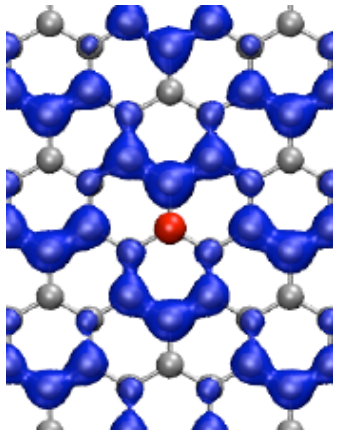
Site-selective chemical control of nanotube's conductivity



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Outline

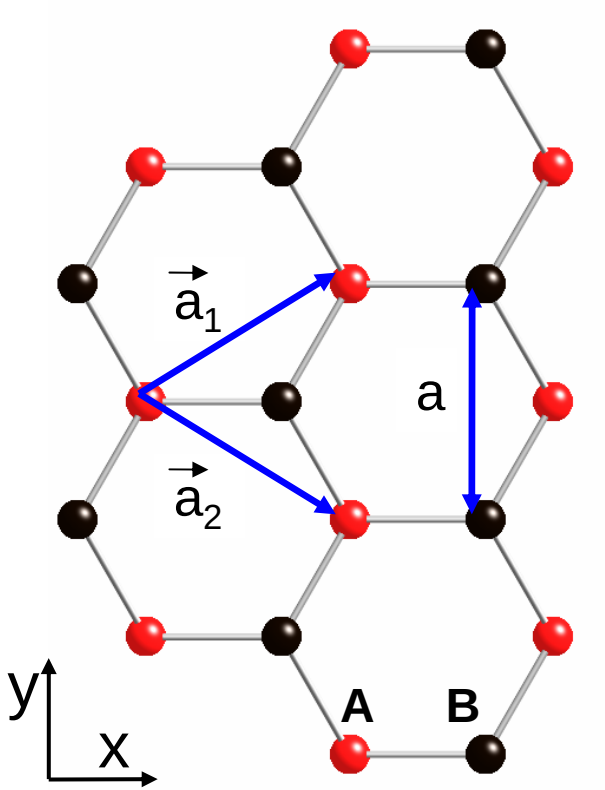
1. Motivation
2. Introduction
3. Calculation Results
4. A simple model to explain the results
5. Outlook

SANES

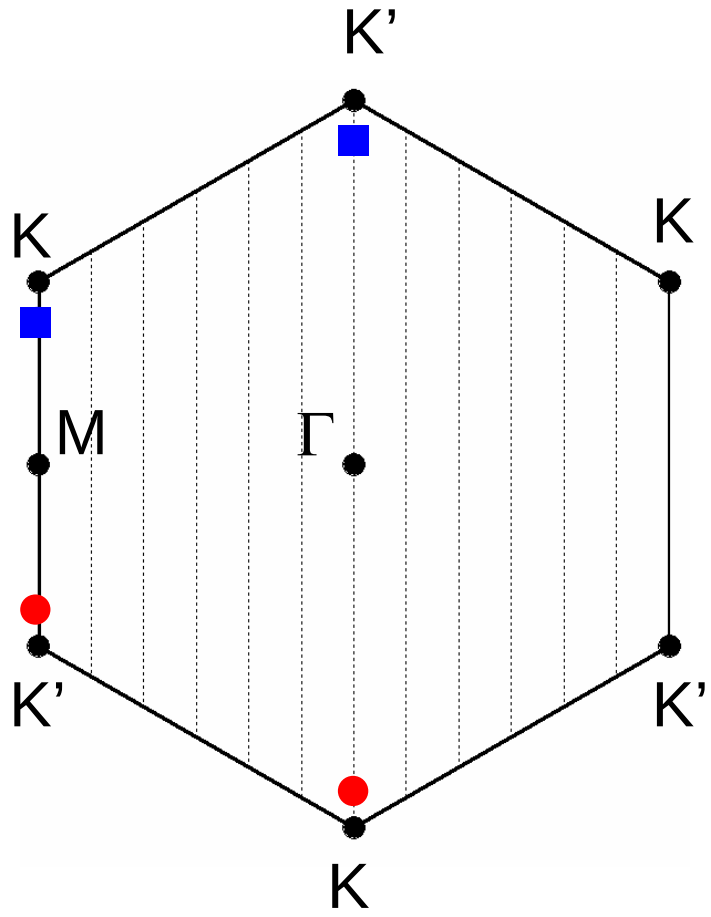
Integrated Self-Adjusting NanoElectronic Sensors

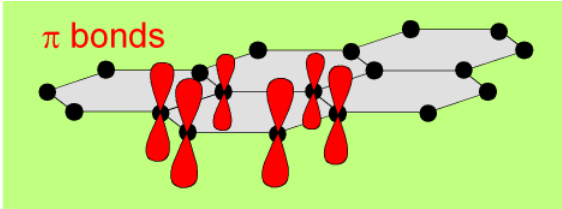
- Main goal: Develop a new integrated self-adjusting nanoelectronic gas sensor based on functionalized carbon nanotubes as active elements.
- Change in conductivity of nanotubes in presence of different gases.
- Sensitivity and selectivity.
- Members: University of Szeged, Rensselaer Polytechnic Institute, University of Oulu, Max-Planck Institute, Laserprobe LP Oy and University of Pais-Vasco.
- Our work: Theoretical models.

