Theoretical Study of Conductance through Monoatomic Nanowires

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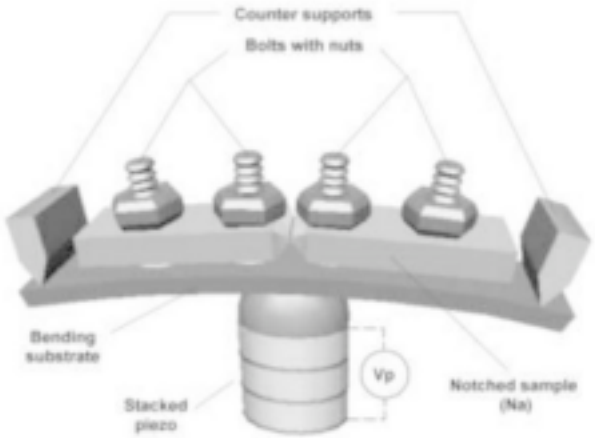
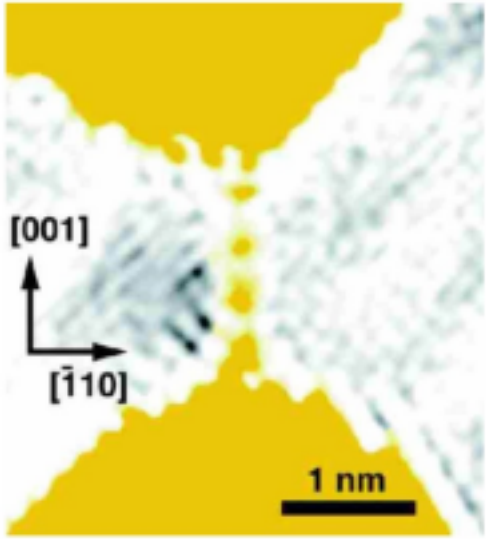
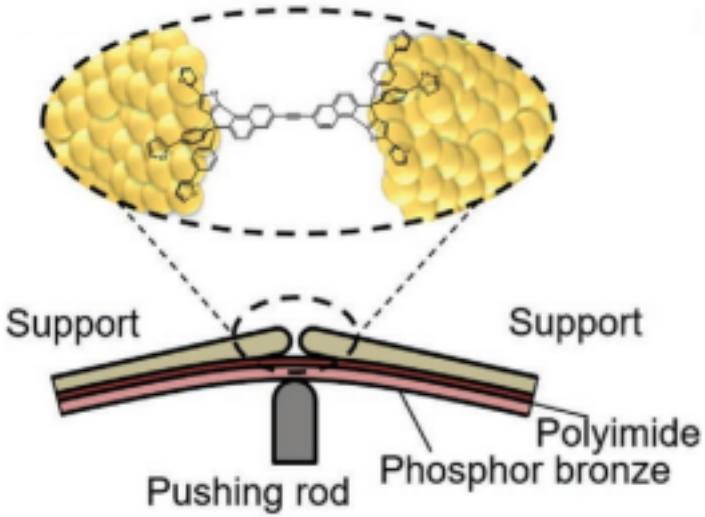
Electronic transport through nanodevices



N. Agraıt et. al. Physics Reports, 377, 81-279 (2003)



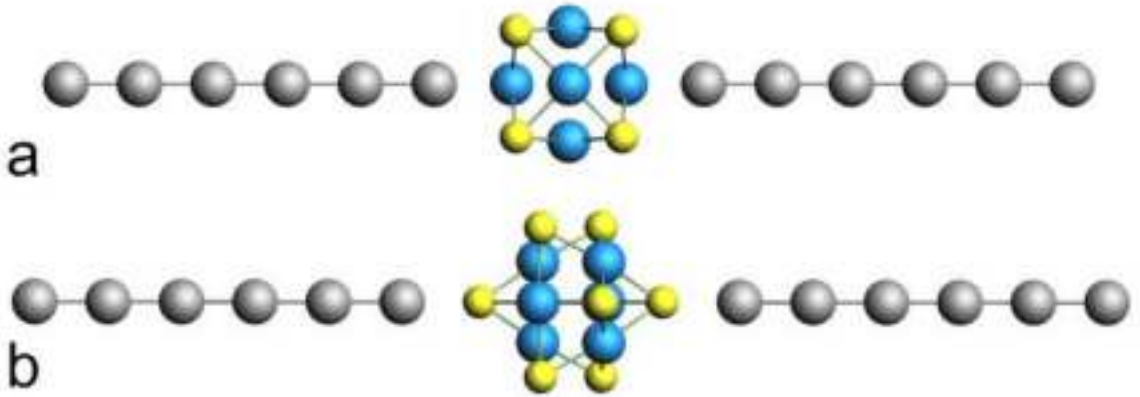
H. Ohnishi et. al. Nature, 395, 780–785, (1998)

