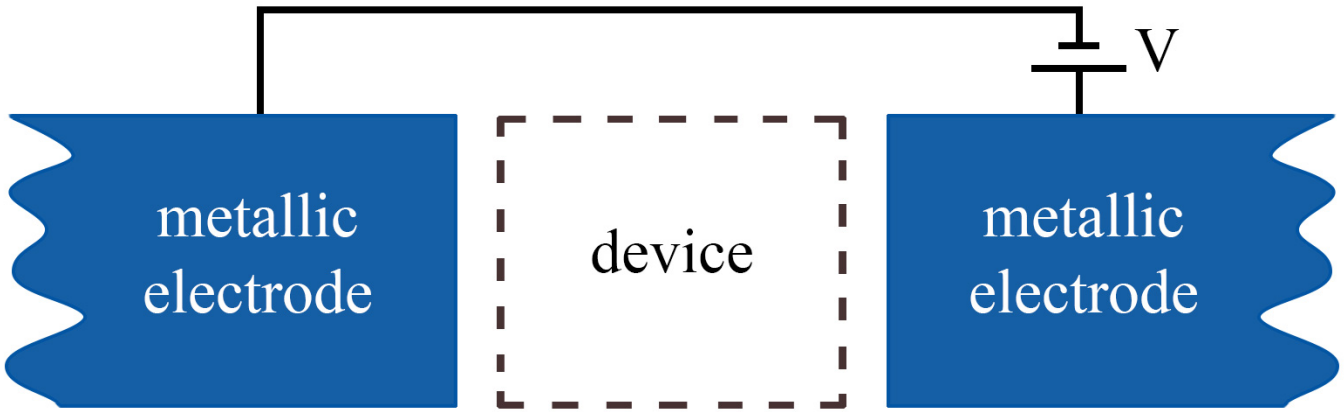
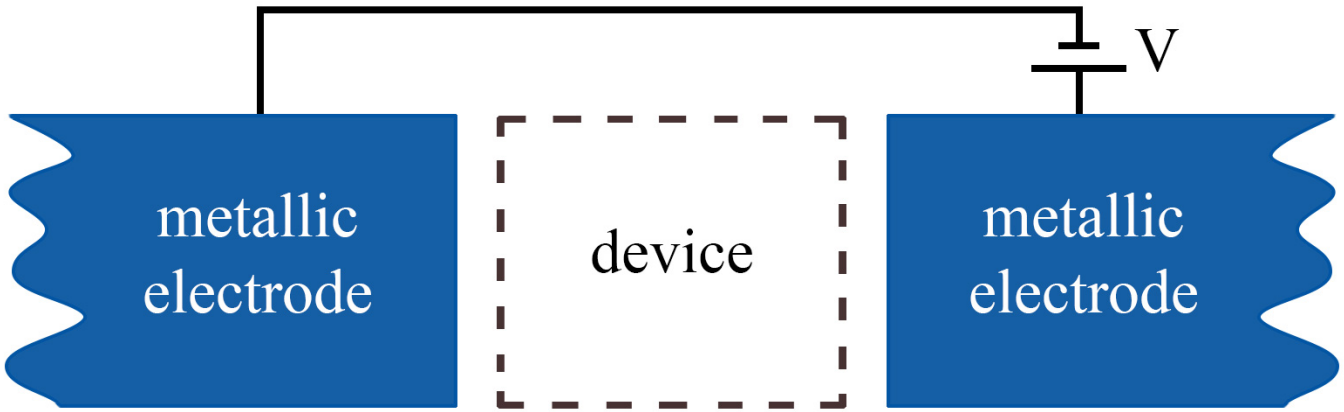
PAMS Second Review
20th November 2015, Brussels

Multi-terminal simulations with TranSIESTA

Pedro Brandimarte


V
metallic electrode
device
metallic electrode

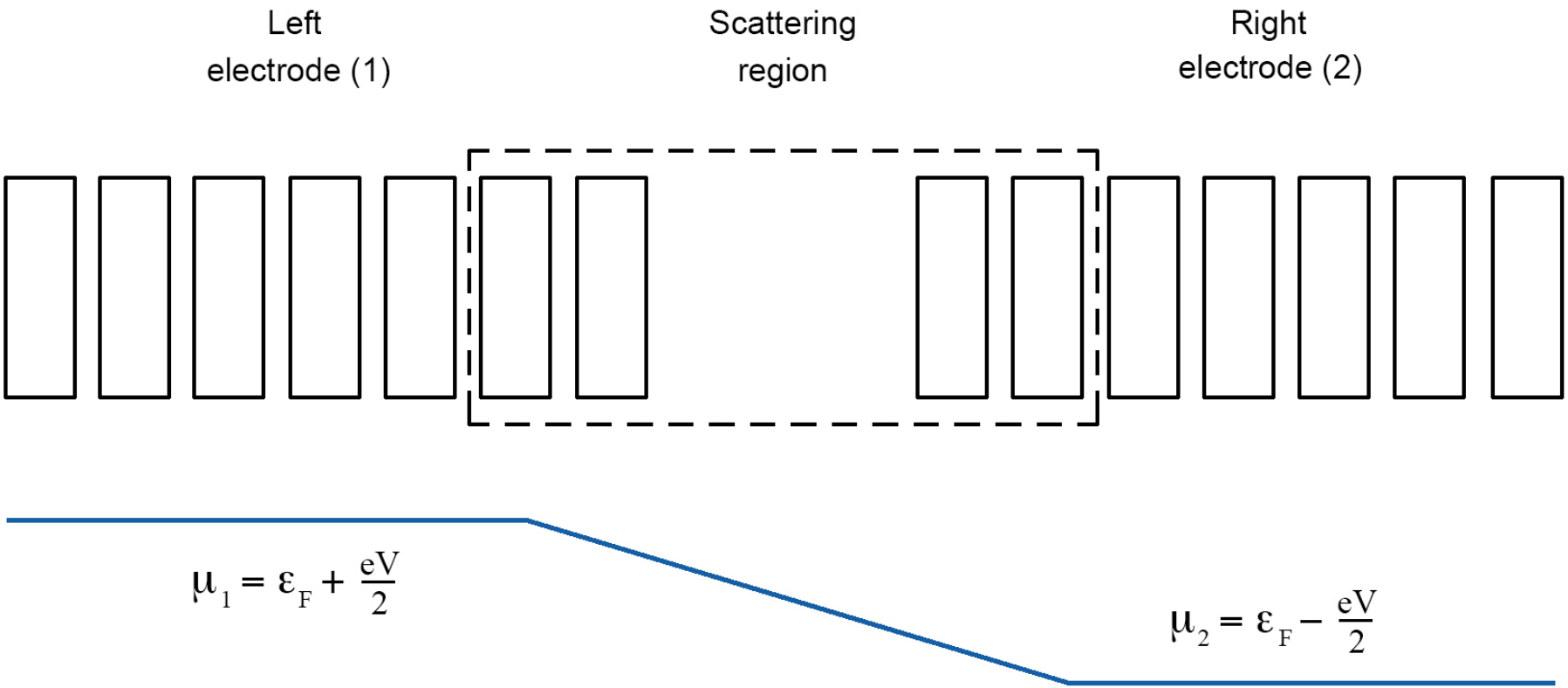


Density-Functional Theory (DFT) **SIESTA**

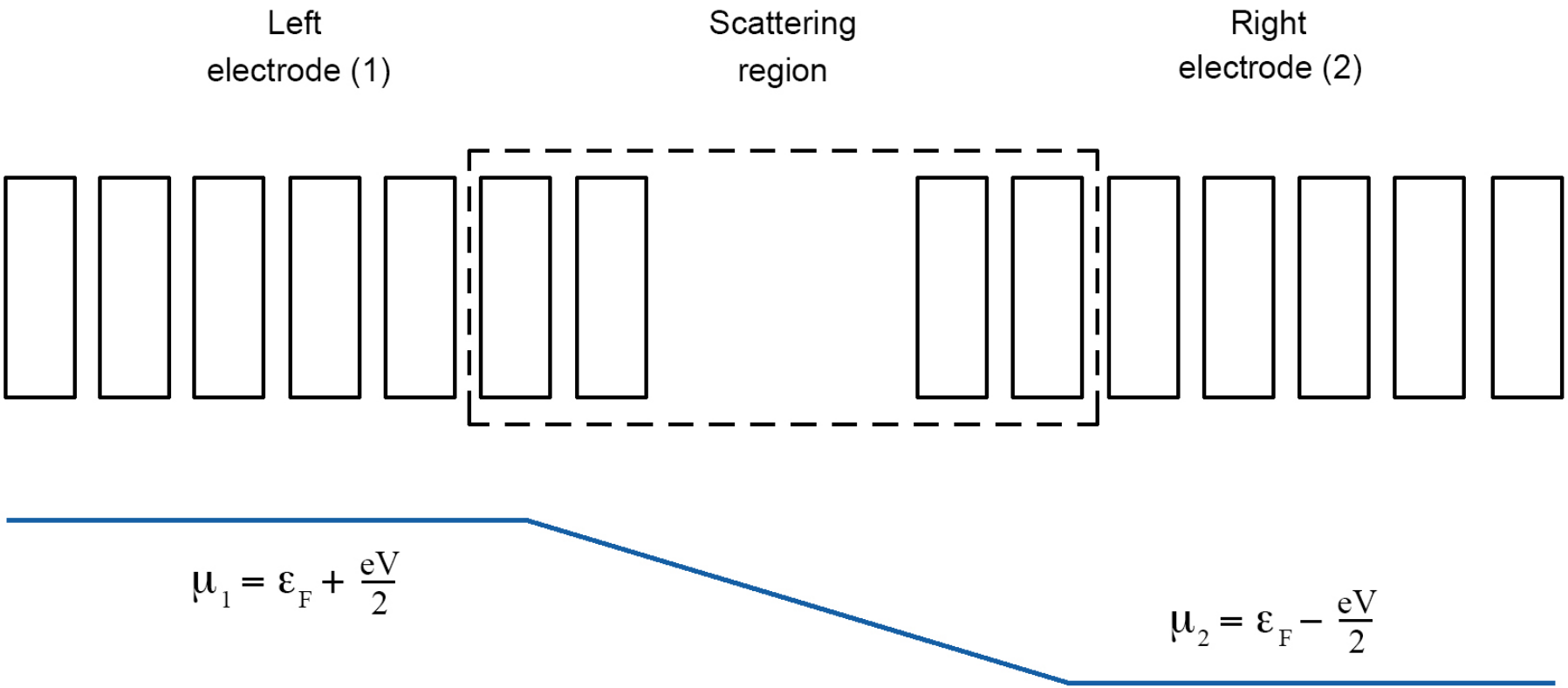
+

Non-Equilibrium Green's Function Formalism (NEGF)