Graphene lattice

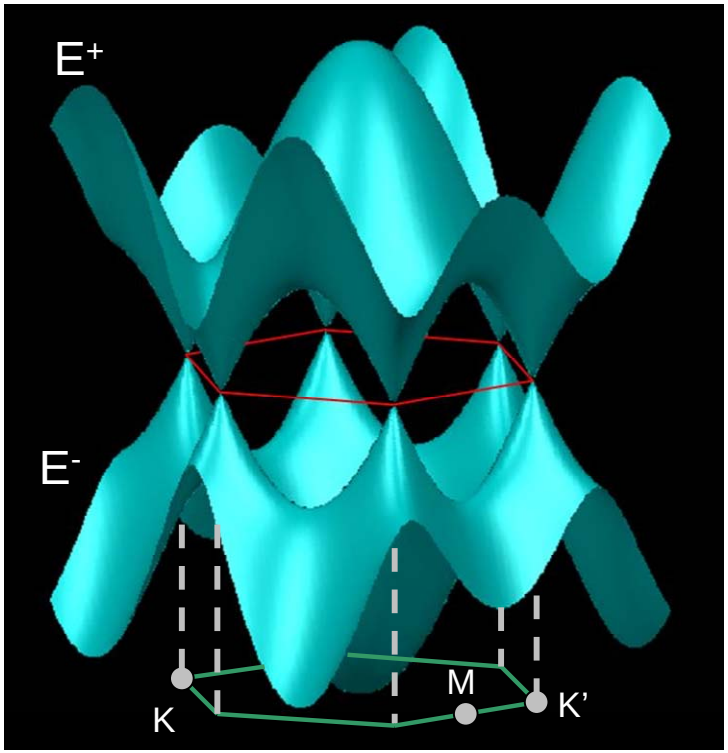


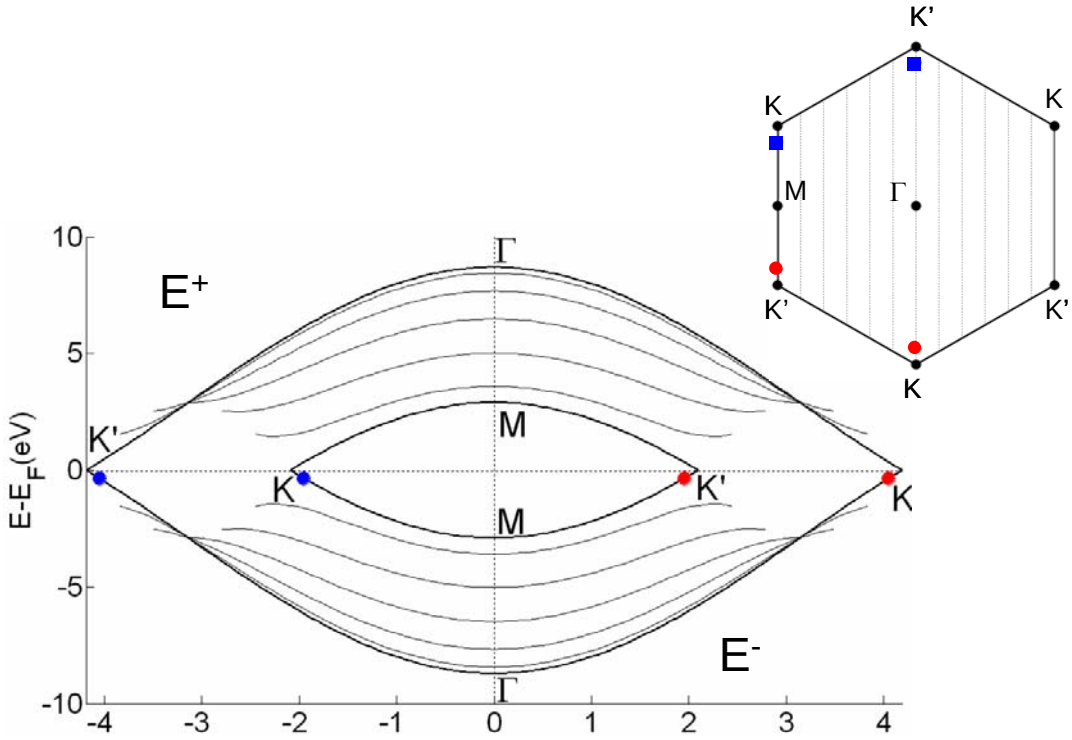
Brillouin Zone





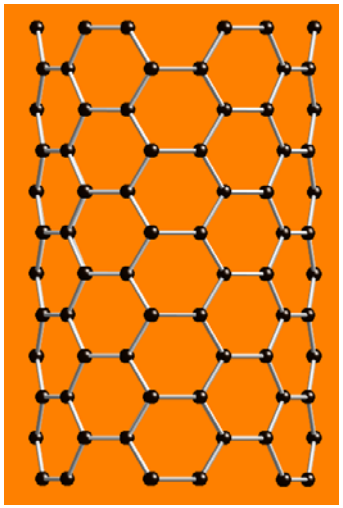
$$E^{\pm}\left(\vec{k}\right) = \pm\gamma_0\sqrt{1+4\cos\frac{\sqrt{3}k_x a}{2}\cos\frac{k_y a}{2}+4\cos^2\frac{k_y a}{2}}$$





There are two available channels to transport electrons

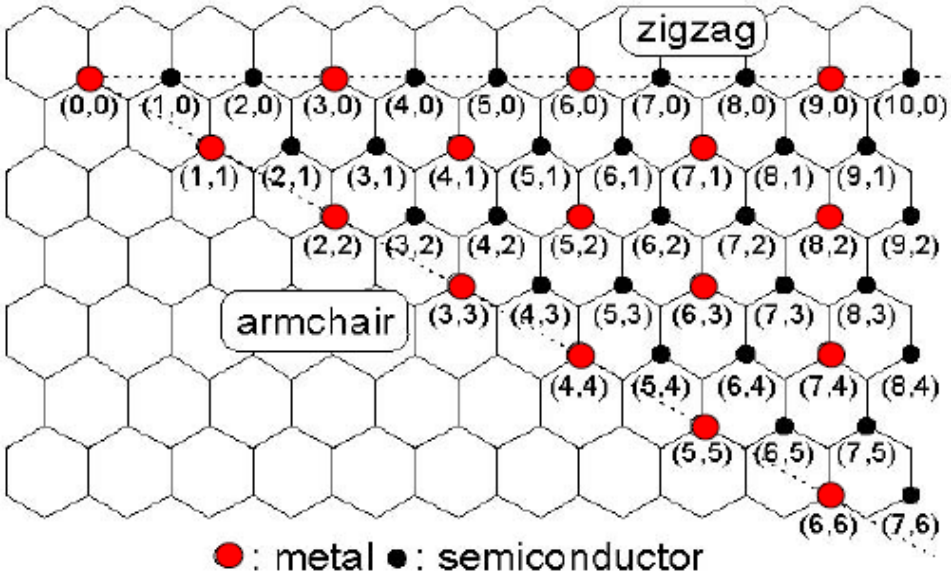
Armchair

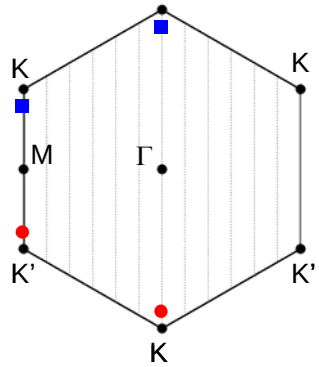


(n,n)

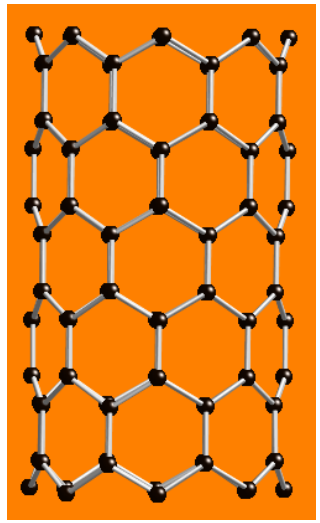
Always metallic

Metallic only if n-m=3p



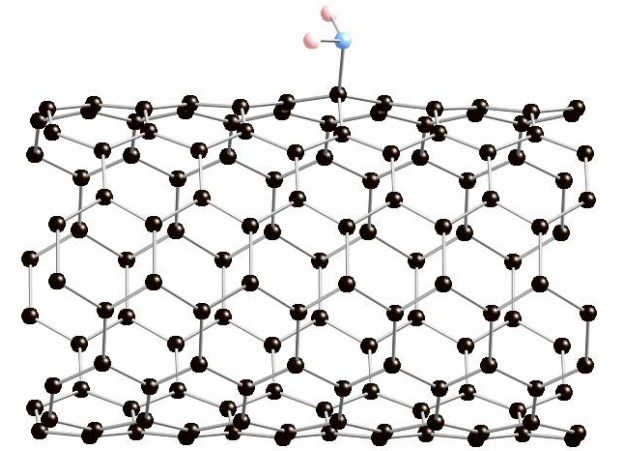


Zigzag



(n,0)

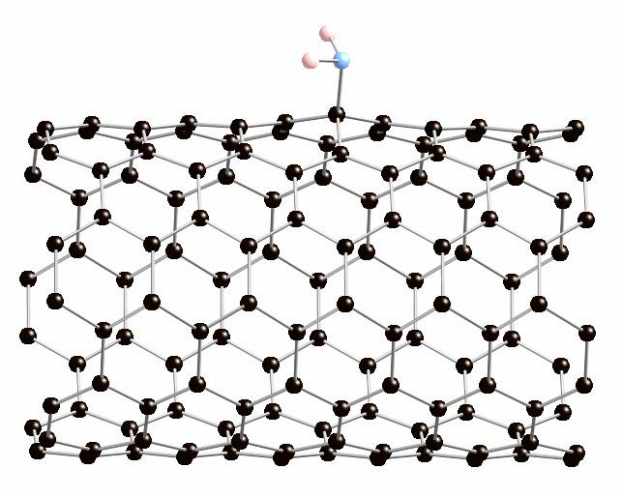
Metallic only if n=3p

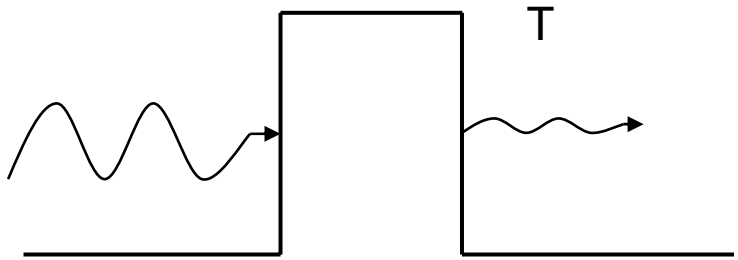


How does the absorption of a molecule affect to the transport properties of a CNT?