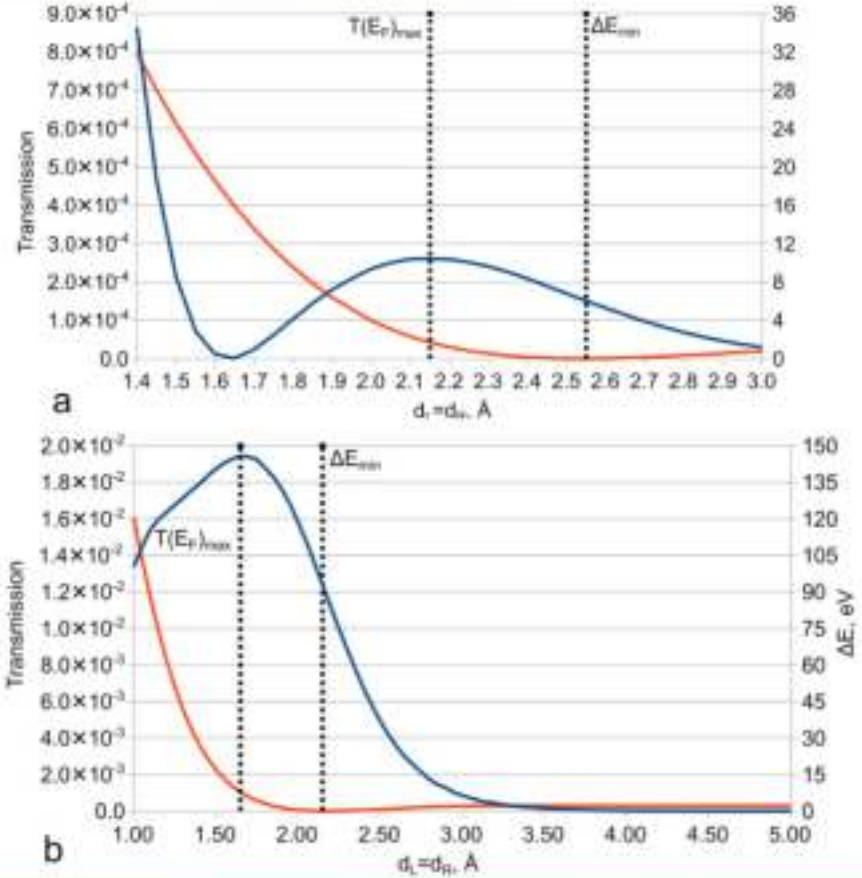


T. Ohto et. al. Small 2021, 17, 2006709

Conductance through clusters

M.R. Ryzhikov, S.G. Kozlova // J. Struct. Chem., 2022, in press



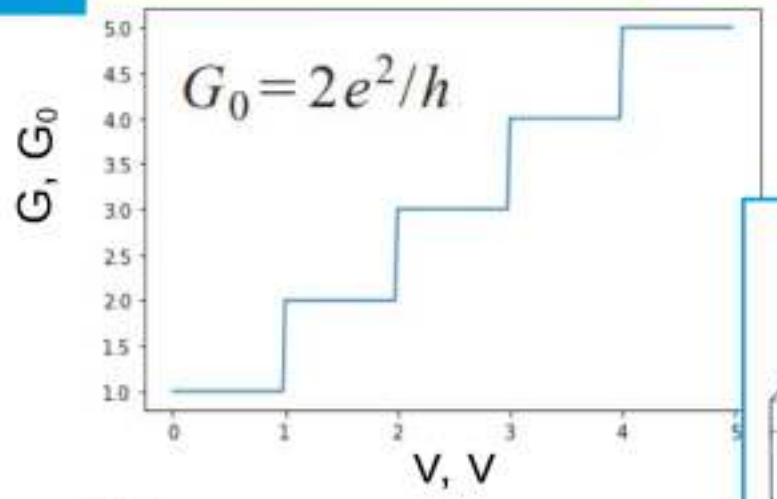


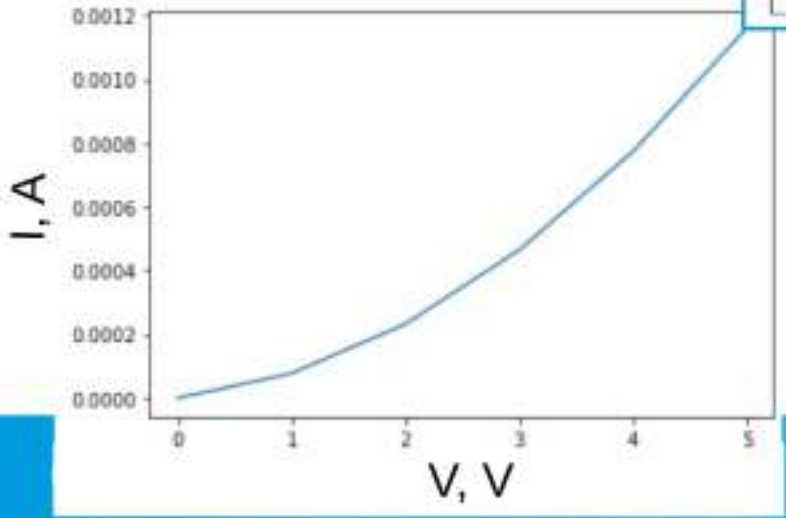
Optimal interatomic distance in infinite nanowires

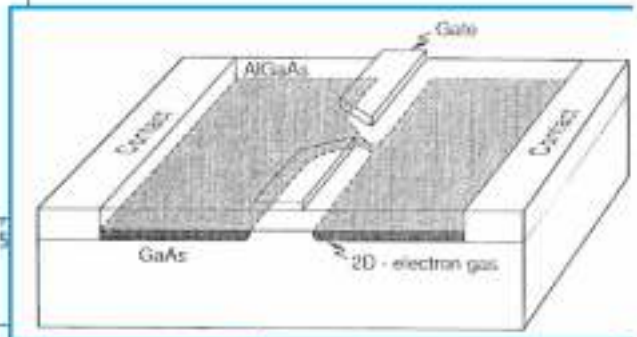
BAND: BLYP/TZ2P

	Cu		Ag		Au		Pt	
	No Disp.	D3(BJ)	No Disp.	D3(BJ)	No Disp.	D3(BJ)	No Disp.	D3(BJ)
Nonrel.	2.384	2.370	2.808	2.793	2.938	2.927	2.865	2.845