TranSIESTA

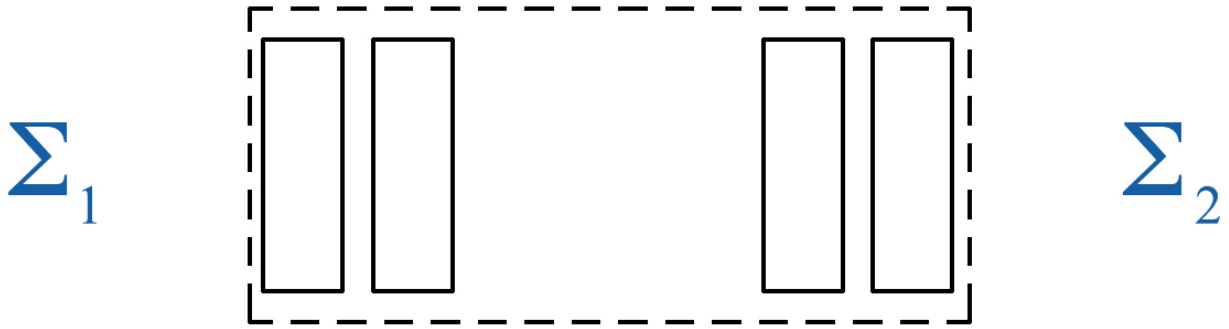

Left
electrode (1)
Scattering
region
Right
electrode (2)
$\mu_1 = \varepsilon_F + \frac{eV}{2}$
$\mu_2 = \varepsilon_F - \frac{eV}{2}$

$$[\varepsilon \mathcal{S} - \mathcal{H}]\, \mathcal{G}^r(E) = \mathbb{1}, \quad \text{where } \varepsilon = \lim_{\eta \to 0^+} E + i\eta$$



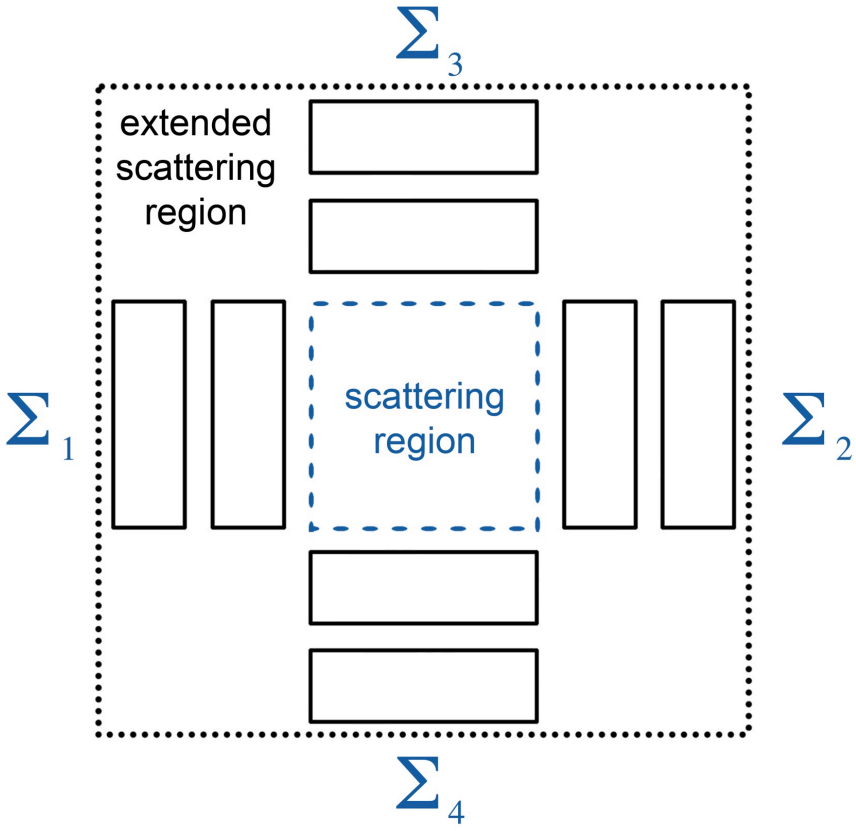
$$[\varepsilon \mathcal{S} - \mathcal{H}]\, \mathcal{G}^r(E) = \mathbb{1}, \quad \text{where } \varepsilon = \lim_{\eta \to 0^+} E + i\eta$$

Left electrode (1) | Scattering region | Right electrode (2)



$$G_M^r = \left[\varepsilon S_M - H_M - \Sigma_1^r - \Sigma_2^r\right]^{-1}$$

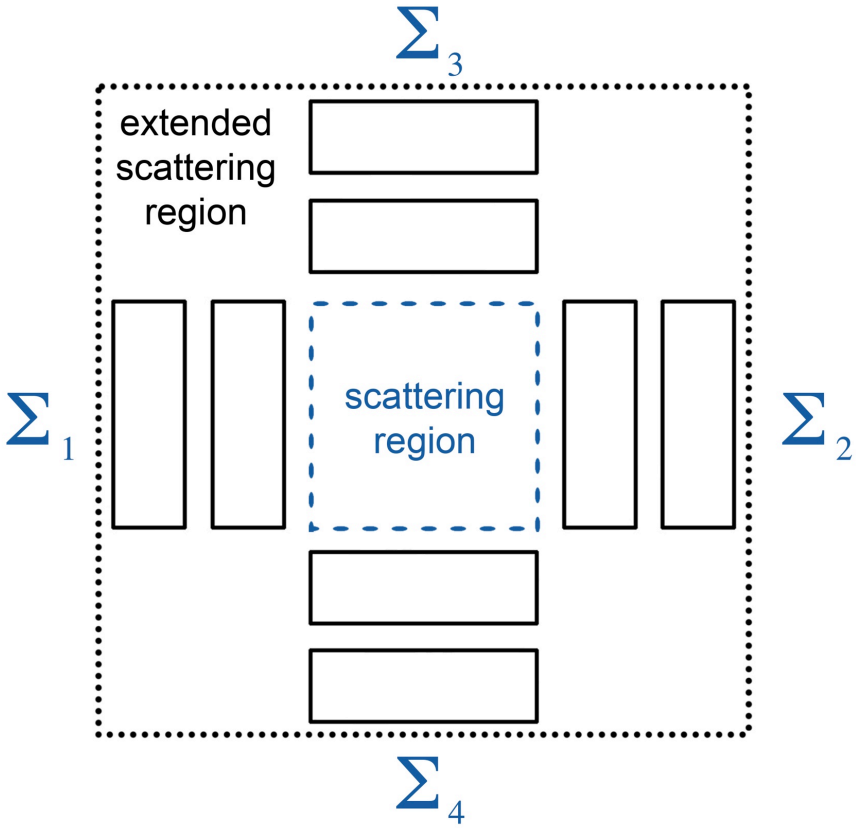

Σ_1
scattering region
Σ_2



DTU Technical University of Denmark

Kamal K. Saha *et al*. *J. Chem. Phys.* **131**, 164105 (2009).

Nick R. Papior. *In preparation* (2015).



$$G^r_M = \left[\varepsilon S_M - H_M - \sum_{j=1}^{N_{el}} \Sigma^r_j \right]^{-1}$$

DTU Technical University of Denmark

Kamal K. Saha *et al*. *J. Chem. Phys.* **131**, 164105 (2009).

Nick R. Papior. *In preparation* (2015).

$$\rho = \frac{1}{2\pi i}\int_{-\infty}^{+\infty} d\epsilon\, G_M^{<} = \frac{1}{2\pi}\int_{-\infty}^{+\infty} d\epsilon\, G_M^{r}\left[\sum_j \Gamma_j f\left(\epsilon-\mu_j\right)\right] G_M^{a}$$

where $\Gamma_j = i\left[\Sigma_j^r - \Sigma_j^{r\dagger}\right]$, $f\left(\epsilon-\mu_j\right) = f_j$ is the Fermi-Dirac distribution.

$$G_M^r = \left[\varepsilon S_M - H_M - \sum_{j=1}^{N_{el}} \Sigma_j^r\right]^{-1}$$

DTU Technical University of Denmark

Kamal K. Saha *et al*. *J. Chem. Phys.* **131**, 164105 (2009).

Nick R. Papior. *In preparation* (2015).

$$\rho = \frac{1}{2\pi i}\int_{-\infty}^{+\infty} d\epsilon\, G_M^{<} = \frac{1}{2\pi}\int_{-\infty}^{+\infty} d\epsilon\, G_M^{r}\left[\sum_j \Gamma_j f\left(\epsilon-\mu_j\right)\right] G_M^{a}$$

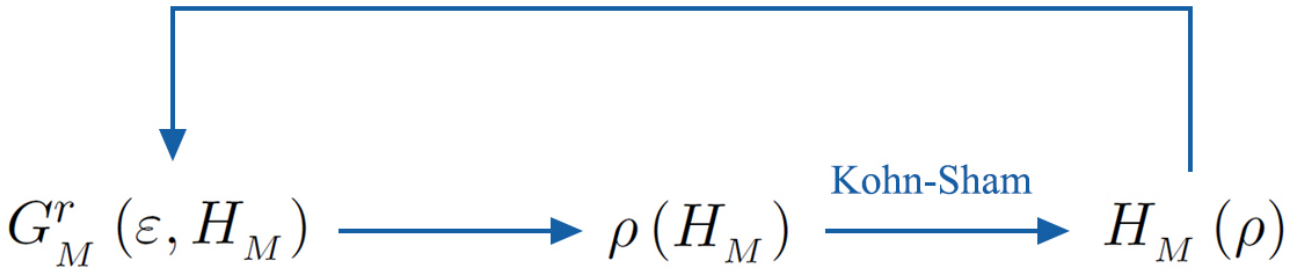
where $\Gamma_j = i\left[\Sigma_j^r - \Sigma_j^{r\dagger}\right]$, $f\left(\epsilon-\mu_j\right) = f_j$ is the Fermi-Dirac distribution.