1. Geometry optimization (DFT calculations) → Expensive part

2. Transport calculations: Non-equilibrium Green's function formalism



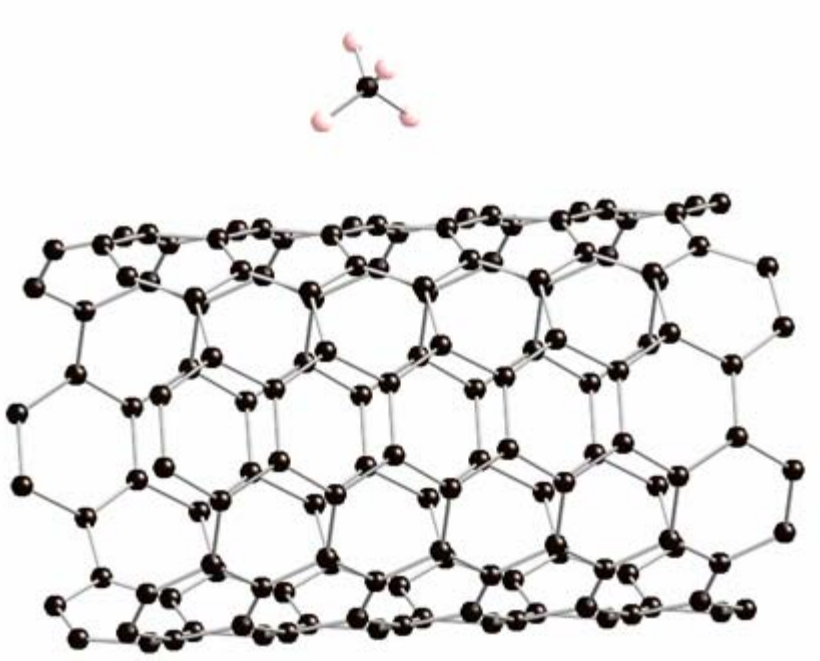


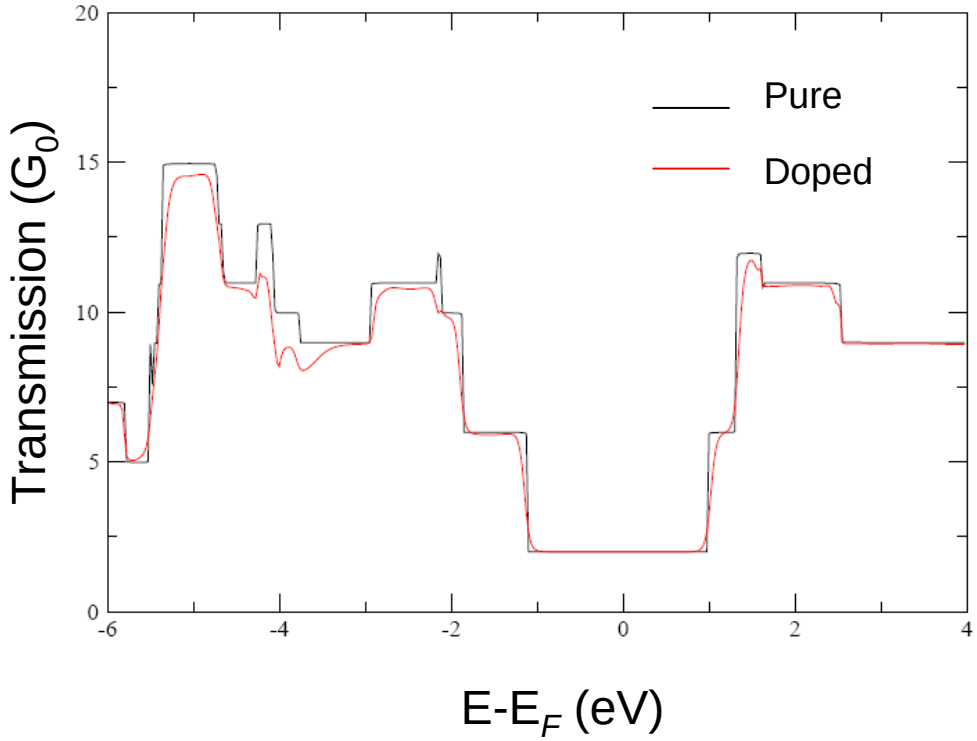
Non-equilibrium Green's function formalism

Pure systems $$G(E) = G_0 N_\perp(E) \qquad G_0 = \frac{2e^2}{h}$$

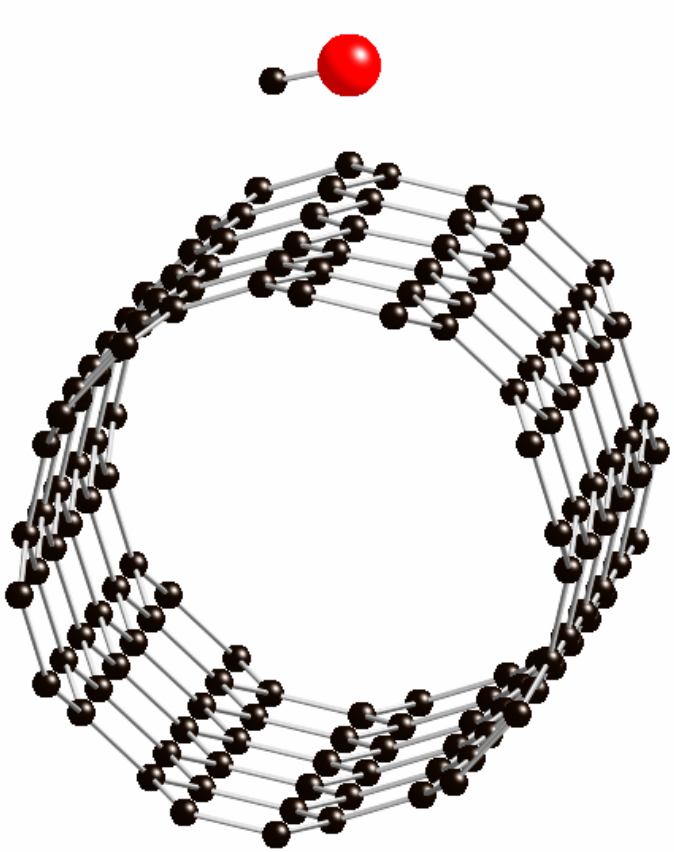
Doped systems $$G(E) = G_0 \sum_{n=1}^{N_\perp} T(E)$$

