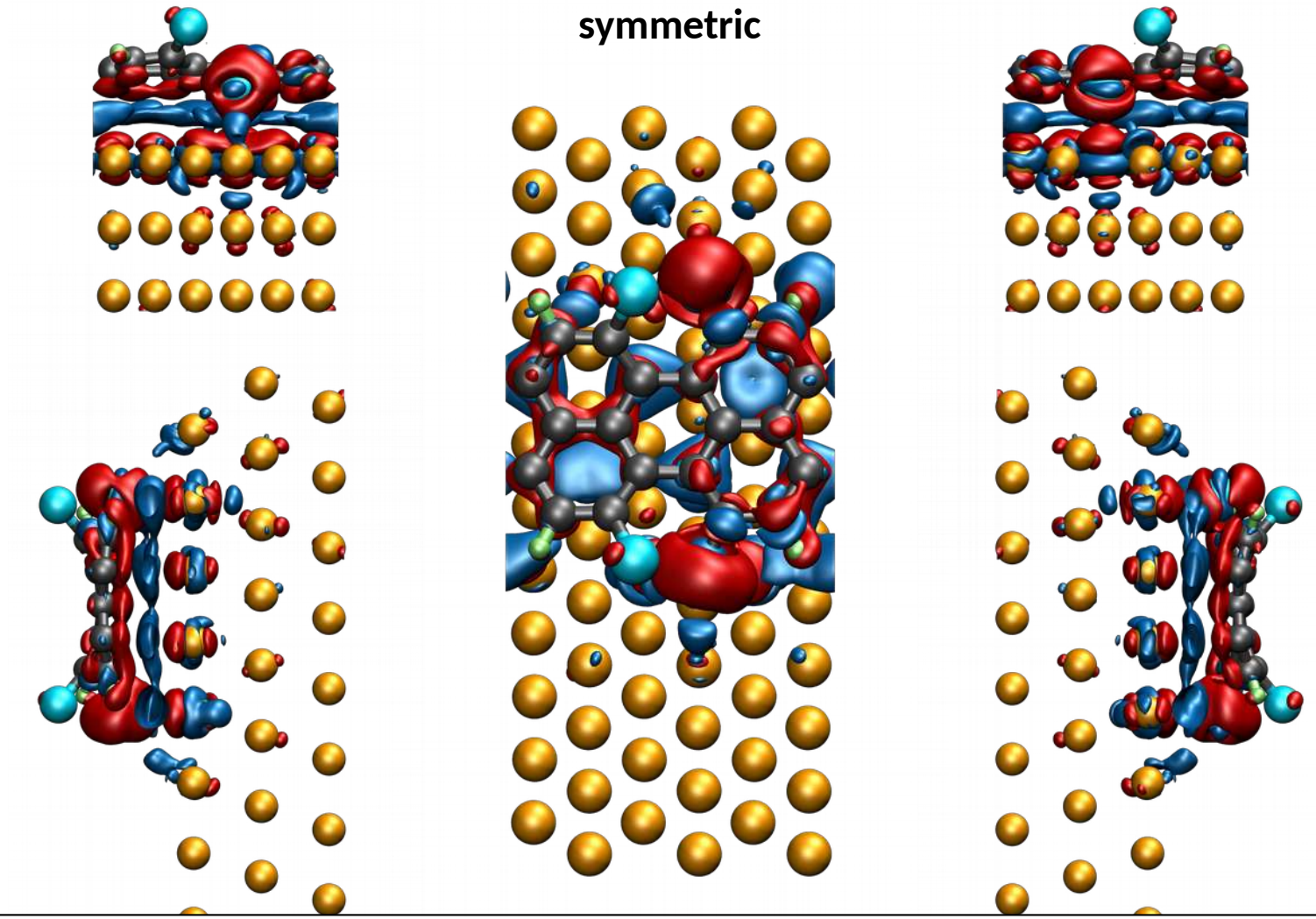
Intermediary
E_{tot} = -157931.18 eV
ΔE_I = -2.989 eV



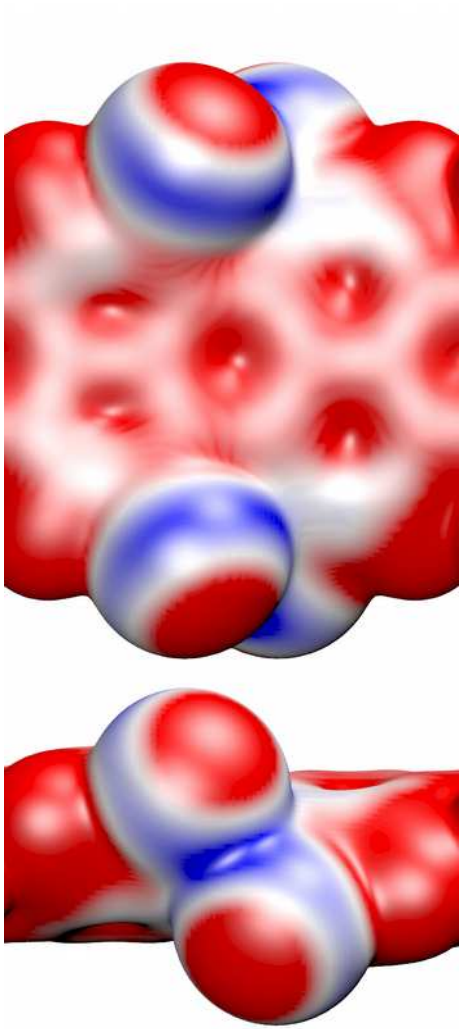
Final
E_{tot} = -157931.53 eV
ΔE_I = -3.104 eV