Scalar ZORA	2.3482	2.3356	2.715	2.705	2.679	2.667	2.445	2.437
SO ZORA	2.3477	2.3352	2.714	2.704	2.650	2.642	2.484	2.473
Bulk exp.	2.556		2.889		2.884		2.772	

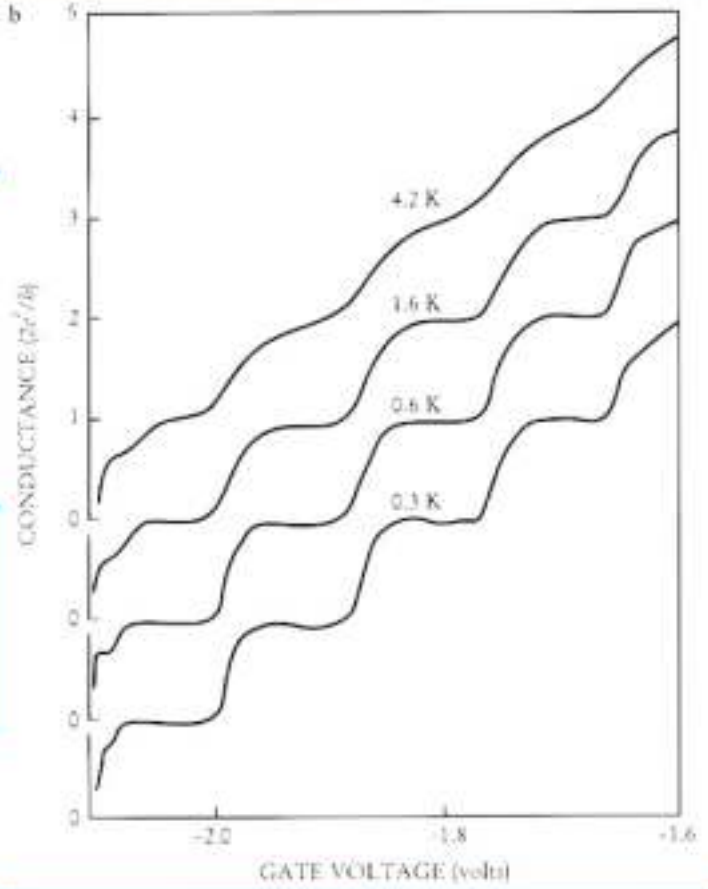
Quantum point contact







H. van Houten & C. Beenakke. Physics Today, 22 (1996)



NEGF method

SIESTA: *M. Brandbyge et. al. Phys. Rev. B 65, 165401 (2002)*

- Calculation of Hamiltonian of infinite bulk leads (DFT).
- Calculation of the self-energies $\Sigma_{L,R}(\epsilon)$ of semi-infinite bulk leads and building corresponding Hamiltonian.