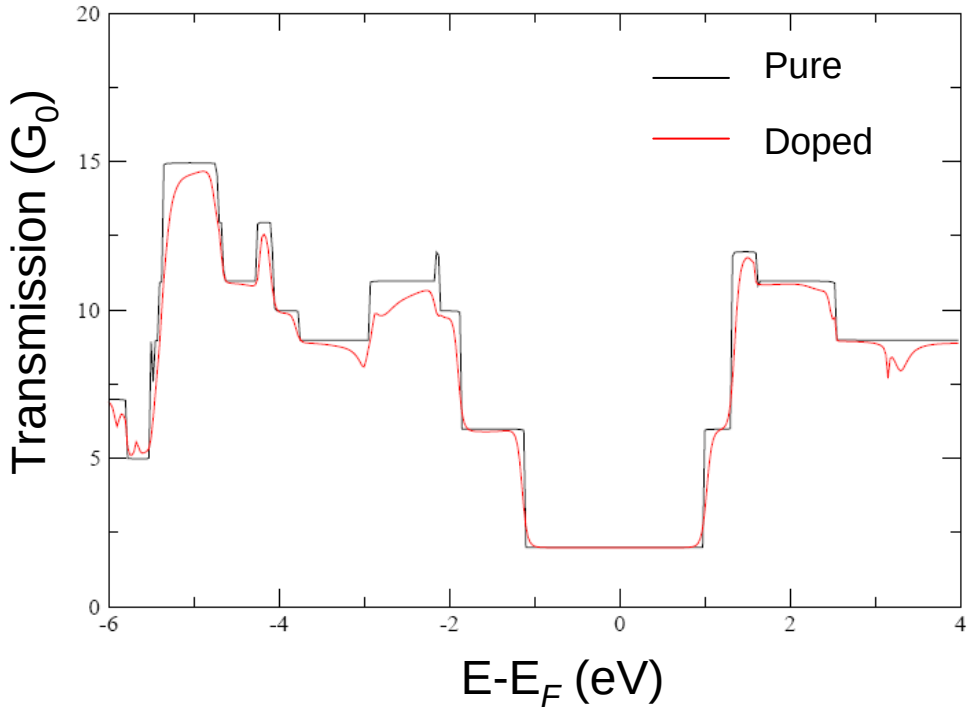
CH_4



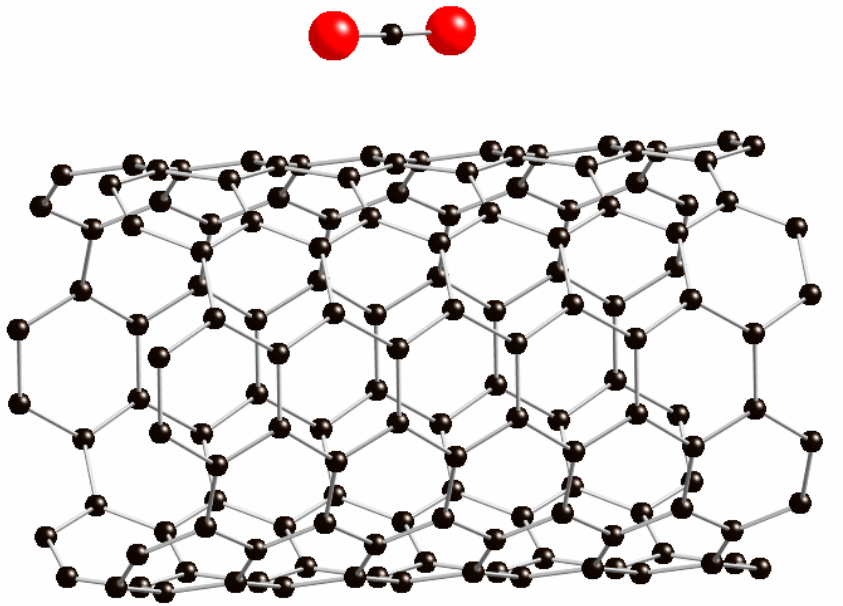


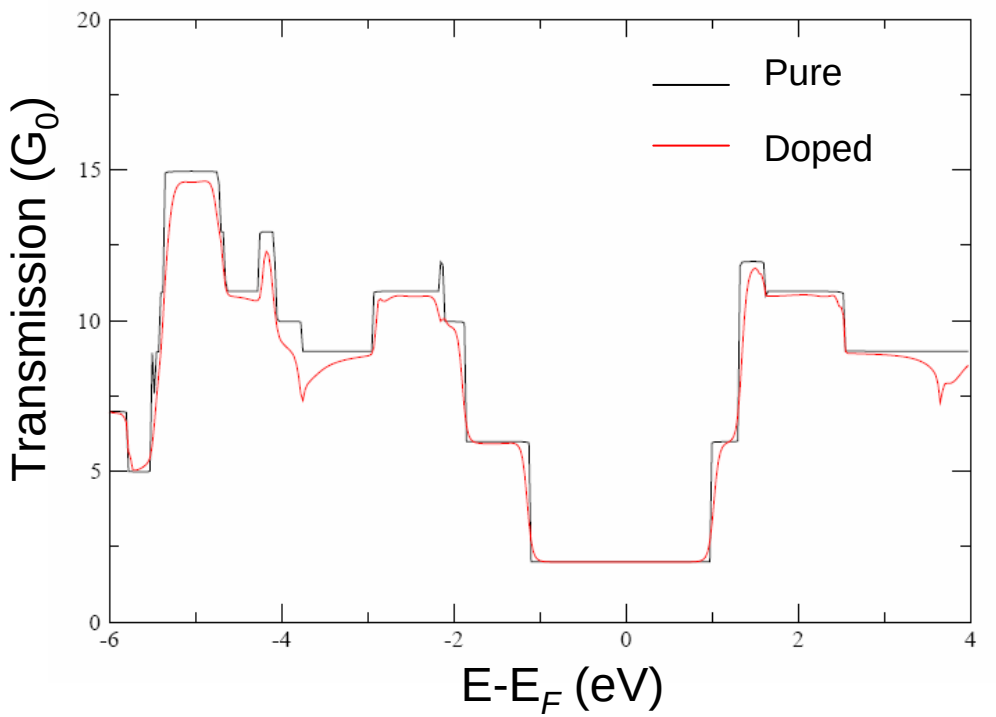
CO



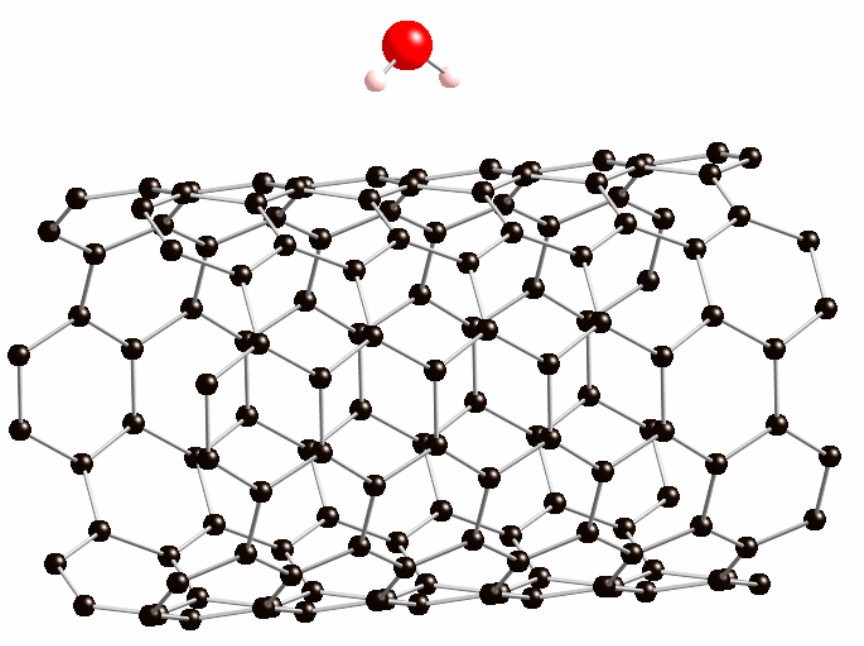


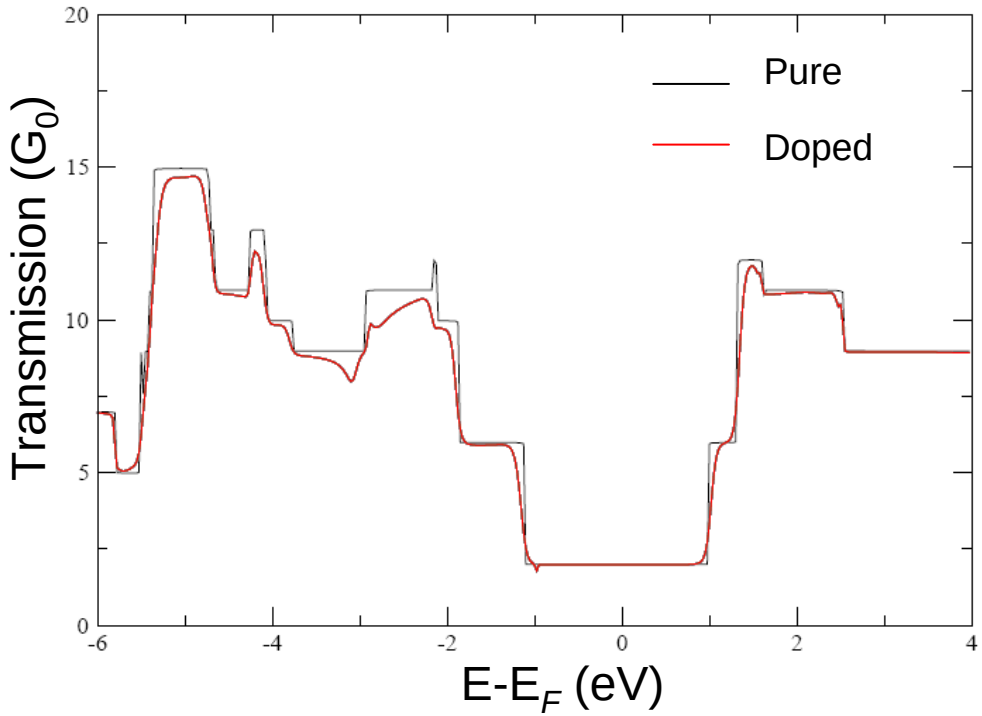
CO_2





H_2O

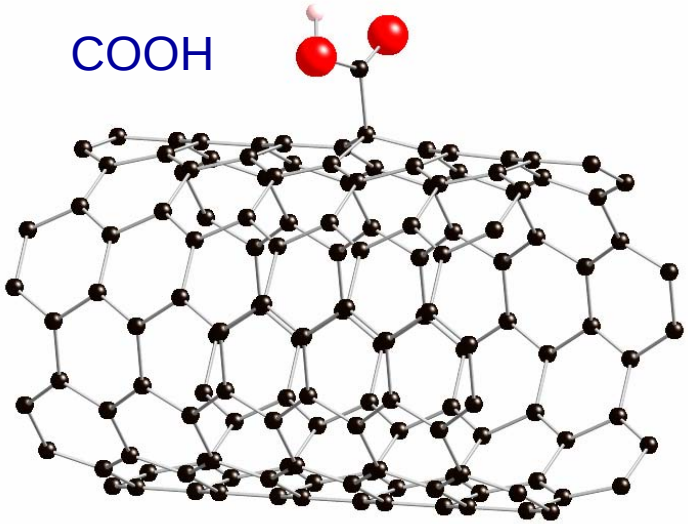