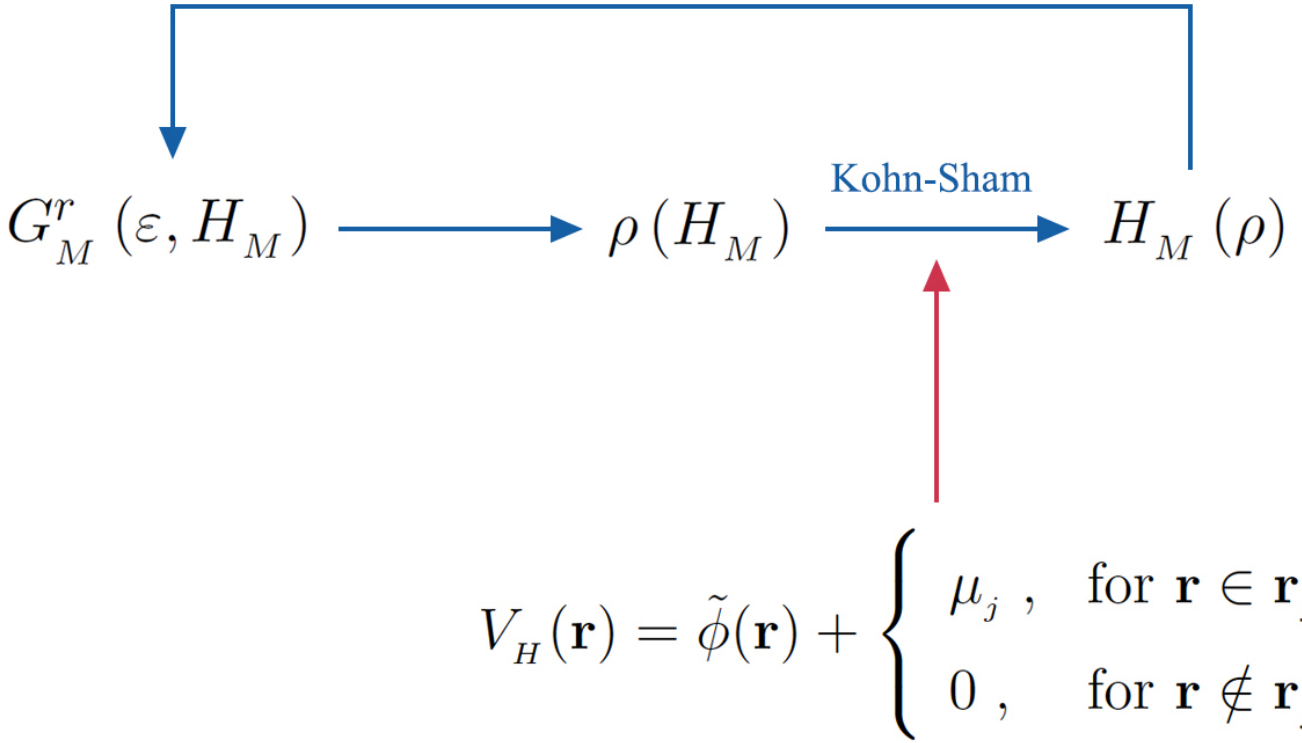
$$G_M^r = \left[\varepsilon S_M - H_M - \sum_{j=1}^{N_{el}} \Sigma_j^r\right]^{-1}$$

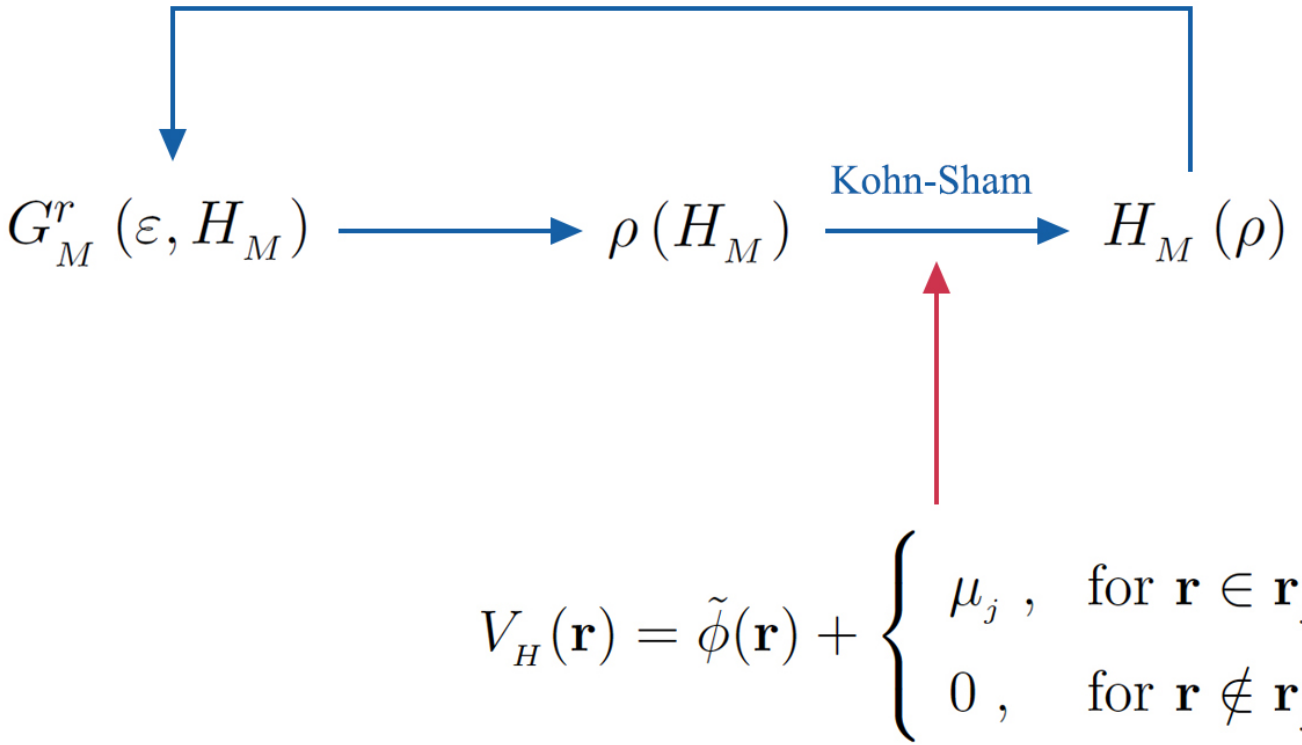
DTU Technical University of Denmark

Kamal K. Saha *et al*. *J. Chem. Phys.* **131**, 164105 (2009).

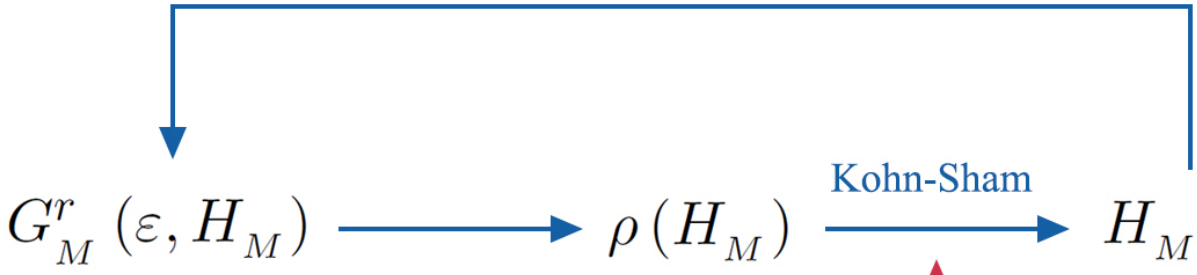
Nick R. Papior. *In preparation* (2015).


$G_M^r(\varepsilon, H_M)$
$\rho(H_M)$
Kohn-Sham
$H_M(\rho)$


$G_M^r(\varepsilon, H_M)$
$\rho(H_M)$
Kohn-Sham
$H_M(\rho)$
$V_H(\mathbf{r}) = \tilde{\phi}(\mathbf{r}) + \begin{cases} \mu_j\ , & \text{for } \mathbf{r} \in \mathbf{r}_j \\ 0\ , & \text{for } \mathbf{r} \notin \mathbf{r}_j \end{cases}$