Dyson equation: $G \equiv G_0 + G_0 \Sigma G$

Propagator

Undressed (unperturbed) propagator

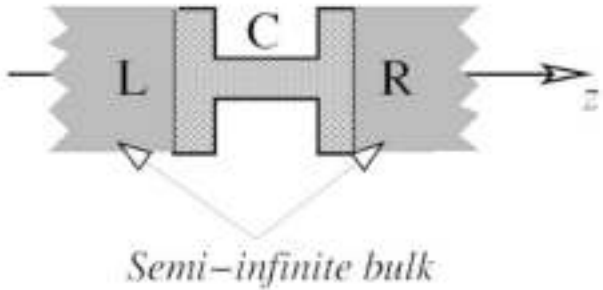
Self-energy

J. Henk and W. Schattke. Comput. Phys. Commun. 77, 69 (1993)

NEGF method

- Calculation of Hamiltonian of infinite bulk leads (DFT).
- Calculation of the self-energies $\Sigma_{L,R}(\epsilon)$ of semi-infinite bulk leads and building corresponding Hamiltonian.
- Calculation of initial Green's function of the system

$$(\mathbf{G})^{-1} = \begin{pmatrix} \mathbf{H}_L + \mathbf{\Sigma}_L & \mathbf{V}_L & 0 \\ \mathbf{V}_L^{\dagger} & \mathbf{H}_C & \mathbf{V}_R \\ 0 & \mathbf{V}_R^{\dagger} & \mathbf{H}_R + \mathbf{\Sigma}_R \end{pmatrix}$$



NEGF method

- Calculation of Hamiltonian of infinite bulk leads (DFT).
- Calculation of the self-energies $\Sigma_{L,R}(\epsilon)$ of semi-infinite bulk leads and building corresponding Hamiltonian.
- Calculation of initial Green's function of the system
- Self-consistent calculation of the non-equilibrium density matrix of the system (leads+device).

$$\mathbf{D}_{\mu\nu} = \mathbf{D}^{L}_{\mu\nu} + \Delta^{R}_{\mu\nu} \qquad \mathbf{D}_{\mu\nu} = w_{\mu\nu}(\mathbf{D}^{L}_{\mu\nu} + \Delta^{R}_{\mu\nu}) + (1 - w_{\mu\nu})(\mathbf{D}^{R}_{\mu\nu} + \Delta^{L}_{\mu\nu})$$

$$\mathbf{D}_{\mu\nu} = \mathbf{D}^{R}_{\mu\nu} + \Delta^{L}_{\mu\nu} \qquad w_{\mu\nu} = \frac{(\Delta^{L}_{\mu\nu})^2}{(\Delta^{L}_{\mu\nu})^2 + (\Delta^{R}_{\mu\nu})^2}$$

NEGF method

- Calculation of Hamiltonian of infinite bulk leads (DFT).
- Calculation of the self-energies $\Sigma_{L,R}(\epsilon)$ of semi-infinite bulk leads and building corresponding Hamiltonian.
- Calculation of initial Green's function of the system
- Self-consistent calculation of the non-equilibrium density matrix of the system (leads+device).
- Calculation of the transmission T(ϵ).

$$\mathbf{\Gamma}_L(z) \equiv i[\mathbf{\Sigma}_L(\varepsilon) - \mathbf{\Sigma}_L(\varepsilon)^\dagger]/2$$

$$T(\varepsilon) = \mathrm{Tr}[\mathbf{\Gamma}_L(\varepsilon)\mathbf{G}^\dagger(\varepsilon)\mathbf{\Gamma}_R(\varepsilon)\mathbf{G}(\varepsilon)]$$