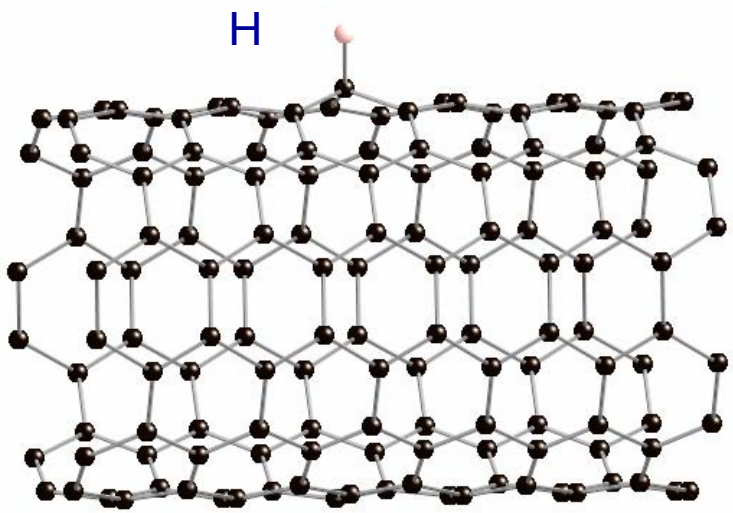
Calculation results

Chemisorbed molecules

COOH

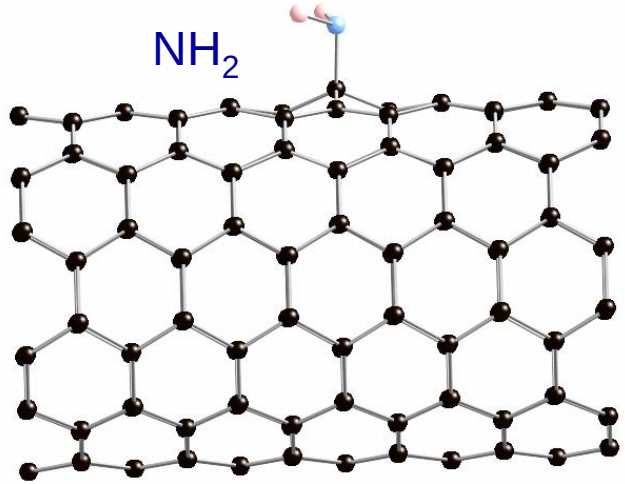


H



OH

NH_2



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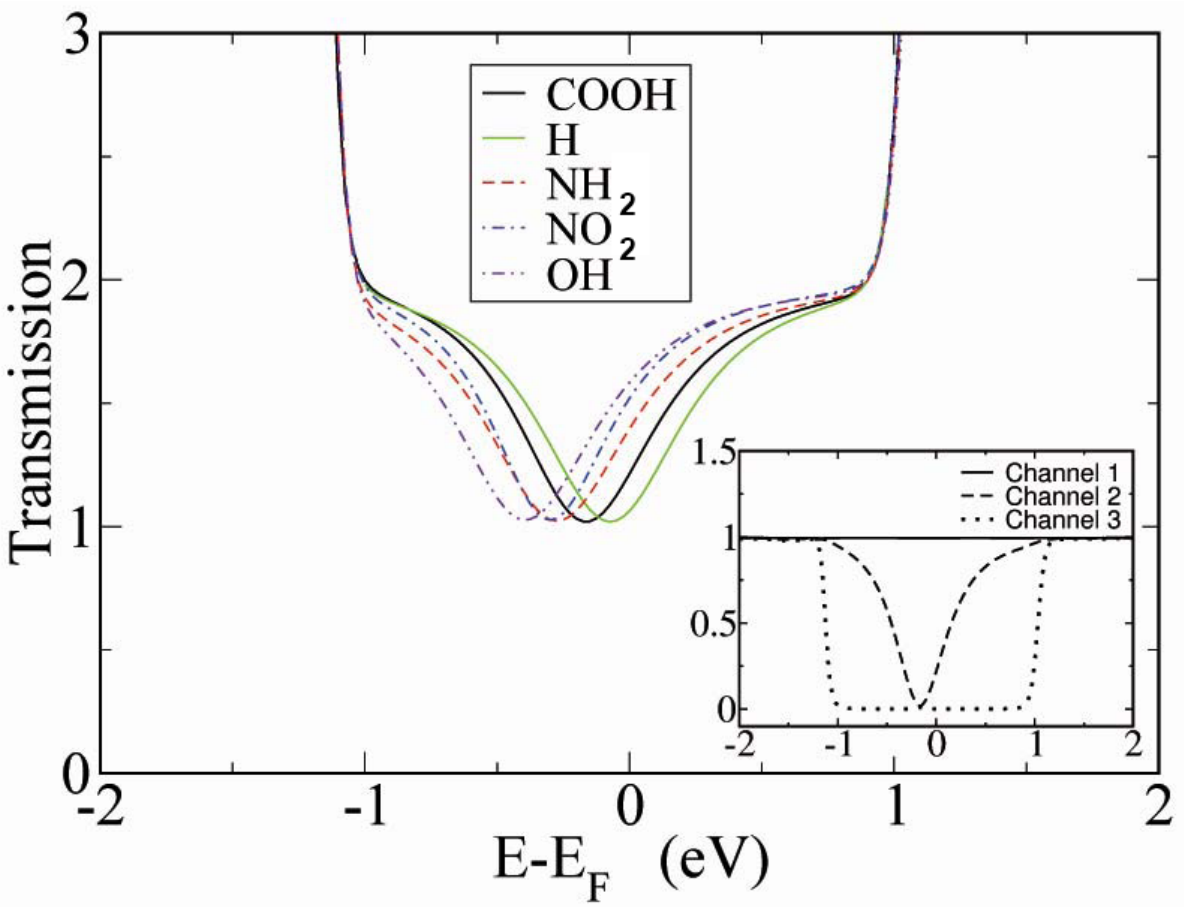
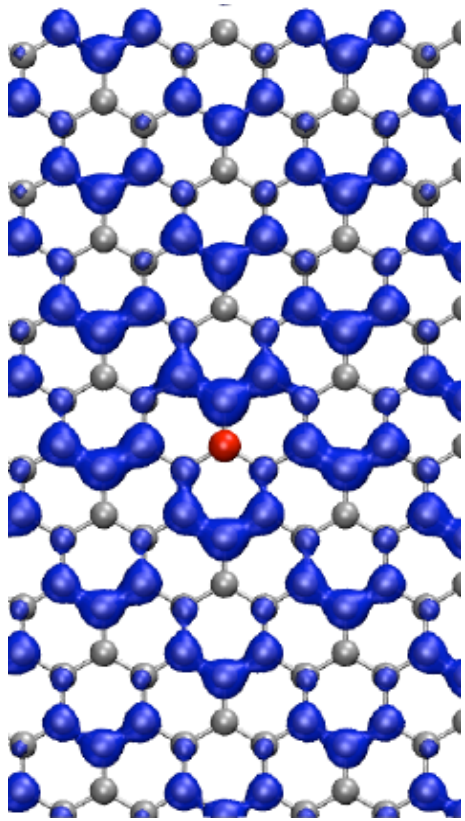
Calculation results