Induced charge upon adsorption

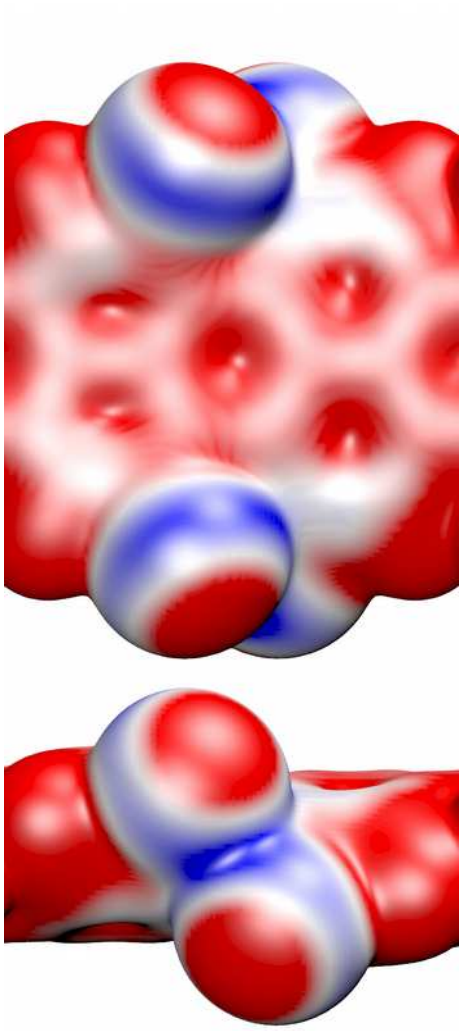


Electrostatic potential (mapped on charge density surface)

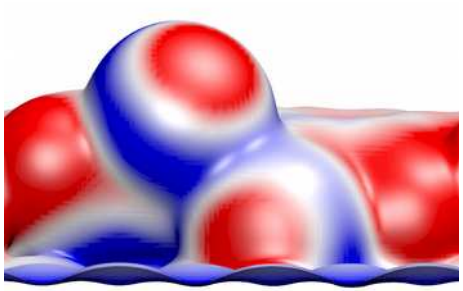


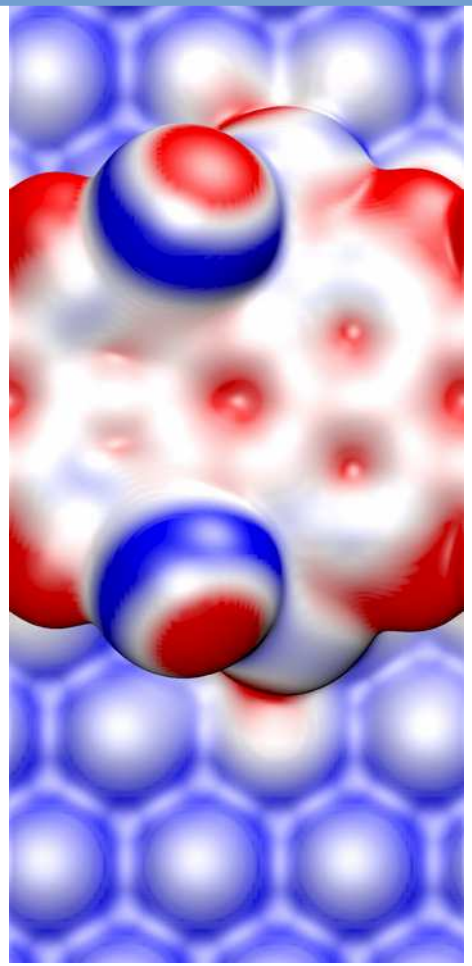
symmetric

Electrostatic potential (mapped on charge density surface)