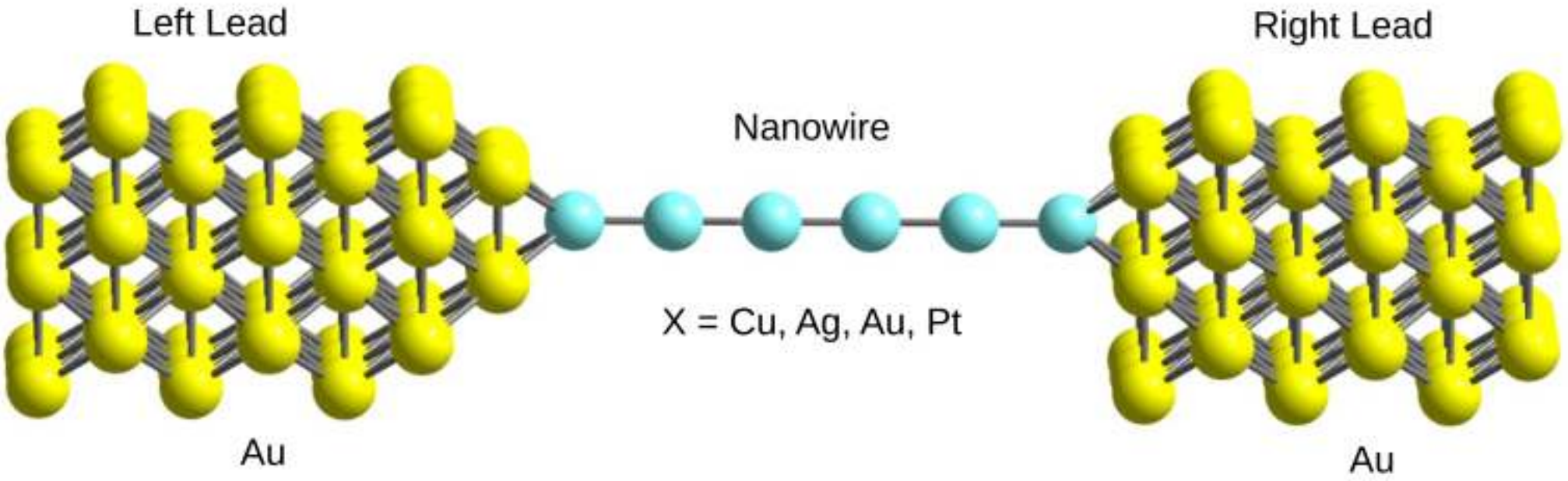
NEGF method

- Calculation of Hamiltonian of infinite bulk leads (DFT).
- Calculation of the self-energies $\Sigma_{L,R}(\epsilon)$ of semi-infinite bulk leads and building corresponding Hamiltonian.
- Calculation of initial Green's function of the system
- Self-consistent calculation of the non-equilibrium density matrix of the system (leads+device).
- Calculation of the transmission T(ϵ).
- Calculation of the current.