Chemisorbed molecules



Channel 1



Transmission direction

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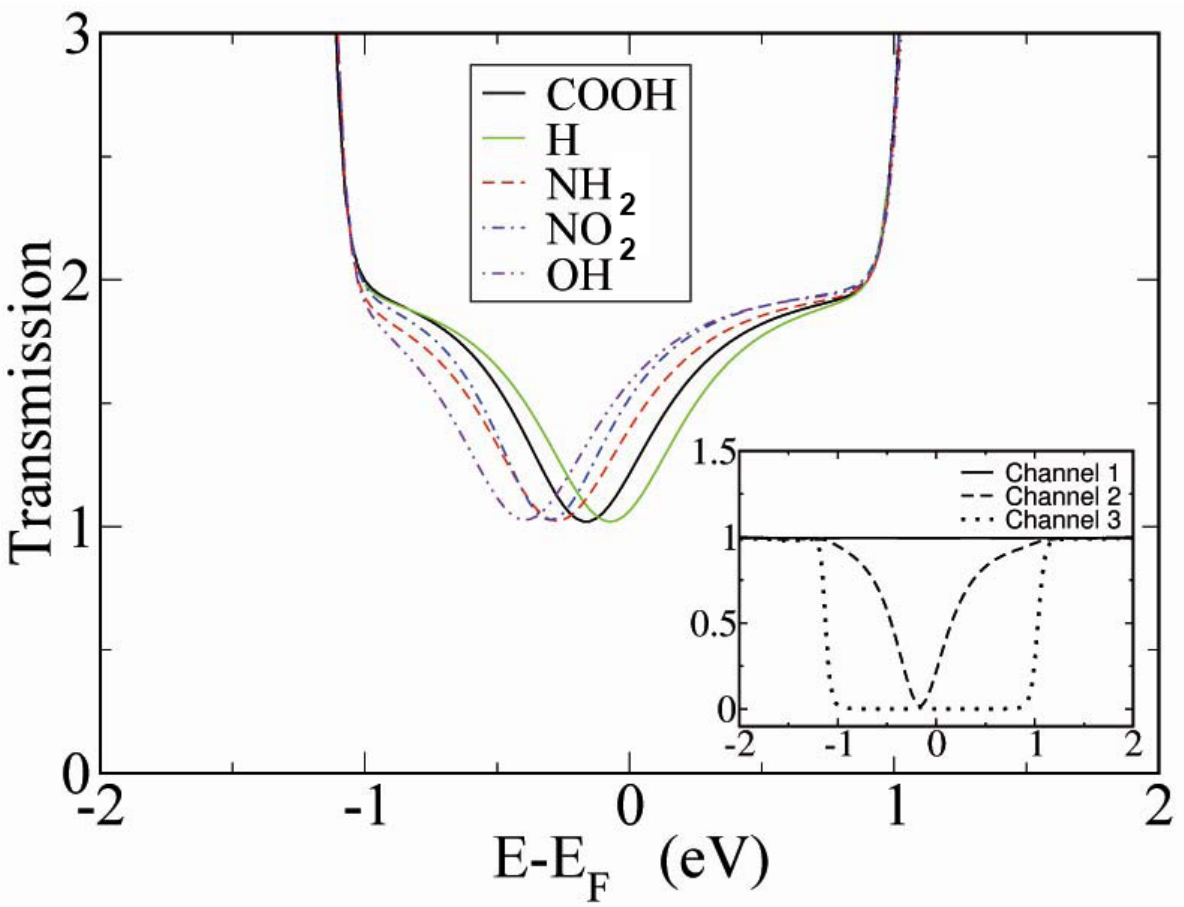
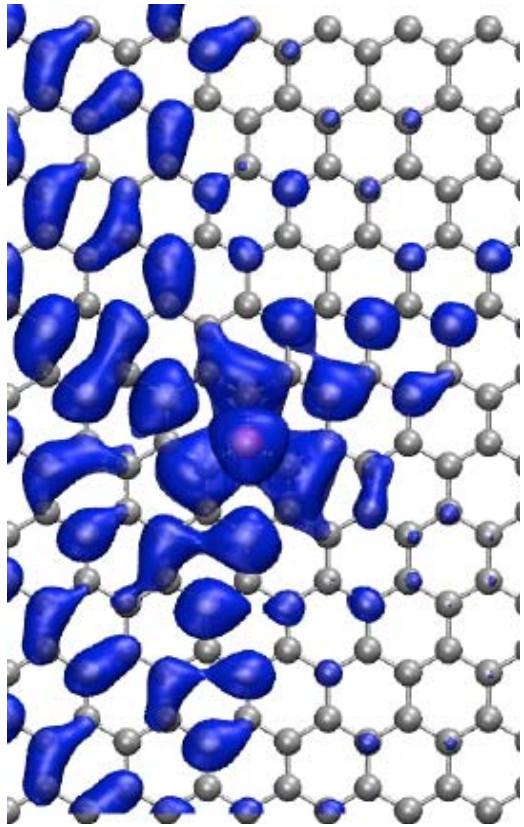
Calculation results

Chemisorbed molecules



Channel 2



Transmission direction

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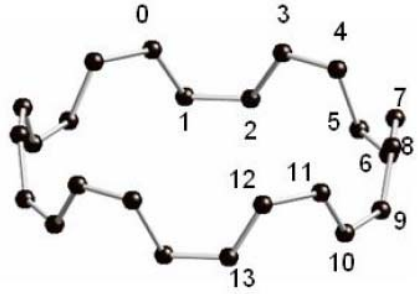
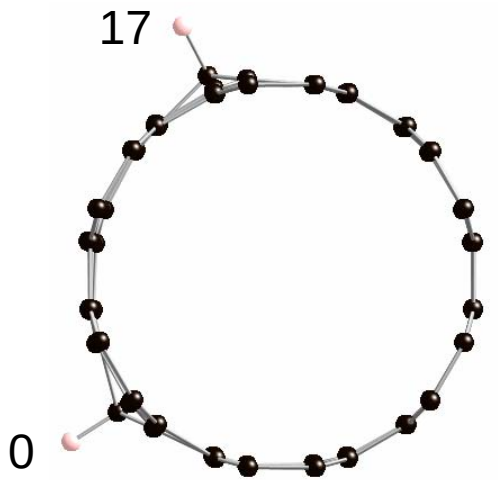
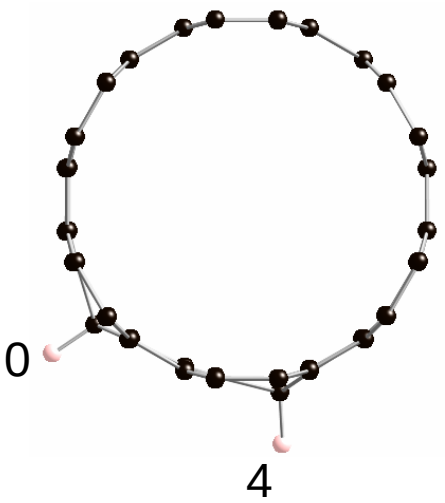
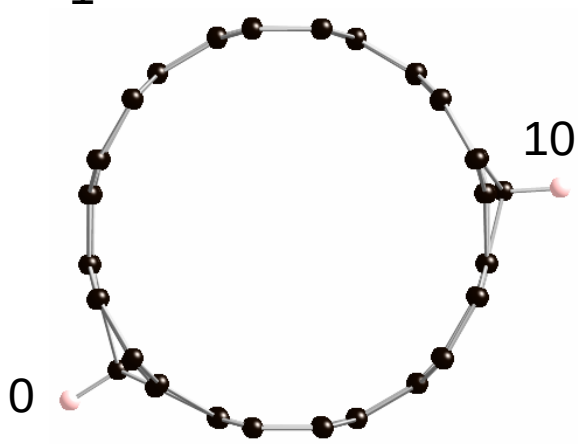
Calculation results