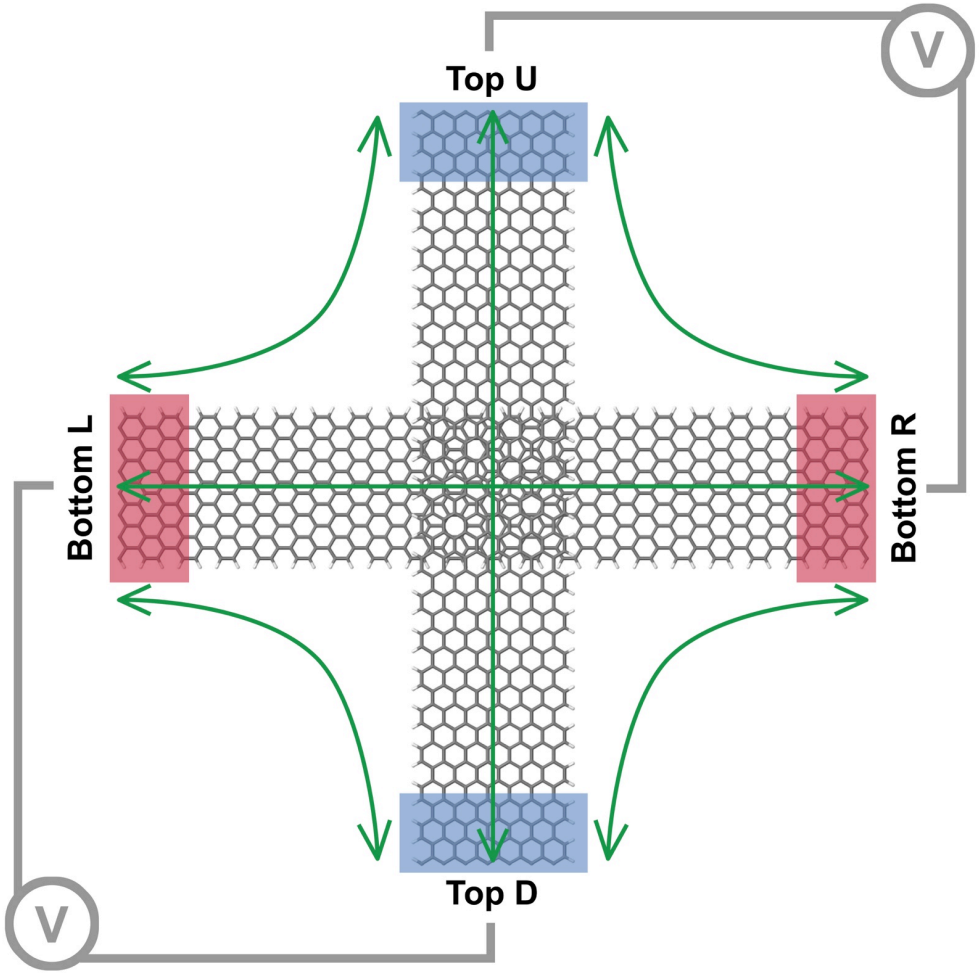
$$I_j = \frac{2e}{h} \sum_{j'} \int_{-\infty}^{+\infty} d\epsilon \, \mathrm{Tr}\left[\Gamma_j G^r_M{}^{\dagger} \Gamma_{j'} G^r_M\right] \left(f_j - f_{j'}\right)$$



$$V_H(\mathbf{r}) = \tilde{\phi}(\mathbf{r}) + \begin{cases} \mu_j\ , & \text{for } \mathbf{r} \in \mathbf{r}_j \\ 0\ , & \text{for } \mathbf{r} \notin \mathbf{r}_j \end{cases}$$

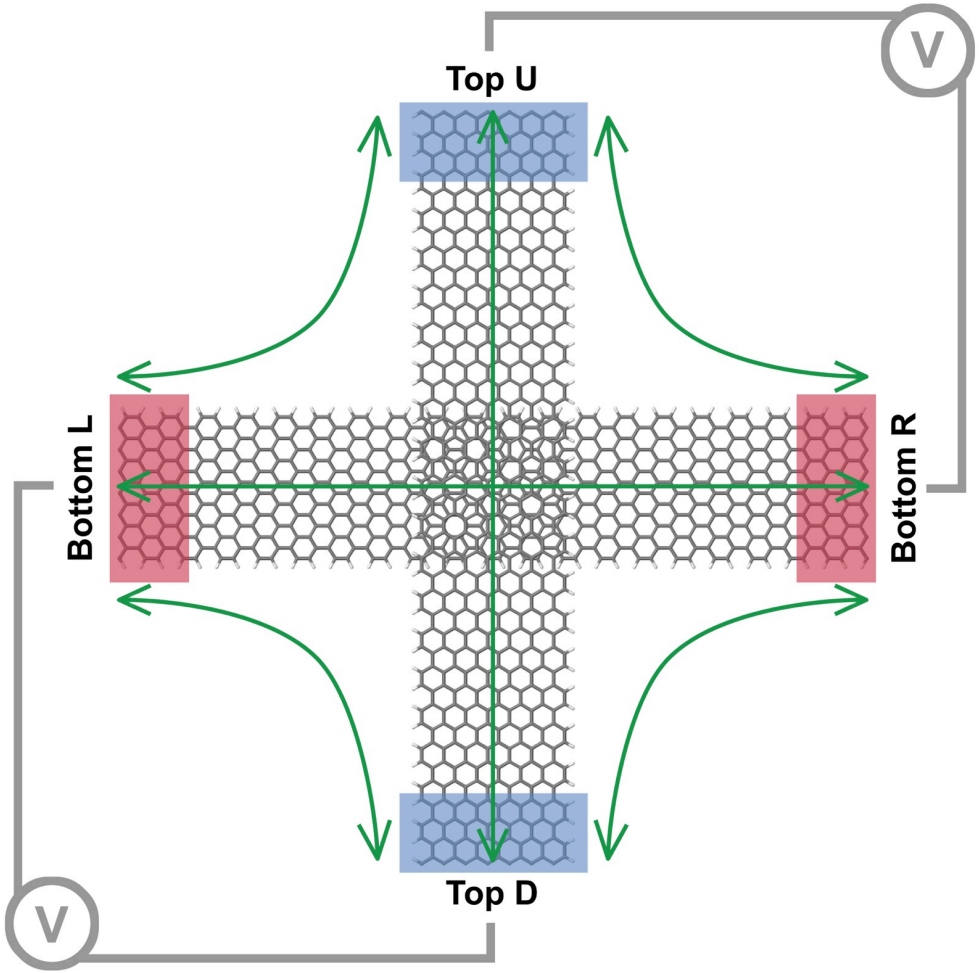
$$I_j = \frac{2e}{h} \sum_{j'} \int_{-\infty}^{+\infty} d\epsilon \, \mathrm{Tr}\left[\Gamma_j G^r_M{}^{\dagger} \Gamma_{j'} G^r_M\right] \left(f_j - f_{j'}\right)$$