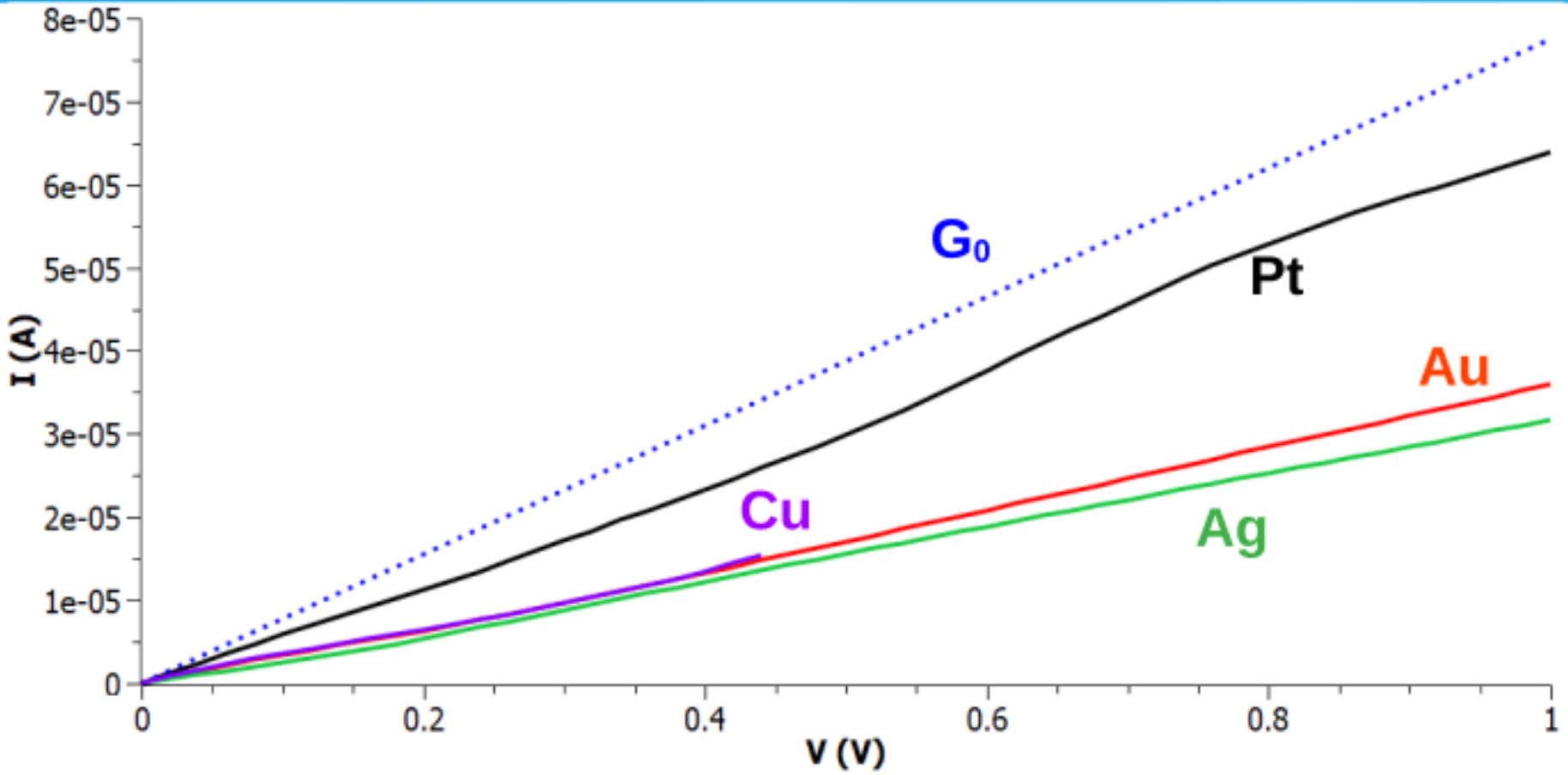
$$G_0 = 2e^2/h$$

$$I(V) = G_0 \int_{-\infty}^{\infty} d\varepsilon [n_F(\varepsilon - \mu_L) - n_F(\varepsilon - \mu_R)] T(\varepsilon)$$

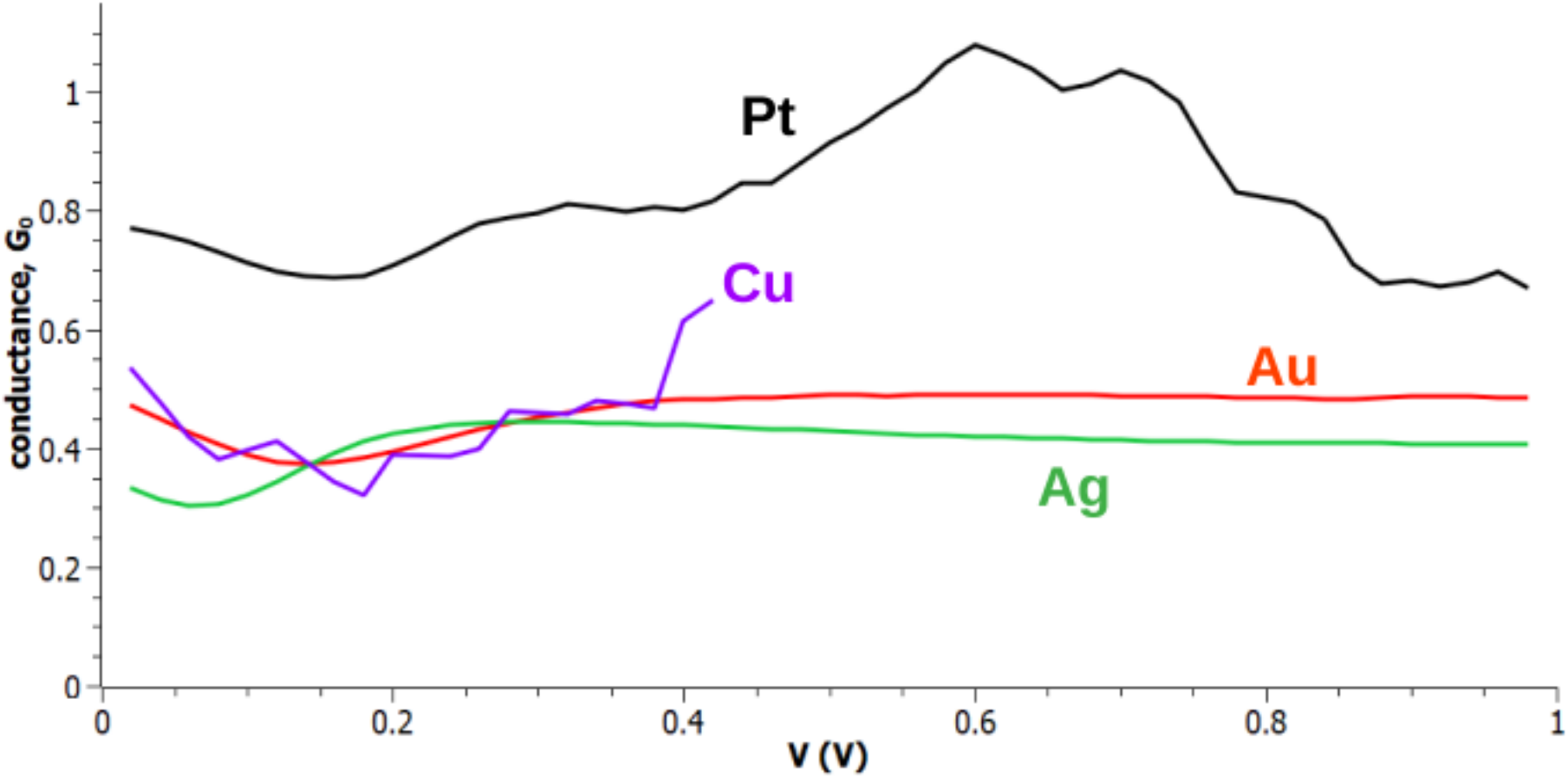
SIESTA: PBE / Scalar Rel. / SZP / TM2 PPs