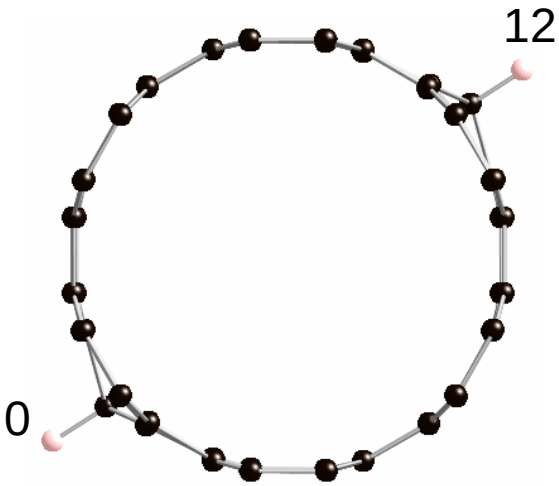
Chemisorbing two molecules











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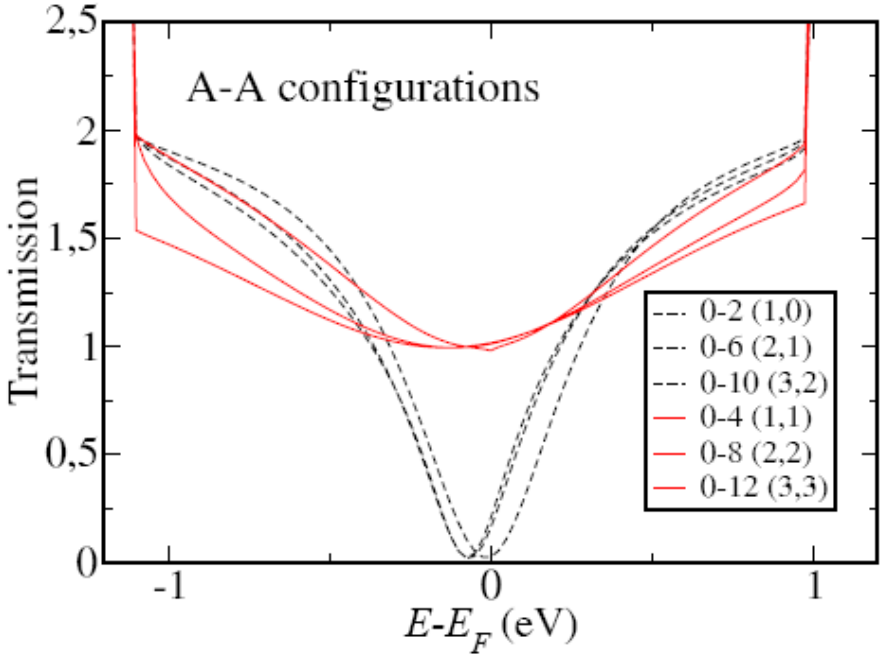
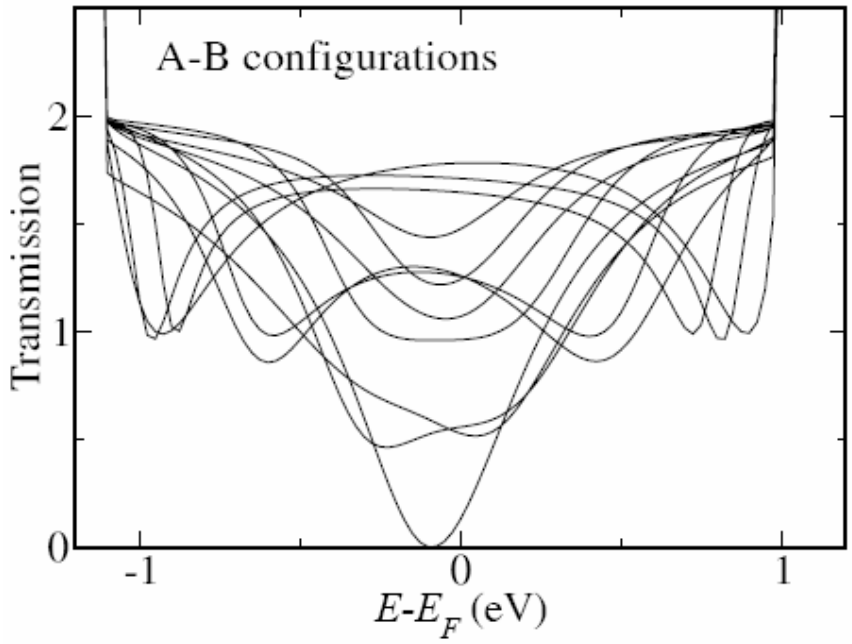
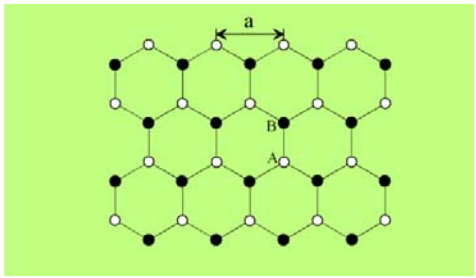
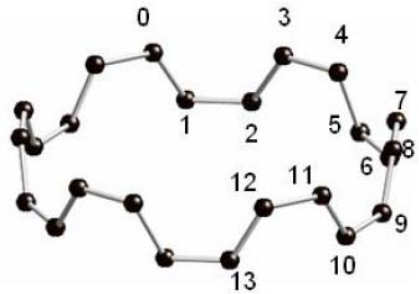
Calculation results