Crossed 14-AGNR



M. Masum Habib and Roger K. Lake. *Phys. Rev. B* **86**, 045418 (2012).

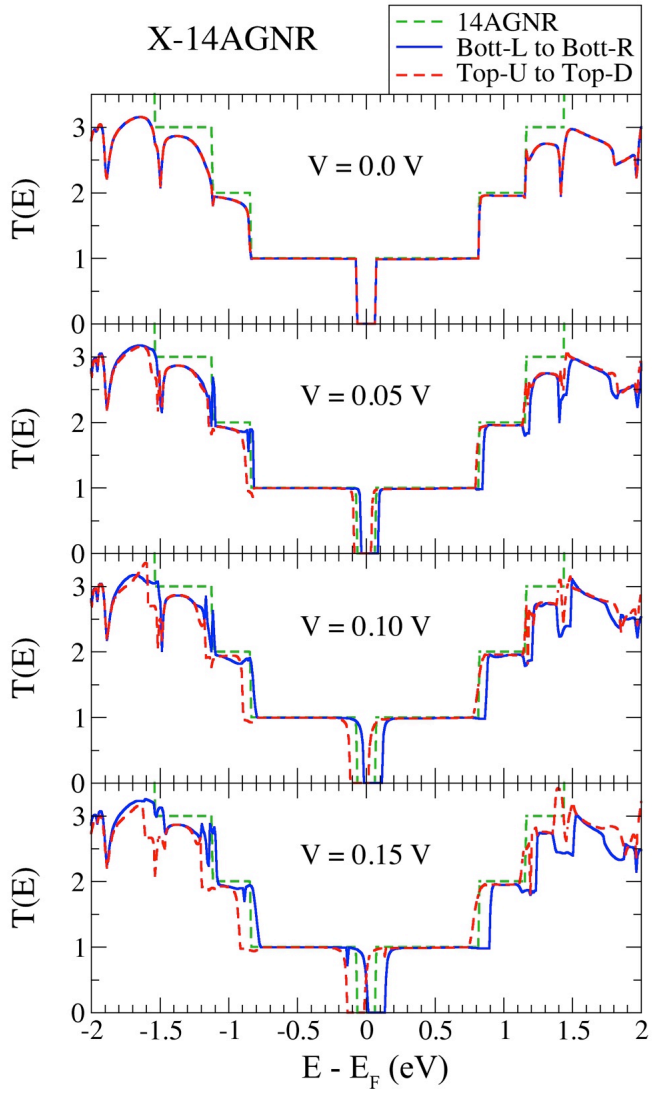
Crossed 14-AGNR

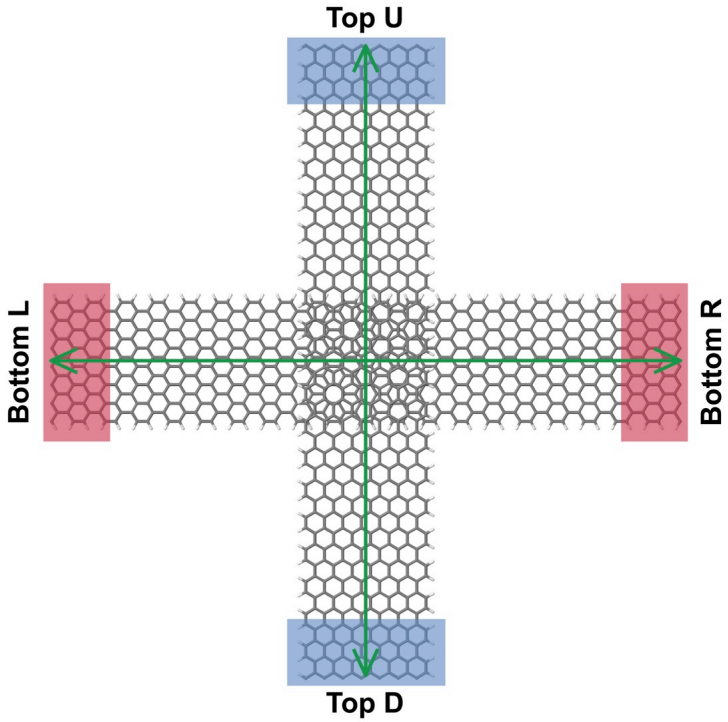


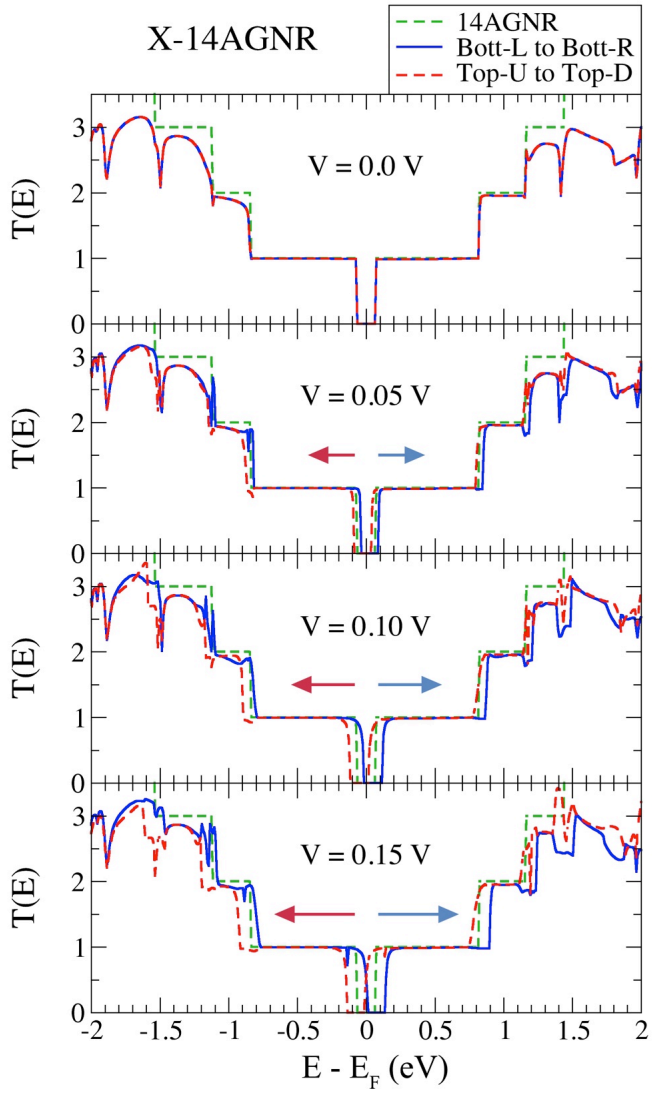
Simulation characteristics:

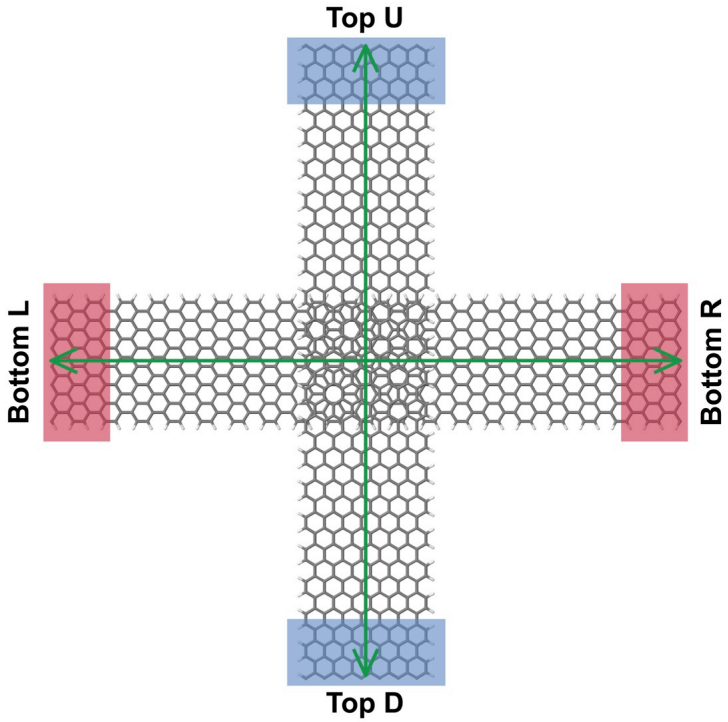
- 1280 atoms;
- double-ζ (9280 orbitals);
- vdW (optB88);
- real space grid cutoff: 350 Ry;
- forces < 5 meV/Å;
- interlayer distance: 3.34 Å.

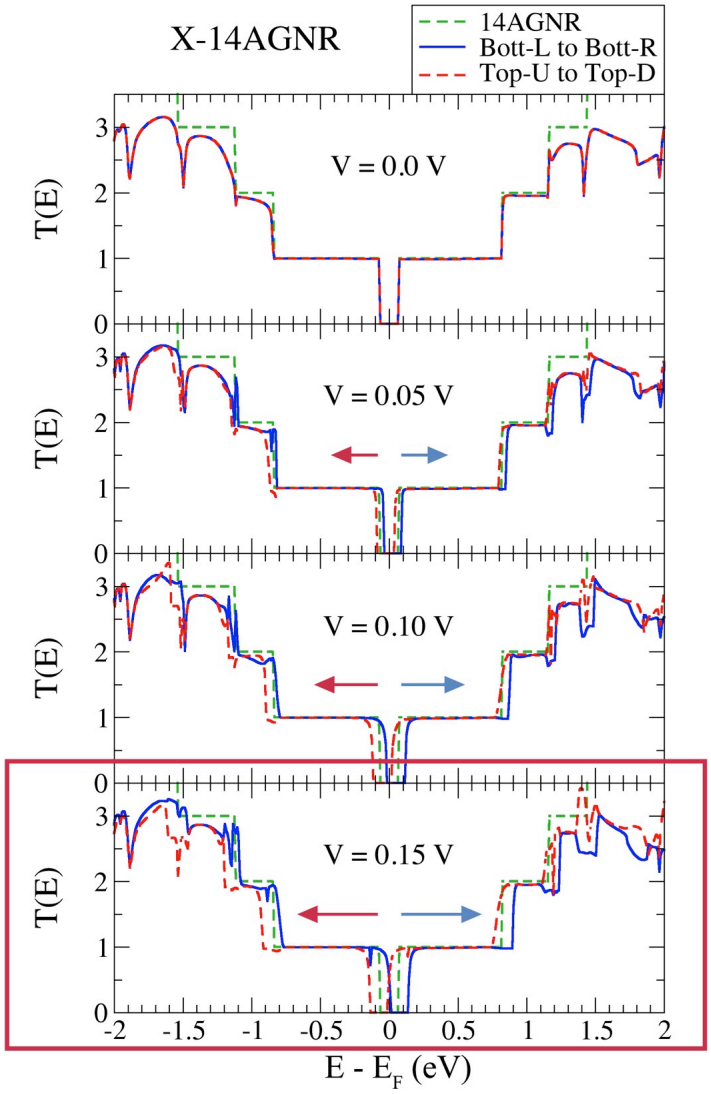
M. Masum Habib and Roger K. Lake. *Phys. Rev. B* **86**, 045418 (2012).

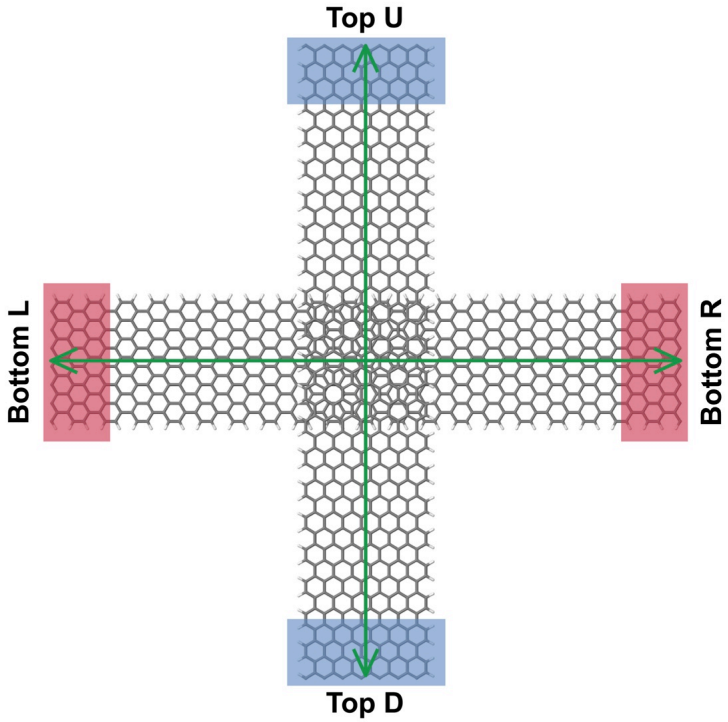

X-14AGNR
14AGNR
Bott-L to Bott-R
Top-U to Top-D
V = 0.0 V
V = 0.05 V
V = 0.10 V
V = 0.15 V
T(E)
E - E_F (eV)