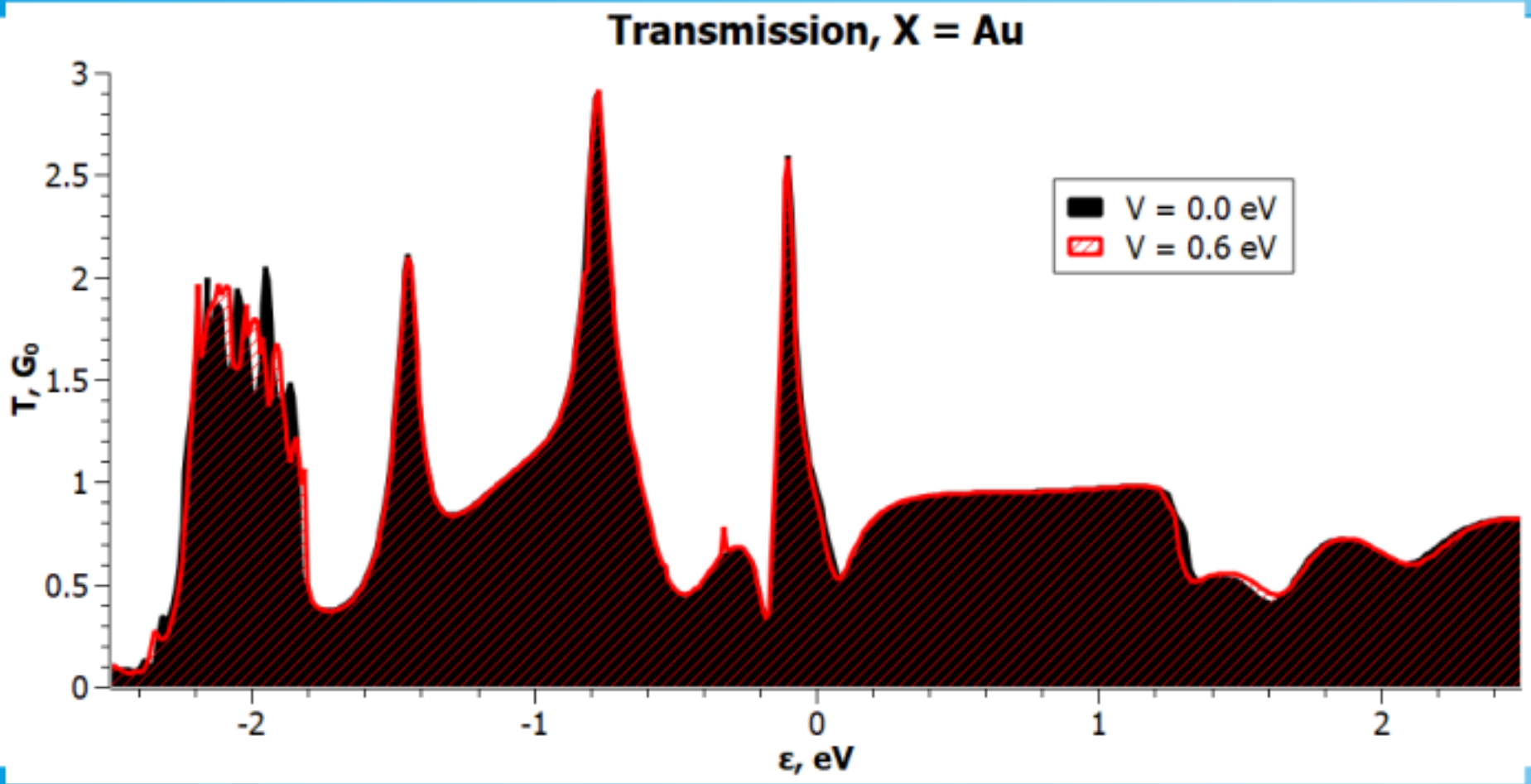
I-V curves


8e-05
7e-05
6e-05
5e-05
4e-05
3e-05
2e-05
1e-05
0
I (A)
0
0.2
0.4
0.6
0.8
1
V (V)
G0
Pt
Au
Cu
Ag