Chemisorbing two molecules









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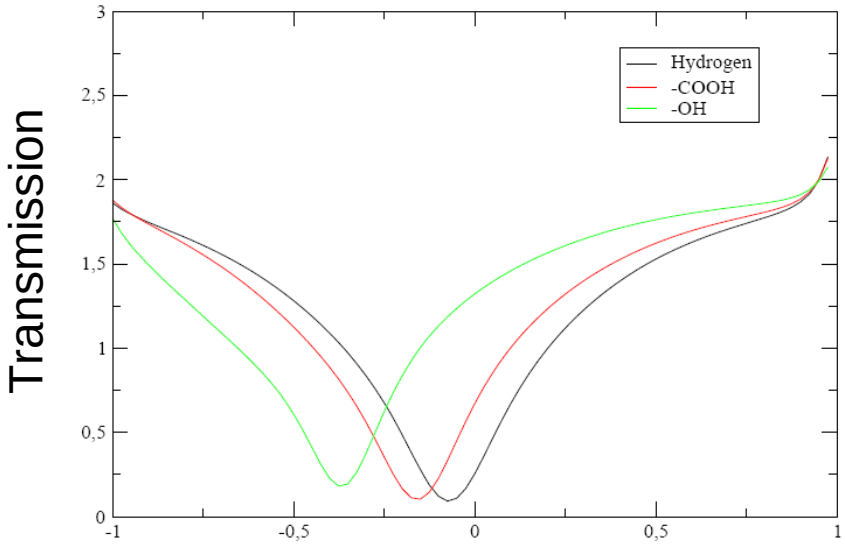
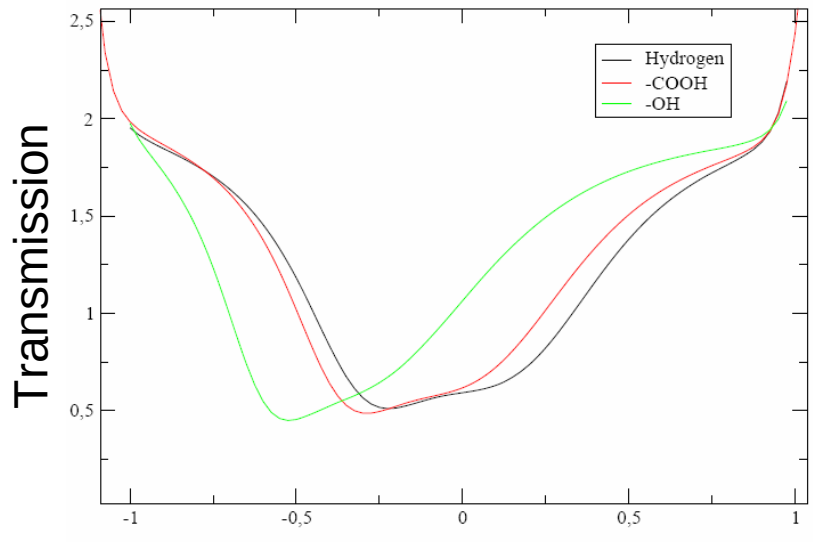
A-A (0-10) pairs



A-B (0-11) pairs

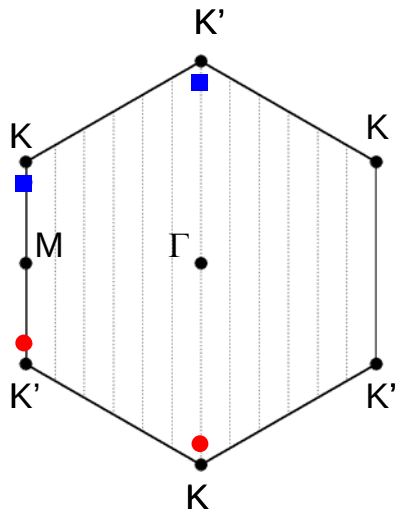


1) Physisorbed molecules do not affect the conductivity close to Fermi level
2) Chemisorbed molecules: One channel is cancelled
3) Universal behaviour for chemisorbed molecules
4) Two molecules: Transmission depends strongly on the relative position of the molecules

Tight-Binding Model

$|K_+\rangle \quad |K'_-\rangle \quad |K'_+\rangle \quad |K_-\rangle$

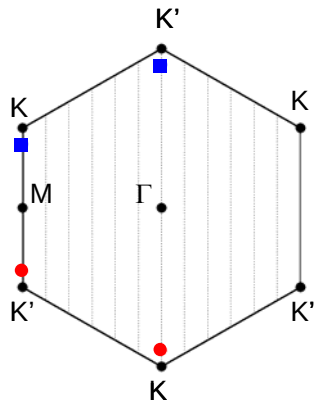
$$H = \begin{pmatrix} 0 & 0 & 0 & 0 & t \\ 0 & 0 & 0 & 0 & t \\ 0 & 0 & 0 & 0 & t \\ 0 & 0 & 0 & 0 & t \\ t & t & t & t & \varepsilon_0 \end{pmatrix}$$



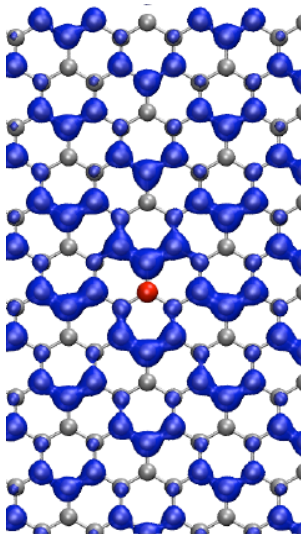
A simple model to explain the results

One molecule

	Eigenvalue	$\|K_+\rangle$	$\|K'_-\rangle$	$\|K'_+\rangle$	$\|K_-\rangle$	$\|\varepsilon_0\rangle$
1)	0	0	1	0	-1	0
2)	0	-1	0	1	0	0
3)	0	-2	1	0	1	0
4)	E^+	t/E^+	t/E^+	t/E^+	t/E^+	1
5)	E^-	t/E^-	t/E^-	t/E^-	t/E^-	1



$$E^{\pm} = \frac{\varepsilon_0 \pm \sqrt{\varepsilon_0^2 + 16t^2}}{2}$$



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A simple model to explain the results

Two molecules

$$H_1 = \begin{array}{c} \begin{array}{cccccc} |K_+\rangle & |K'_-\rangle & |K'_+\rangle & |K_-\rangle & & \end{array} \\ \begin{pmatrix} 0 & 0 & 0 & 0 & t & t\cdot f_1 \\ 0 & 0 & 0 & 0 & t & t\cdot f_2 \\ 0 & 0 & 0 & 0 & t & t\cdot f_3 \\ 0 & 0 & 0 & 0 & t & t\cdot f_4 \\ t & t & t & t & \varepsilon_0 & 0 \\ t\cdot f_1^* & t\cdot f_2^* & t\cdot f_3^* & t\cdot f_4^* & 0 & \varepsilon_0 \end{pmatrix} \end{array}$$

$$f_1 = e^{-i\frac{2\pi}{3}(n-m)} \qquad f_2 = e^{i\frac{2\pi}{3}(n-m)} \qquad f_3 = s\cdot e^{-i\frac{2\pi}{3}(n-m+3m)} \qquad f_4 = s\cdot e^{i\frac{2\pi}{3}(n-m+3n)}$$

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A simple model to explain the results

Two molecules

$$H_2 = \begin{array}{c} \begin{array}{cccccc} |K_+\rangle & |K'_-\rangle & |K'_+\rangle & |K_-\rangle & & \end{array} \\ \begin{pmatrix} 0 & 0 & 0 & 0 & t & t\cdot f_1 \\ 0 & 0 & 0 & 0 & t & t\cdot f_2 \\ 0 & 0 & 0 & 0 & t & t\cdot f_3 \\ 0 & 0 & 0 & 0 & t & t\cdot f_4 \\ t & t & t & t & \varepsilon_0 & 0 \\ t\cdot f_1^* & t\cdot f_2^* & t\cdot f_3^* & t\cdot f_4^* & 0 & \varepsilon_0 \end{pmatrix} \end{array}$$

$$f_1 = e^{-i\frac{2\pi}{3}(n-m)} \qquad f_2 = e^{i\frac{2\pi}{3}(n-m)} \qquad f_3 = s\cdot e^{-i\frac{2\pi}{3}(n-m+3m)} \qquad f_4 = s\cdot e^{i\frac{2\pi}{3}(n-m+3n)}$$

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1. When the second impurity is at an A site such that the relative distance R fulfils the condition:

$$R = n \cdot \vec{a}_1 + m \cdot \vec{a}_2, n - m = 3p,\ p\ being\ an\ \text{integer}$$

all the f parameters are 1 and the corresponding eigenvectors of H_2 have the same form as those of H_1

2. If the second impurity is placed at an A site, but does not satisfy the condition all the eigenvectors are non-propagating.

3. If the second impurity is placed at a B site the form of the eigenvectors depend strongly on the actual adsorption site.

Outlook

One and two molecules adsorbed is not enough for SANES project, but…

We have found a nice property that could be useful:

- Nanoswitches
- Memories
- Self-Assembly

Thanks for your attention!

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