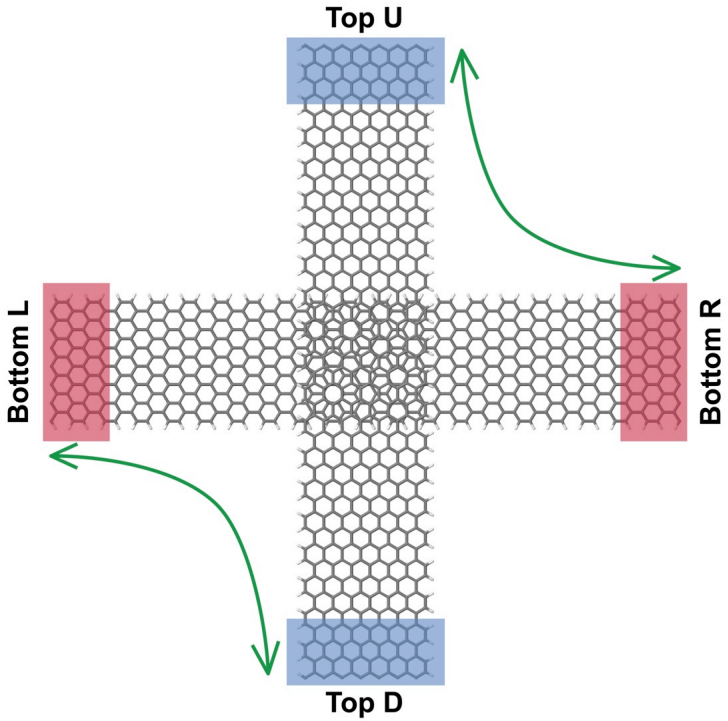

Top U
Bottom L
Bottom R
Top D

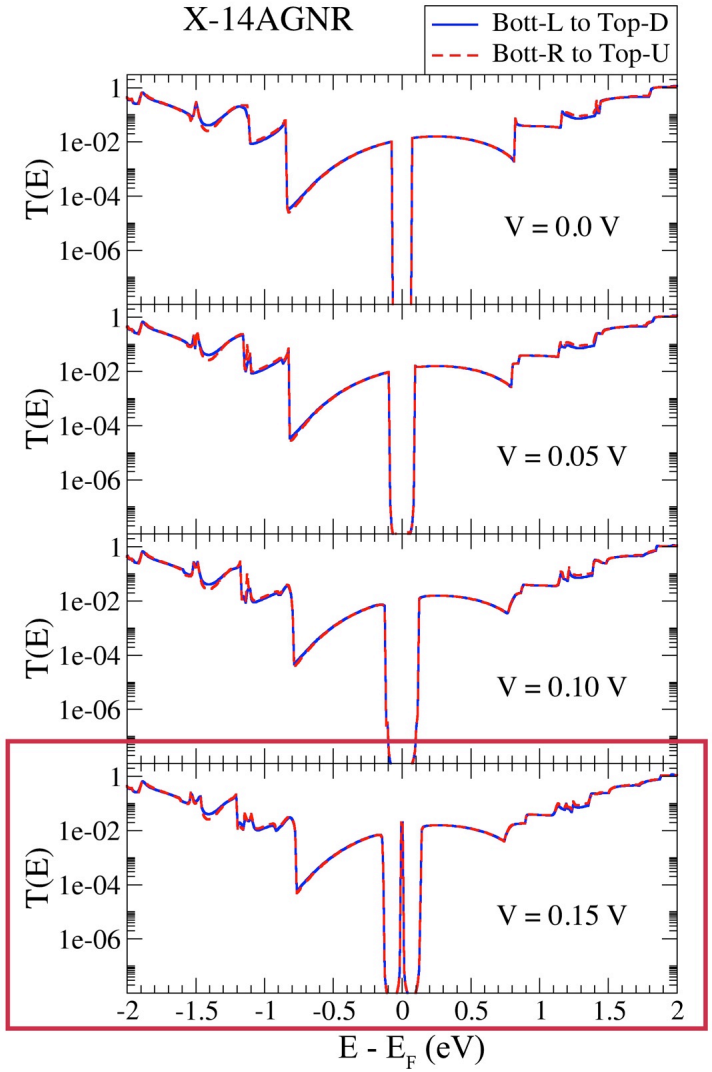

X-14AGNR
14AGNR
Bott-L to Bott-R
Top-U to Top-D
V = 0.0 V
V = 0.05 V
V = 0.10 V
V = 0.15 V
T(E)
E - E_F (eV)

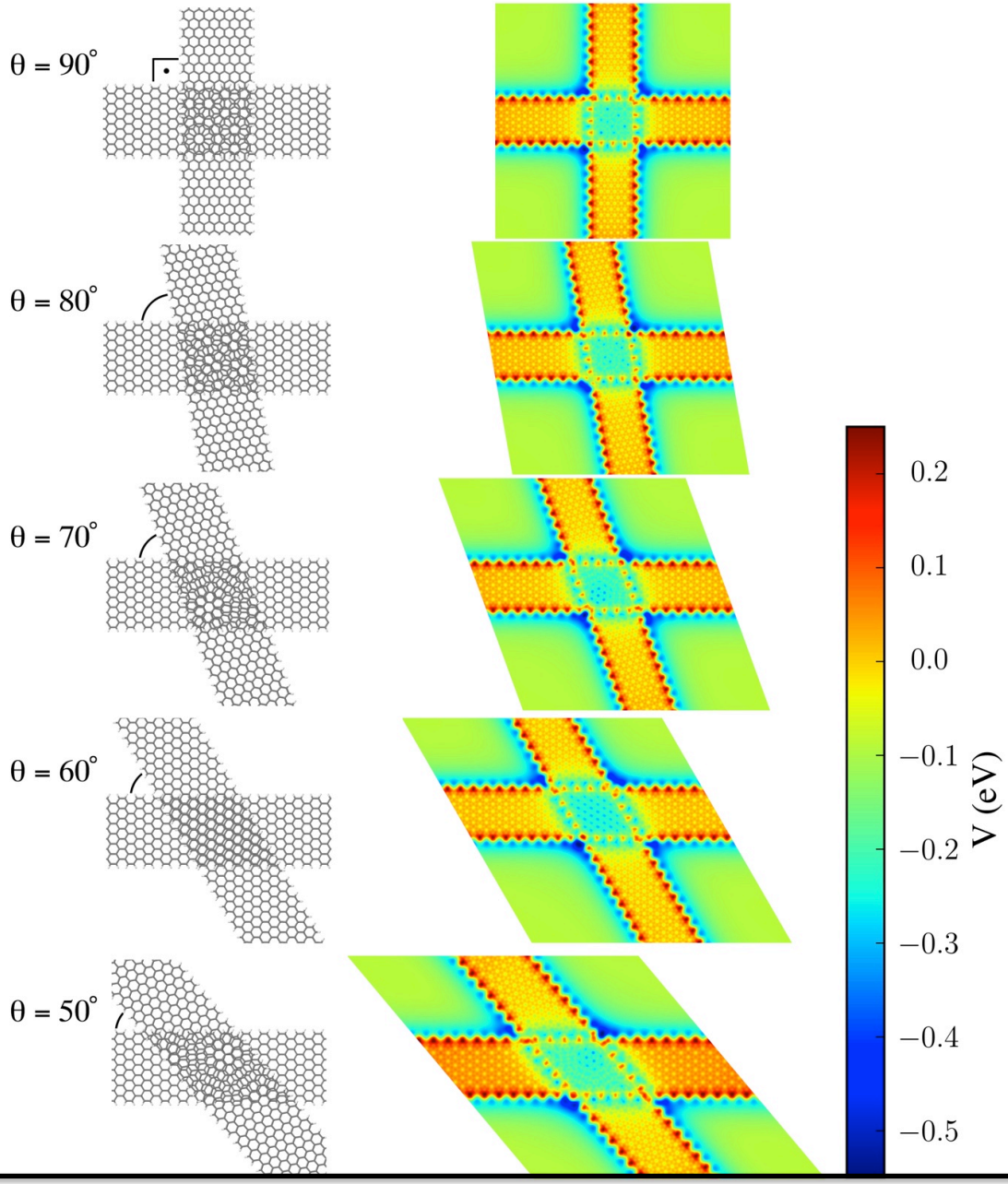

Top U
Bottom L
Bottom R
Top D

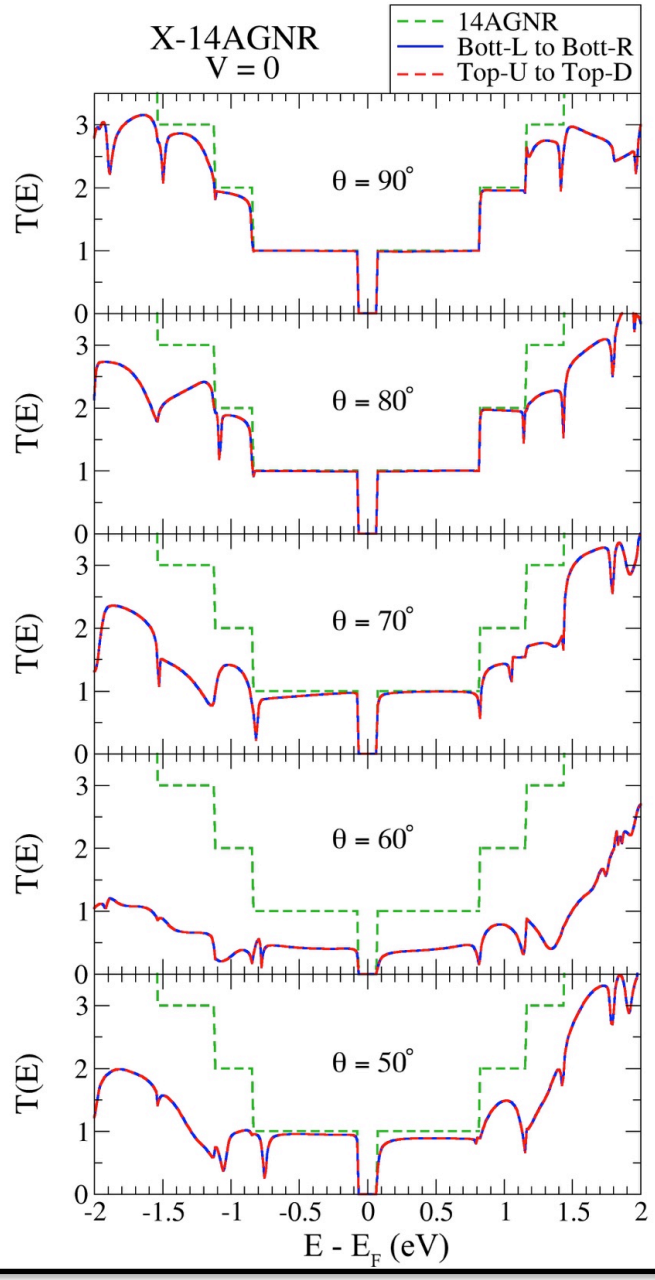

X-14AGNR
14AGNR
Bott-L to Bott-R
Top-U to Top-D
V = 0.0 V
V = 0.05 V
V = 0.10 V
V = 0.15 V
T(E)
E - E_F (eV)