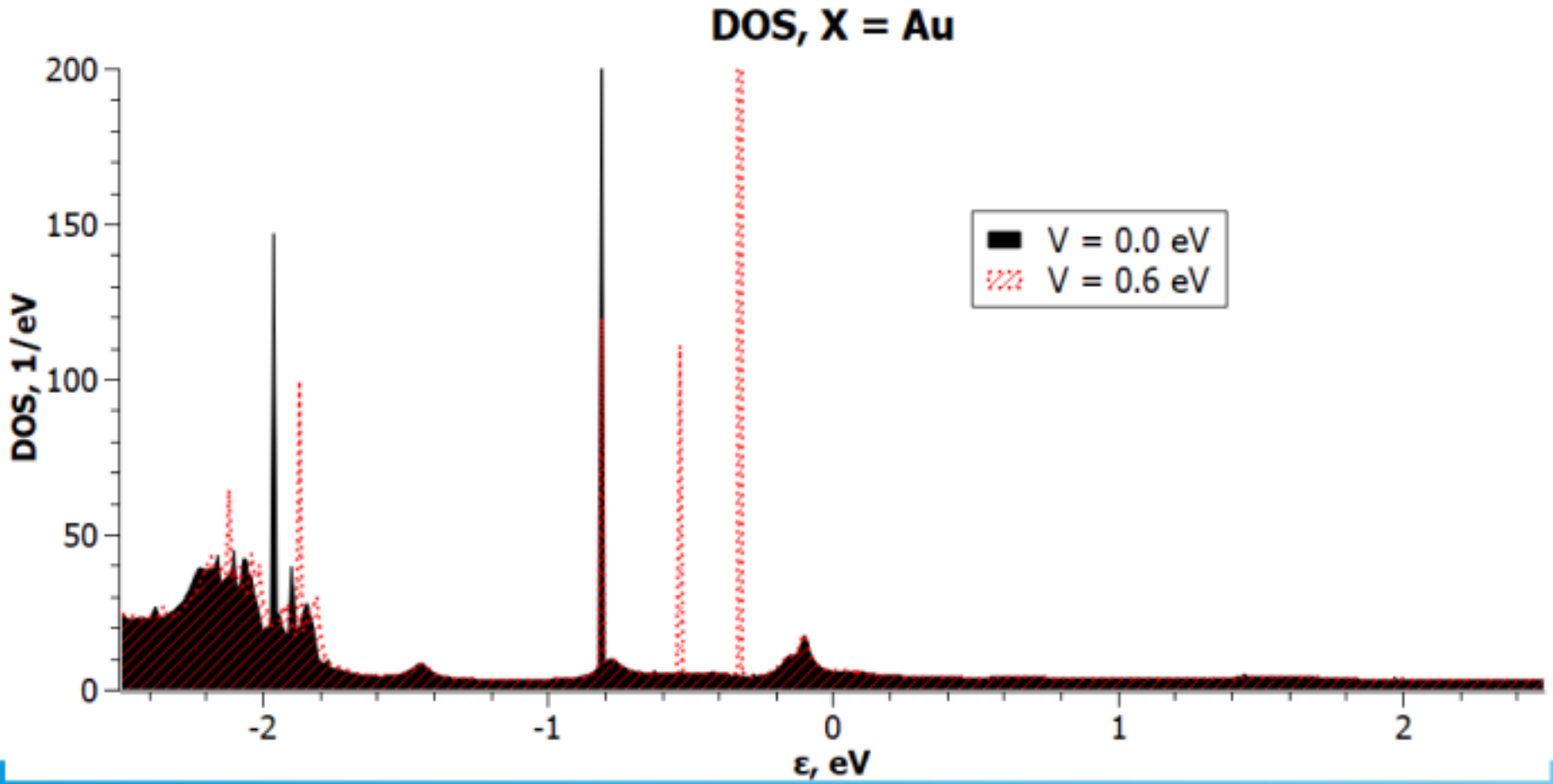
Conductance



Transmission



Density of States



Conclusion

- Optimized interatomic distances in monoatomic nanowires of Cu, Ag, Au and Pt are less then in corresponding bulk materials.
- Scalar relativistic effects are noticeable even for Cu nanowires.
- Spin-Orbit relativistic corrections shorten the interatomic distances for Cu, Ag and Au, but enlarges the interatomic distances in Pt nanowires.
- Calculated conductance of Cu, Ag, Au and Pt nanowires shows nonlinear effects. Conductance of Cu, Ag and Au wires is ~0.5 G_0 while for Pt it reaches 1 G_0 at certain voltage range.
- Considered in this work Cu-Au system is, probably, too unrealistic.

Acknowledgments

- The work was supported by the Russian Science Foundation, project №22-23-00245.

Thank you for your attention!