symmetric





5-AGNR realized with one step reaction

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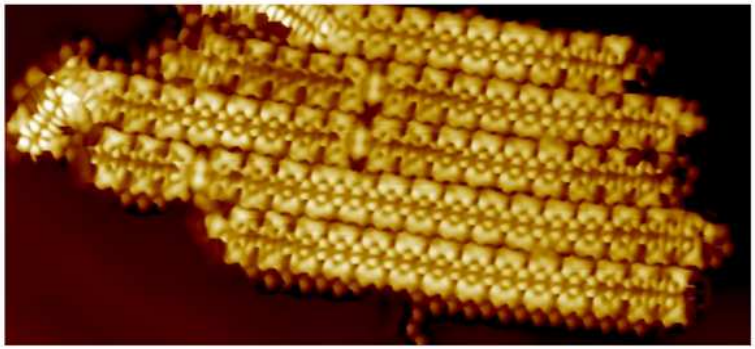
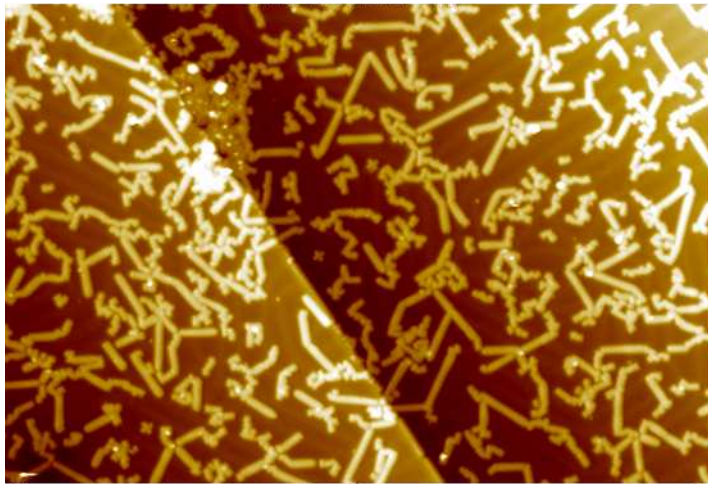
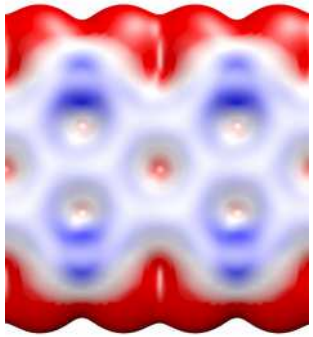
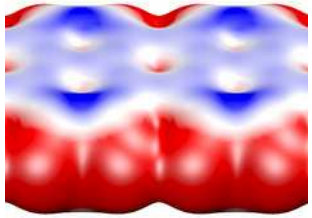




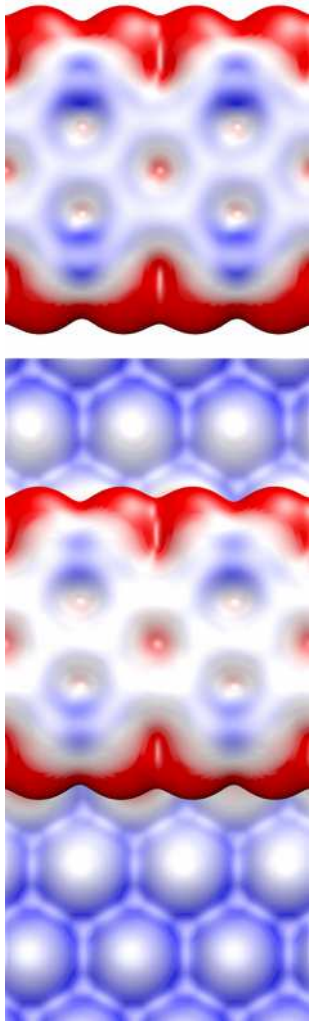
Electrostatic potential (mapped on charge density surface)



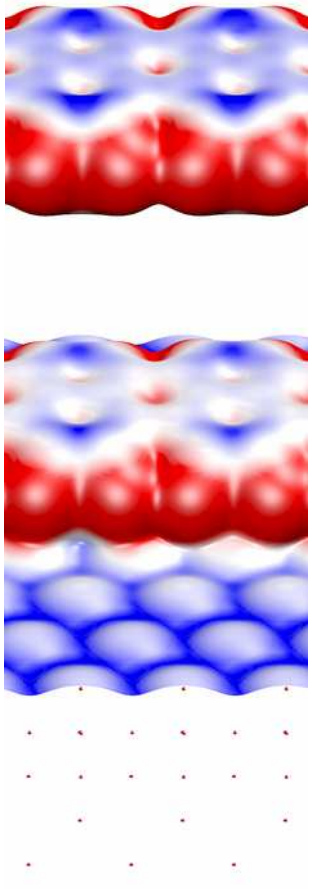
Pristine 5-AGNR

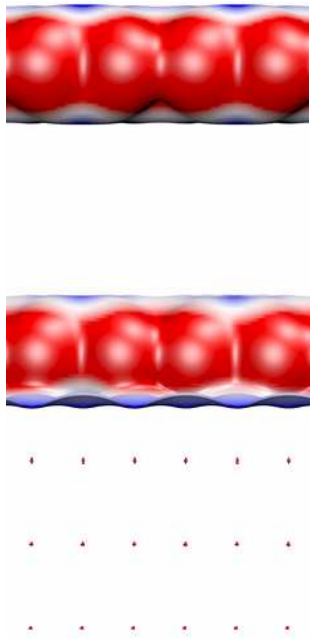


Electrostatic potential (mapped on charge density surface)



Pristine 5-AGNR





Thank you for your attention!