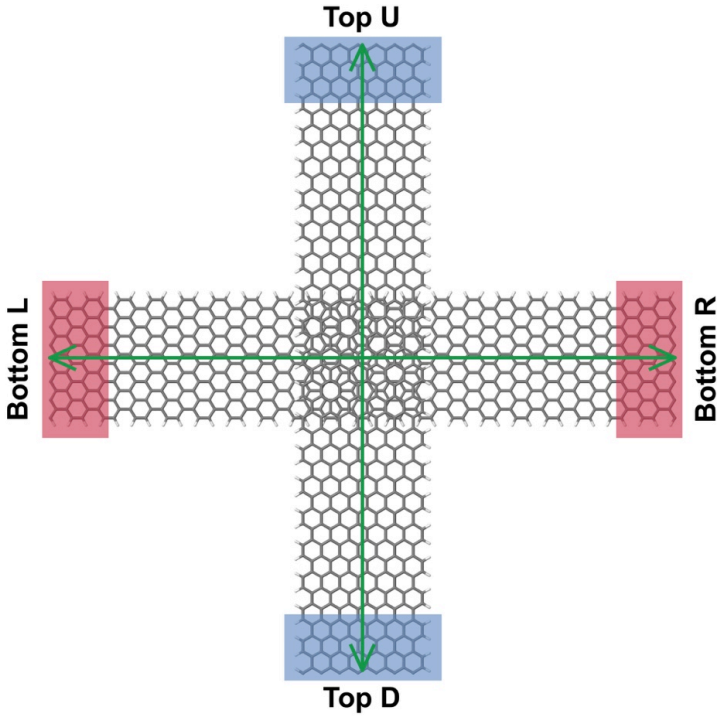

Top U
Bottom L
Bottom R
Top D

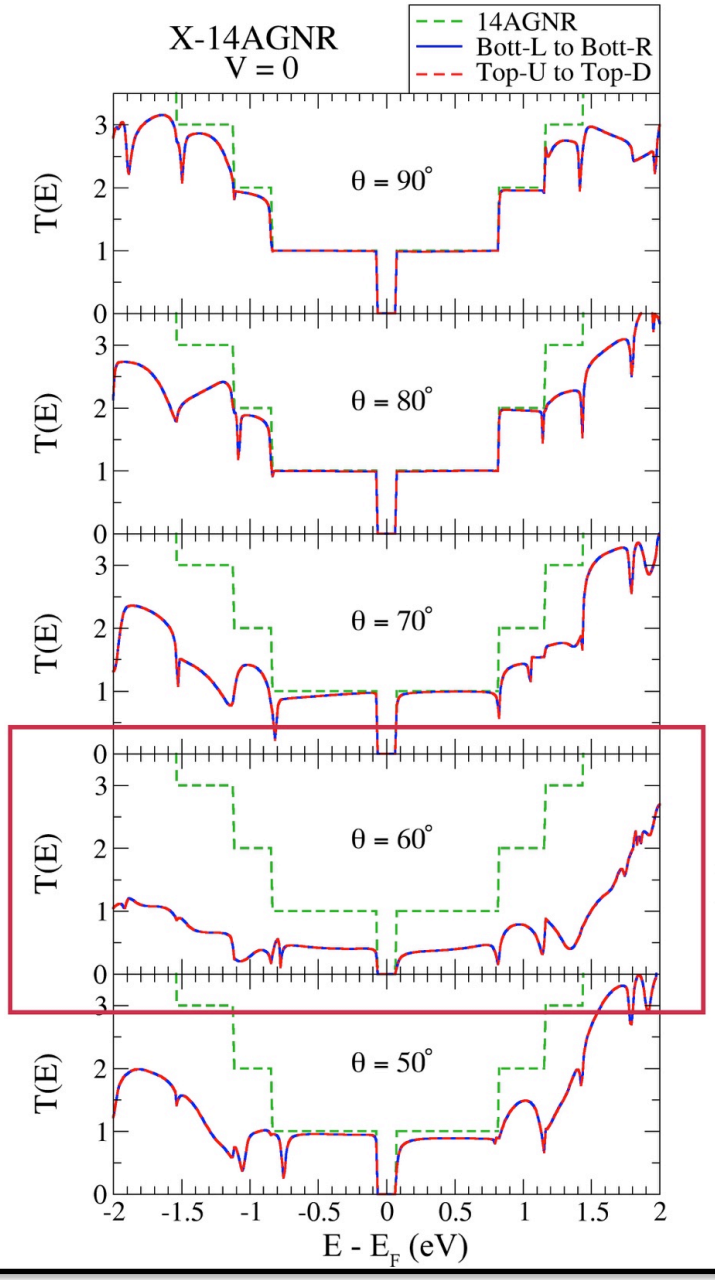

Top U
Bottom L
Bottom R
Top D

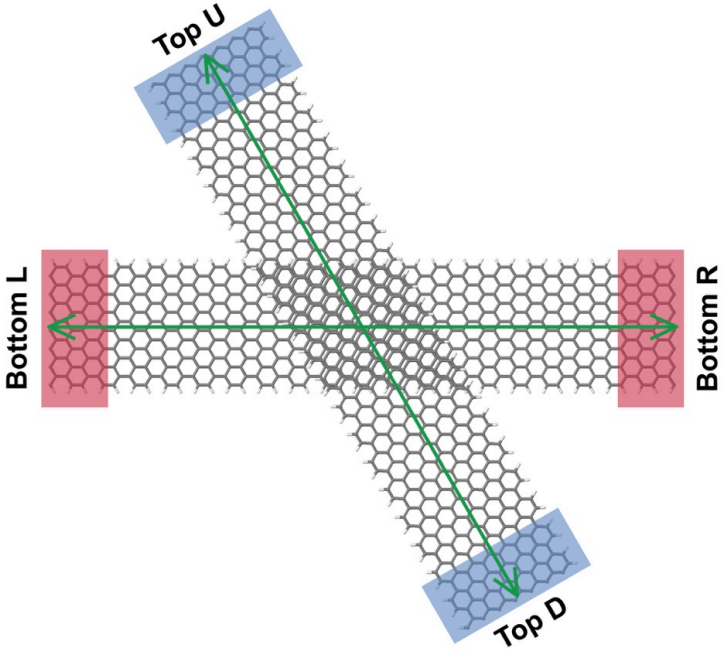

X-14AGNR
Bott-L to Top-D
Bott-R to Top-U
T(E)
V = 0.0 V
V = 0.05 V
V = 0.10 V
V = 0.15 V
1
1e-02
1e-04
1e-06
-2
-1.5
-1
-0.5
0
0.5
1
1.5
2
E - E_F (eV)

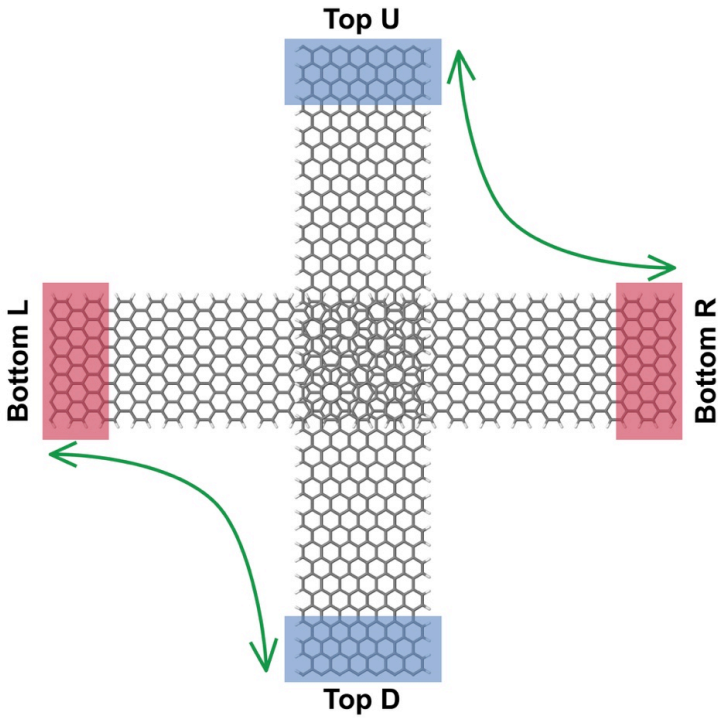

θ = 90°
θ = 80°
θ = 70°
θ = 60°
θ = 50°
0.2
0.1
0.0
−0.1
−0.2
−0.3
−0.4
−0.5
V (eV)

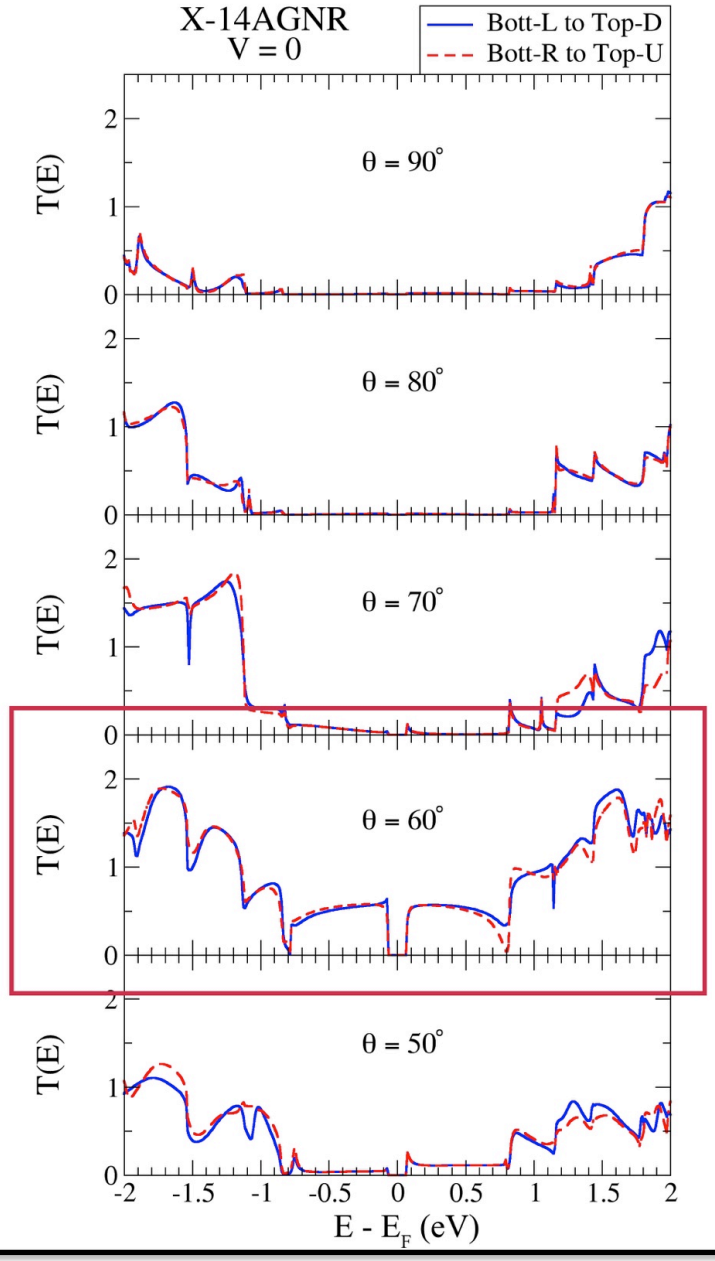

X-14AGNR
V = 0
14AGNR
Bott-L to Bott-R
Top-U to Top-D
θ = 90°
θ = 80°
θ = 70°
θ = 60°
θ = 50°
T(E)
E - E_F (eV)

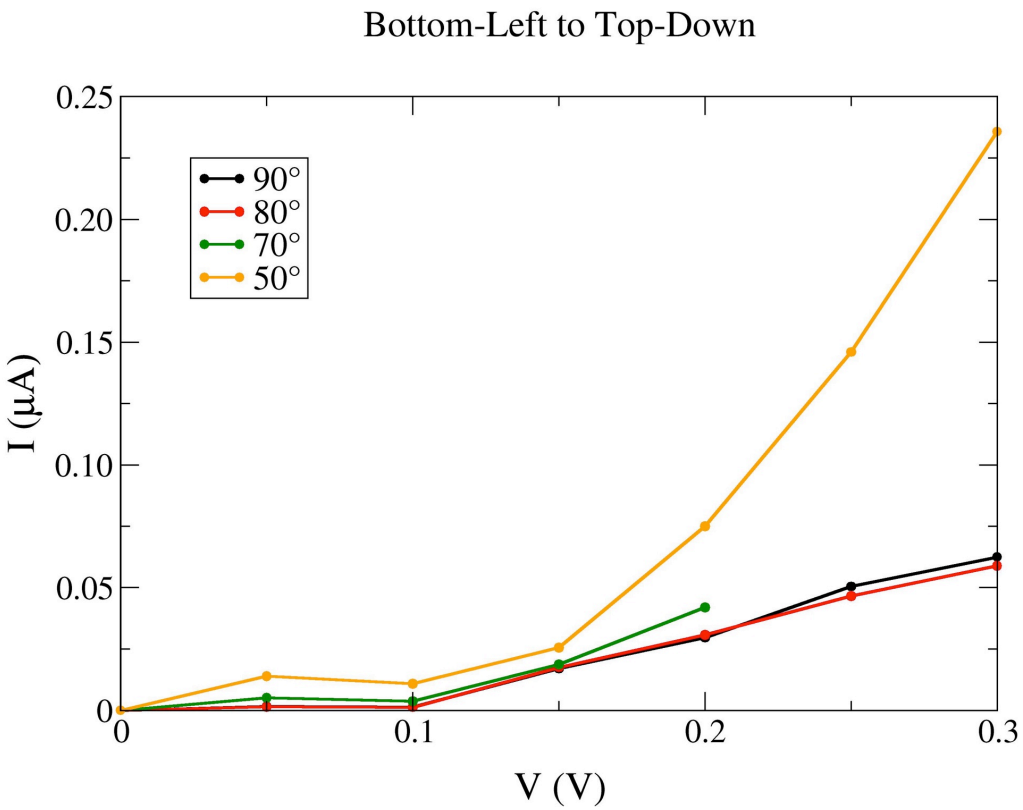

Top U
Bottom L
Bottom R
Top D

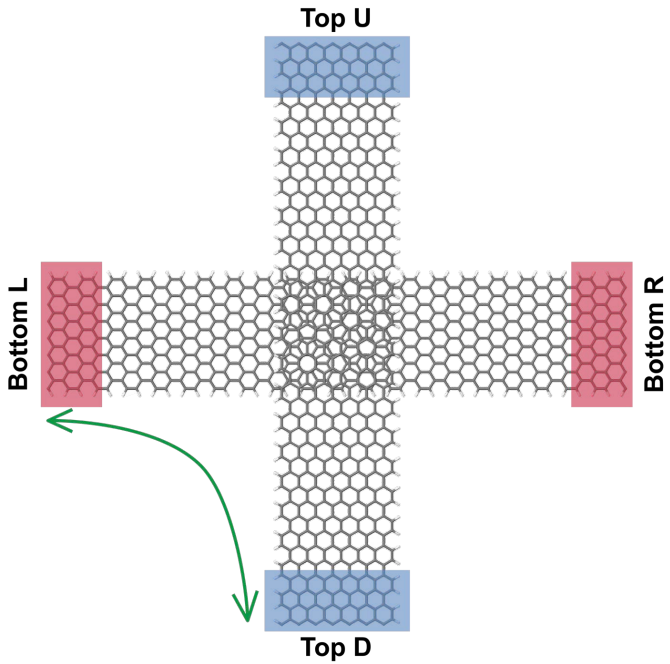

X-14AGNR
V = 0
14AGNR
Bott-L to Bott-R
Top-U to Top-D
θ = 90°
θ = 80°
θ = 70°
θ = 60°
θ = 50°
T(E)
E - E_F (eV)

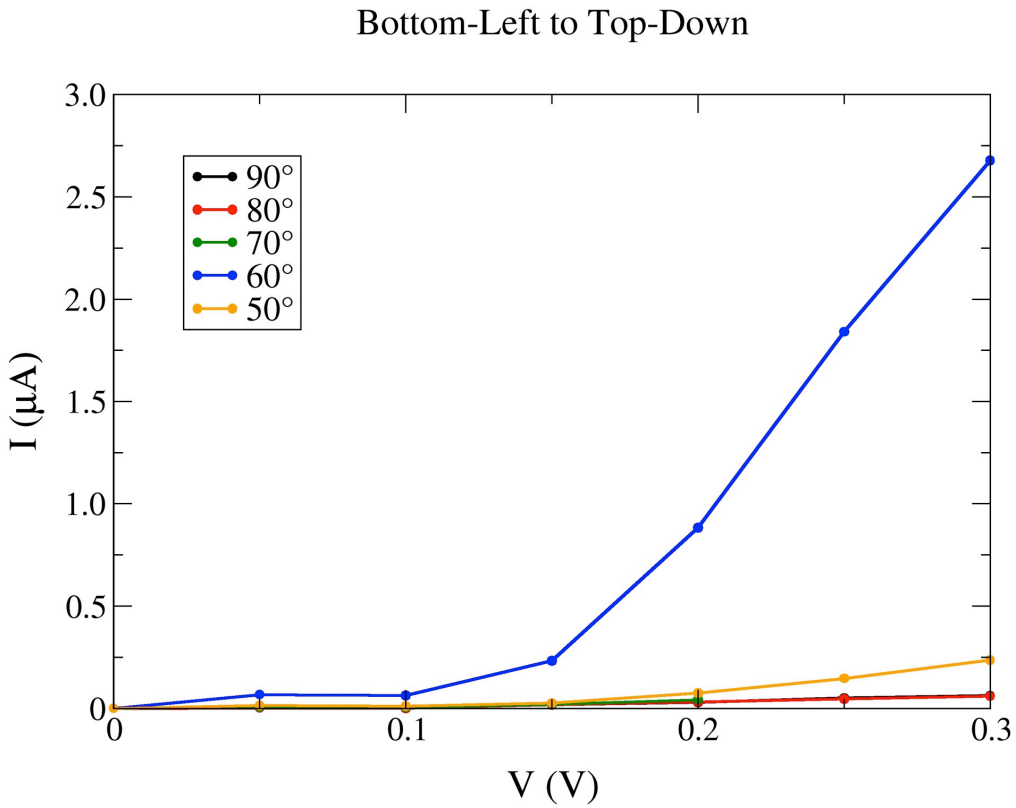

Top U
Bottom L
Bottom R
Top D

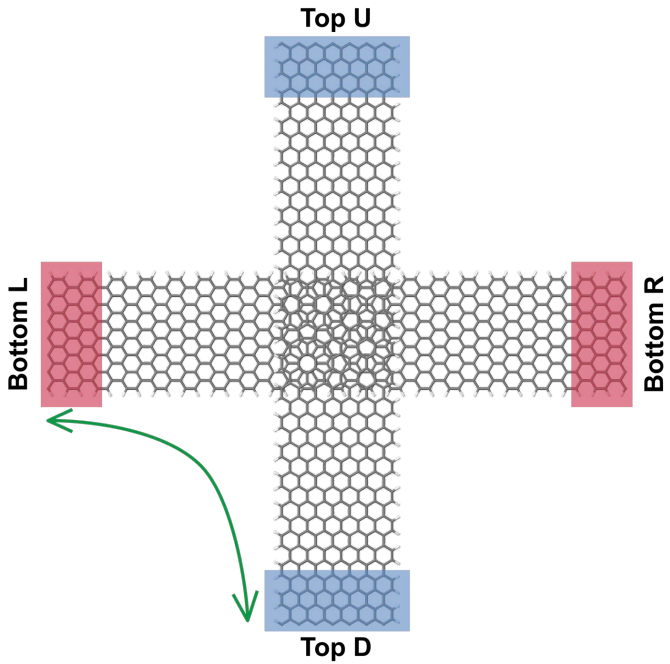

Top U
Bottom L
Bottom R
Top D


X-14AGNR
V = 0
Bott-L to Top-D
Bott-R to Top-U
θ = 90°
θ = 80°
θ = 70°
θ = 60°
θ = 50°
T(E)
E - E_F (eV)


Bottom-Left to Top-Down
0.25
0.20
0.15
0.10
0.05
0
I (μA)
90°
80°
70°
50°
0
0.1
0.2
0.3
V (V)


Top U
Bottom L
Bottom R
Top D


Bottom-Left to Top-Down
3.0
2.5
2.0
1.5
1.0
0.5
0
I (μA)
0
0.1
0.2
0.3
V (V)
90°
80°
70°
60°
50°


Top U
Bottom L
Bottom R
Top D